USER'S GUIDE FOR EVALUATING SUBSURFACE VAPOR INTRUSION INTO BUILDINGS

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DISCLAIMER

This document presents technical and policy recommendations based on current understanding of the phenomenon of subsurface vapor intrusion. This guidance does not impose any requirements or obligations on the U.S. Environmental Protection Agency (EPA) or on the owner/operators of sites that may be contaminated with volatile and toxic compounds. The sources of authority and requirements for addressing subsurface vapor intrusion are the applicable and relevants statutes and regulations.. This guidance addresses the assumptions and limitations that need to be considered in the evaluation of the vapor intrusion pathway. This guidance provides instructions on the use of the vapor transport model that originally was developed by P. Johnson and R. Ettinger in 1991 and subsequently modified by EPA in 1998, 2001, and again in November 2002. On November 29, 2002 EPA published Draft Guidance for Evaluating the Vapor Intrusion to Indoor Air Pathway from Groundwater and Soils (Federal Register: November 29, 2002 Volume 67, Number 230 Page 71169-71172). This document is intended to be a companion for that guidance. Users of this guidance are reminded that the science and policies concerning vapor intrusion are complex and evolving.

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ACKNOWLEDGMENT

Environmental Quality Management, Inc. (EQ) via Industrial Economics Incorporated (IEC) Subcontract No. 3073-002 prepared this document and the accompanying spreadsheets for the U.S. Environmental Protection Agency (EPA). Mr. Tom Robertson (EQ Project Manager) and Mr. Henry Roman (IEC Project Manager) managed the project. The work was completed on behalf of the U.S. EPA Office of Solid Waste. Ms. Janine Dinan was the government's Project Manager.

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WHAT'S NEW IN THIS VERSION!

This revised version of the User's Guide corresponds with the release of Version 3.1 of the Johnson and Ettinger (1991) model (J&E) spreadsheets for estimating subsurface vapor intrusion into buildings. Several things have changed within the models since Version 2 was released in December 2000 and since the original version was released in September 1998. The following represent the major changes in Version 3.1 to be consistent with Draft Guidance for Evaluating the Vapor Intrusion to Indoor Air Quality from Groundwater and Soils dated November 25, 2002 as referenced below:

1. Table 1 lists the chemicals that are commonly found at contaminated sites. This list has been expanded from the list of chemicals included in Version 2 of the model. We have also applied certain criteria to determine whether it is appropriate to run the model for these contaminants. Only those contaminants for which all of the toxicological or physical chemical properties needed to make an assessment of the indoor inhalation risk are included in the spreadsheets. A chemical is considered to be sufficiently toxic if the vapor concentration of the pure component poses an incremental life time cancer risk greater than 1×10^{-6} or the noncancer hazard index is greater than 1. A chemical is considered to be sufficiently volatile if its Henry's law constant is 1×10^{-5} atm-m^3/mole or greater. The final chemical list for Version 3 includes 108 chemicals.

2. **Chemical Property Data** - The source of chemical data used in the calculation is primarily EPA's Superfund Chemical Data Matrix (SCDM) database. EPA's WATER9 database is used for chemicals not included in the SCDM database. Appendix B contains other data sources. Henry's Law value for cumene is incorrect in the above listed reference. The correct value was determined by using EPA's system performs automated reasoning in chemistry algorithms found in "Prediction of Chemical Reactivity Parameters and Physical Properties of Organic Compounds from Molecular Structure Using SPARE." EPA-2003.

3. **Toxicity Values –** EPA's Integrated Risk Information System (IRIS) is the generally preferred source of carcinogenic unit risks and non-carcinogenic reference concentrations (RfCs) for inhalation exposure.[1] The following two sources were consulted, in order of preference, when IRIS values were not available: provisional toxicity values recommended by EPA's National Center for Environmental Assessment (NCEA) and EPA's Health Effects Assessment Summary Tables (HEAST). If no inhalation toxicity data could be obtained from IRIS, NCEA, or HEAST, extrapolated unit risks and/or RfCs using toxicity data for oral exposure (cancer slope factors and/or reference doses, respectively) from these same sources

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[1] U.S. EPA. 2002. Integrated Risk Information System (IRIS). http://www.epa.gov/iriswebp/iris/index.html. November.

using the same preference order were used.[2] Note that for most compounds, extrapolation from oral data introduces considerable uncertainty into the resulting inhalation value. Values obtained from inhalation studies or from pharmacokinetic modeling applied to oral doses will be less uncertain than those calculated using the equations noted in footnote 2.

IRIS currently does not include carcinogenicity data for trichloroethylene (TCE), a volatile contaminant frequently encountered at hazardous waste sites. The original carcinogenicity assessment for TCE, which was based on a health risk assessment conducted in the late 1980's, was withdrawn from IRIS in 1994. The Superfund Technical Support Center has continued to recommend use of the cancer slope factor from the withdrawn assessment, until a reassessment of the carcinogenicity of TCE is completed. In 2001, the Agency published a draft of the TCE toxicity assessment for public comment.[3] Using this guidance, TCE target concentrations for the draft vapor intrusion guidance were calculated using a cancer slope factor identified in that document, which is available on the NCEA web site. This slope factor was selected because it is based on state-of-the-art methodology. However, because this document is still undergoing review, the slope factor and the target concentrations calculated for TCE are subject to change and should be considered "provisional" values.

Toxicity databases such as IRIS are routinely updated as new information becomes available; the data included in the lookup tables are current as of December 2003. Users of these models are strongly encouraged to research the latest toxicity values for contaminants of interest from the sources noted above. In the next year, IRIS reassessments are expected for several contaminants commonly found in subsurface contamination whose inhalation toxicity values are currently based on extrapolation.

4. Assumption and Limitations

The Johnson and Ettinger (J&E) Model was developed for use as a screening level model and, consequently, is based on a number of simplifying assumptions regarding contaminant distribution and occurrence, subsurface characteristics, transport mechanisms, and building construction. The assumptions of the J&E Model as implemented in EPA's spreadsheet version are listed in Section 2.11, Section 5, and

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[2] The oral-to-inhalation extrapolations assume an adult inhalation rate (IR) of 20 m^3/day and an adult body weight (BW) of 70 kg. Unit risks (URs) were extrapolated from cancer slope factors (CSFs) using the following equation:

$$UR\ (\mu g/m^3)^{-1} = CSF\ (mg/kg/d)^{-1} * IR\ (m^3/d) * (1/BW)(kg^{-1})* (10^{-3}\ mg/\mu g)$$

Reference concentrations (RfCs) were extrapolated from reference doses (RfDs) using the following equation:

$$RfC\ (mg/m^3) = RfD\ (mg/kg/d) * (1/IR)\ (m3/d)^{-1}\ (\ BW\ (kg)$$

[3] US EPA, Trichloroethylene Health Risk Assessment: Synthesis and Characterization – External Review Draft, Office of Research and Development, EPA/600/P-01-002A, August, 2001.

Table 12 along with an assessment of the likelihood that the assumptions can be verified through field evaluation.

5. Soil Parameters

A list of generally reasonable, yet conservative, model input parameters for selected soil and sampling related parameters are provided in Tables 7 and 8. These tables also provide the practical range, typical or mean value (if applicable), and most conservative value for these parameters. For building parameters with low uncertainty and sensitivity, only a single "fixed" value corresponding to the mean or typical value is provided in Table 9. Soil-dependent properties are provided in Table 10 for soils classified according to the US Soil Conservation Soil (SCS) system. If site soils are not classified according to the US SCS, Table 11 can be used to assist in selecting an appropriate SCS soil type corresponding to the available site lithologic information. Note that the selection of the soil texture class should be biased towards the coarsest soil type of significance, as determined by the site characterization program. These input parameters were developed considering soil-physics science, available studies of building characteristics, and expert opinion. Consequently, the input parameters listed in Tables 7 and 8 are considered default parameters for a first-tier assessment, which should in most cases provide a reasonably (but not overly) conservative estimate of the vapor intrusion attenuation factor for a site. The soil water filled porosity (θ_w) is dependent on the soil type and the default value was removed from the model set up. Users must define soil type or input a value for the porosity.

6. Building Parameters

Building Air Exchange Rate (Default Value = 0.25 hr^{-1})

Results from 22 studies for which building air exchange data are available were summarized in Hers et al. (2001). When all the data were analyzed, the 10th, 50th, and 90th percentile values were 0.21, 0.51, and 1.48 air exchanges per hour (AEH). Air exchange rates varied depending on season and climatic region. For example, for the winter season and coldest climatic area (Region 1, Great Lakes area and extreme northeast US), the 10th, 50th, and 90th percentile values were 0.11, 0.27, and 0.71 AEH. In contrast, for the winter season and warmest climatic area [Region 4 (southern California, Texas, Florida, Georgia)], the 10th, 50th, and 90th percentile values were 0.24, 0.48, and 1.13 AEH. For this guidance, a default value of 0.25 for air exchange rate was selected to represent the lower end of these distributions. The previous version of the guidance included a default value of 0.45 exchanges per hour.

Building Area and Subsurface Foundation Area (Default Value = 10 m by 10 m)

A Michigan study indicates that a 111.5 m^2 area approximately corresponds to the 10^{th} percentile floor space area for residential single family dwellings, based on statistics compiled by the U.S. Department of Commerce (DOC) and U.S. Housing and Urban Development (HUD). The previous median value was 9.61 m x 9.61 m.

Building Mixing Height (Default Value = 2.44 m for slab-on-grade scenario; = 3.66 m for basement scenario)

The J&E Model assumes that subsurface volatiles migrating into the building are completely mixed within the building volume, which is determined by the building area and mixing height. The building mixing height will depend on a number of factors including the building height, the heating, ventilation and air conditioning (HVAC) system operation, environmental factors such as indoor-outdoor pressure differentials and wind loading, and seasonal factors. For a single-story house, the variation in mixing height can be approximated by the room height. For a multi-story house or apartment building, the mixing height will be greatest for houses with HVAC systems that result in significant air circulation (e.g., forced-air heating systems). Mixing heights will be less for houses using electrical baseboard heaters. It is likely that mixing height is, to some degree, correlated to the building air exchange rate.

There are little data available that provide for direct inference of mixing height. There are few sites, with a small number of houses where indoor air concentrations were above background, and where both measurements at ground level and the second floor were made (CDOT, Redfields, Eau Claire). Persons familiar with the data sets for these sites indicate that in most cases a fairly significant reduction in concentrations (factor of two or greater) was observed, although at one site (Eau Claire, "S” residence), the indoor TCE concentrations were similar in both the basement and second floor of the house. For the CDOT site apartments, there was an approximate five-fold reduction between the concentrations measured for the first floor and second floor units. Less mixing would be expected for an apartment because there are less cross-floor connections than for a house. The default value chosen for a basement house scenario (3.66 m) would be representative of a two-fold reduction or attenuation in vapor concentrations between floors.

Crack Width (0.1 cm) and Crack Ratio (Default Value = 0.0002 for basement house; = 0.0038 for slab-on-grade house)

The crack width and crack ratio are related. Assuming a square house and that the only crack is a continuous edge crack between the foundation slab and wall (“perimeter crack”), the crack ratio and crack width are related as follows:

$$Crack\,Ratio = \frac{4(CrackWidth / \sqrt{Subsurface\,Foundation\,Area}}{Subsurface\,Foundation\,Area}$$

There is little information available on crack width or crack ratio. One approach used by radon researchers is to back calculate crack ratios using a model for soil gas flow through cracks and the results of measured soil gas flow rates into a building. For example, the back-calculated values for a slab/wall edge crack based on soil gas-entry rates reported in Nazaroff (1992), Revzan et al. (1991), and Nazaroff et al. (1985) range from approximately 0.0001 to 0.001. Another possible approach is to measure crack openings although this, in practice, is difficult to do. Figley and Snodgrass (1992) present data from ten houses where edge crack measurements were made. At the eight houses where cracks were observed, the cracks' widths ranged from hairline cracks up to 5 mm wide, while the total crack length per house ranged from 2.5 m to 17.3 m. Most crack widths were less than 1 mm. The suggested defaults for crack ratio is regulatory guidance, literature and models also vary. In ASTM E1739-95, a default crack ratio of 0.01 is used. The crack ratios suggested in the VOLASOIL model (developed by the Dutch Ministry of Environment) range from 0.0001 to 0.0000001. The VOLASOIL model values correspond to values for a "good" and "bad" foundation, respectively. The crack ratio used by J&E (1991) for illustrative purposes ranged from 0.001 to 0.01. The selected default values fall within the ranges observed.

Q_{soil} *(Default Value = 5 L/min)*

The method used to estimate the vapor flowrate into a building (Q_{soil}) is an analytical solution for two-dimensional soil gas flow to a small horizontal drain (Nazaroff 1992) ("Perimeter Crack Model"). Use of this model can be problematic in that Q_{soil} values are sensitive to soil-air permeability and consequently a wide range in flows can be predicted.

An alternate empirical approach was selected to determine the Q_{soil} value. This new approach is based on trace tests (i.e., mass balance approach). When soil gas advection is the primary mechanism for tracer intrusion into a building, the Q_{soil} value is estimated by measuring the concentrations of a chemical tracer in indoor air, outdoor air, and in soil vapor below a building, and measuring the building ventilation rate (Hers et al. 2000a; Fischer et al. 1996; Garbesi et al. 1993; Rezvan et al. 1991; Barbesi and Sectro 1989). The Q_{soil} values measured using this technique were compared to predicted rates using the Perimeter Crack model, for sites with coarse-grained soils. The Perimeter Crack model predictions are both higher and lower than the measured values, but overall are within one order of magnitude of the measured values. Although the Q_{soil} predicted by the models and measured using field tracer tests are uncertain, the results suggest that a "typical" range for houses on coarse-grained soils is on the order of 1 to 10 L/min. A disadvantage with the tracer test approach is that there are only limited data, and there do not appear to be any tracer studies for field sites with fine-grained soils.

Because the advective flow zone is relatively limited in extent, the soil type adjacent to the building foundation is of importance. In many cases, coarse-grained imported fill is placed below foundations, and either coarse-grained fill, or disturbed, loose fill is placed adjacent to the foundation walls. Therefore, a conservative approach for the purposes of this guidance is to assume that soil gas flow will be controlled by coarse-grained soil, and not to rely on the possible reduction in flow that would be caused by fine-grained soils near the house foundation. For these reasons, a soil gas flow rate of 5 L/min (midpoint between 1 and 10 L/min) was chosen as the input value.

7. Convenience Changes

- Default values for soil bulk densities have been added to the lookup tables for the various soil types.
- Default values for soil water-filled porosity have been updated within the lookup tables for soil properties for the various soil types.
- The chemical data list has been expanded to include 108 chemicals. Chemical physical properties were reviewed and updated where applicable to provide the user with more accurate values.
- All of the lookup functions within the models were modified to include an exact match parameter, rather than a closest match. The models would previously return data for CAS Numbers not in the lookup tables. Although the DATENTER sheet informed the user that this CAS Number was not found, it would return values on the CHEMPROPS sheet that was the closest match. This caused some confusion and therefore was changed.
- CAS number and soil type pick lists were added to the cells within the models where the user is required to provide data in a specific format. The pick lists were added to assist the user from entering data that are not an acceptable parameter.
- All models were modified to require the user to specify the soil type of each stratum. In addition, a button was added that allows the user to automatically retrieve the default values for the soil type selected. These additions were added as a convenience to the user and soil selection can be ignored should site-specific data be available.
- All models were modified to include an input for the average vapor flow rate into the building (Q_{soil}) in liters/minute (L/min). This value can be left blank and the model will calculate the value of Q_{soil} as was done in previous versions.

- All models were also modified to include a button that will reset the default value on the DATENTER sheet. This button will allow the user to clear all values and reset the default values or reset only those values that have a default value. The user is also allowed to specify whether the values should be reset for the basement or slab-on-grade scenario.

SECTION 1

INTRODUCTION TO THE VAPOR INTRUSION MODEL THEORY AND APPLICATION

Volatilization of contaminants located in subsurface soils or in groundwater, and the subsequent mass transport of these vapors into indoor spaces constitutes a potential inhalation exposure pathway, which may need to be evaluated when preparing risk assessments. Likewise, this potential indoor inhalation exposure pathway may need evaluation when estimating a risk-based soil or groundwater concentration below which associated adverse health effects are unlikely.

Johnson and Ettinger (J&E) (1991) introduced a screening-level model that incorporates both convective and diffusive mechanisms for estimating the transport of contaminant vapors emanating from either subsurface soils or groundwater into indoor spaces located directly above the source of contamination. In their article, J&E reported that the results of the model were in qualitative agreement with published experimental case histories and in good qualitative and quantitative agreement with detailed three-dimensional numerical modeling of radon transport into houses.

The J&E Model is a one-dimensional analytical solution to convective and diffusive vapor transport into indoor spaces and provides an estimated attenuation coefficient that relates the vapor concentration in the indoor space to the vapor concentration at the source of contamination. The model is constructed as both a steady-state solution to vapor transport (infinite or non-diminishing source) and as a quasi-steady-state solution (finite or diminishing source). Inputs to the model include chemical properties of the contaminant, saturated and unsaturated zone soil properties, and structural properties of the building.

This manual provides documentation and instructions for using the vapor intrusion model as provided in the accompanying spreadsheets.

Model results (both screening and advanced) are provided as either a risk-based soil or groundwater concentration, or as an estimate of the actual incremental risks associated with a user-defined initial concentration. That is to say that the model will reverse-calculate an “acceptable” soil or groundwater concentration given a user-defined risk level (i.e., target risk level or target hazard quotient), or the model may be used to forward-calculate an incremental cancer risk or hazard quotient based on an initial soil or groundwater concentration.

The infinite source models for soil contamination and groundwater contamination should be used as first-tier screening tools. In these models, all but the most sensitive model parameters have been set equal to central tendency or upper bound values. Values for the most sensitive parameters may be user-defined.

More rigorous estimates may be obtained using site-specific data and the finite source model for soil contamination. Because the source of groundwater contamination may be located upgradient of the enclosed structure for which the indoor inhalation pathway is to be assessed, the advanced model for contaminated groundwater is based on an infinite source of contamination, however, site-specific values for all other model parameters may be user-defined.

In addition to the finite and infinite source models referred to above, two models that allow the user to input empirical soil gas concentration and sampling depth information directly into the spreadsheets. These models will subsequently estimate the resulting steady-state indoor air concentrations and associated health risks.

Because of the paucity of empirical data available for either bench-scale or field-scale verification of the accuracy of these models, as well as for other vapor intrusion models, the user is advised to consider the variation in input parameters and to explore and quantify the impacts of assumptions on the uncertainty of model results. At a minimum, a range of results should be generated based on variation of the most sensitive model parameters.

SECTION 2

MODEL THEORY

Chemical fate and transport within soils and between the soil column and enclosed spaces are determined by a number of physical and chemical processes. This section presents the theoretical framework on which the J&E Model is based, taking into account the most significant of these processes. In addition, this section also presents the theoretical basis for estimating values for some of the most sensitive model parameters when empirical field data are lacking. The fundamental theoretical development of this model was performed by J&E (1991).

2.1 MODEL SETTING

Consider a contaminant vapor source (C_{source}) located some distance (L_T) below the floor of an enclosed building constructed with a basement or constructed slab-on-grade. The source of contamination is either a soil-incorporated volatile contaminant or a volatile contaminant in solution with groundwater below the top of the water table.

Figure 1 is a simplified conceptual diagram of the scenario where the source of contamination is incorporated in soil and buried some distance below the enclosed space floor. At the top boundary of contamination, molecular diffusion moves the volatilized contaminant toward the soil surface until it reaches the zone of influence of the building. Here convective air movement within the soil column transports the vapors through cracks between the foundation and the basement slab floor. This convective sweep effect is induced by a negative pressure within the structure caused by a combination of wind effects and stack effects due to building heating and mechanical ventilation.

Figure 2 illustrates the scenario where the source of contamination is below the top of the water table. Here the contaminant must diffuse through a capillary zone immediately above the water table and through the subsequent unsaturated or vadose zone before convection transports the vapors into the structure.

The suggested minimum site characterization information for a first-tier evaluation of the vapor intrusion pathway includes: site conceptual model, nature and extent of contamination distribution, soil lithologic descriptions, groundwater concentrations, and/or possibly near source soil vapor concentrations. The number of samples and measurements needed to establish this information varies by site, and it is not possible to provide a hard and fast rule.

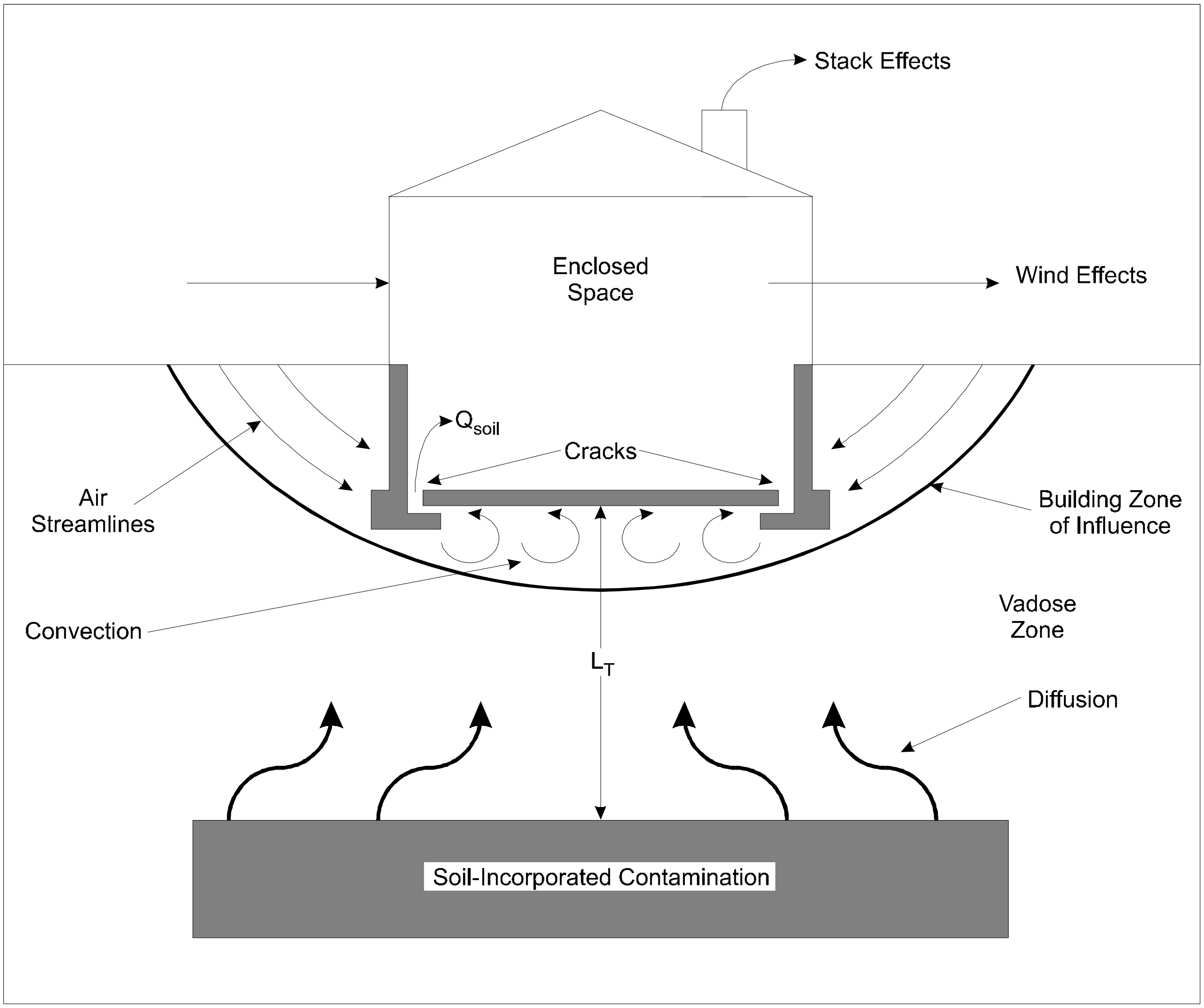


Figure 1. Pathway for Subsurface Vapor Intrusion into Indoor Air

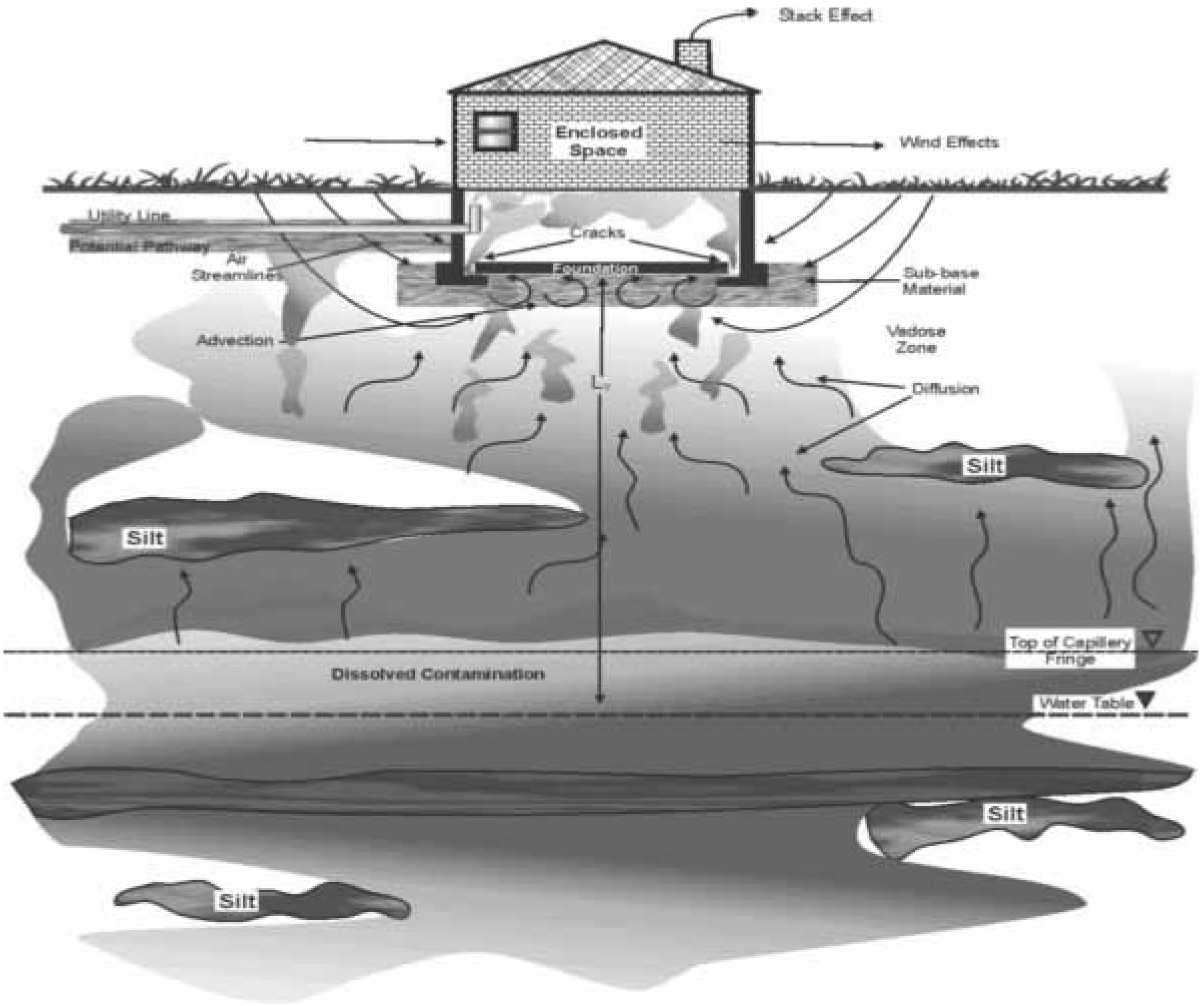


Figure 2. Vapor Pathway into Buildings

Based on the conceptual site model, the user can select the appropriate spreadsheet corresponding to the vapor source at the site and determine whether to use the screening level spreadsheet (which accommodates only one soil type above the capillary fringe) or the more advanced version (which allows up to three layers above the capillary fringe). As most of the inputs to the J&E Model are not collected during a typical site characterization, conservative inputs are typically estimated or inferred from available data and other non-site specific sources of information.

Table 1 lists 114 chemicals that may be found at hazardous waste sites and it indicates whether the chemical is sufficiently toxic and volatile to result in a potentially unacceptable indoor inhalation risk. It also provides a column for checking off the chemicals found or reasonably suspected to be present in the subsurface at a site. Under this approach, a chemical is considered sufficiently toxic if the vapor concentration of the pure component poses an incremental lifetime cancer risk greater than 10^{-6} or results in a non-cancer hazard index greater than one. A chemical is considered sufficiently volatile if its Henry's Law Constant is 1×10^{-5} atm-m^3/mol or greater (EPA, 1991). It is assumed that if a chemical does not meet both of these criteria, it need not be further considered as part of the evaluation. Table 1 also identifies six chemicals that meet the toxicity and volatility criteria but are not included in the vapor intrusion models because one or more of the needed physical or chemical properties has not been found in the literature.

The rate of soil gas entry (Q_{soil}) or average vapor flow rate into the building is a function solely of convection; however, the vapor concentration entering the structure may be limited by either convection or diffusion depending upon the magnitude of the source-building separation (L_T).

2.2 VAPOR CONCENTRATION AT THE SOURCE OF CONTAMAINATION

With a general concept of the problem under consideration, the solution begins with an estimate of the vapor concentration at the source of contamination.

In the case of soil contamination, the initial concentration (C_R) does not contain a residual-phase (e.g., nonaqueous-phase liquid or solid); and in the case of contaminated groundwater, the initial contaminant concentration (C_W) is less than the aqueous solubility limit (i.e., in solution with water).

Given these initial conditions, C_{source} for soil contamination may be estimated from Johnson et al. (1990) as:

$$C_{source} = \frac{H'_{TS}\, C_R\, \rho_b}{\theta_w + K_d \rho_b + H'_{TS}\, \theta_a} \qquad (1)$$

where C_{source} = Vapor concentration at the source of contamination, g/cm^3-v

H'_{TS} = Henry's law constant at the system (soil) temperature, dimensionless

TABLE 1. SCREENING LIST OF CHEMICALS

CAS No.	Chemical	Is Chemical Sufficiently Toxic?[1]	Is Chemical Sufficiently Volatile?[2]	Check Here if Known or Reasonably Suspected to be Present [3]
83329	Acenaphthene	YES	YES	
75070	Acetaldehyde	YES	YES	
67641	Acetone	YES	YES	
75058	Acetronitrile	YES	YES	
98862	Acetophenone	YES	YES	
107028	Acrolein	YES	YES	
107131	Acrylonitrile	YES	YES	
309002	Aldrin	YES	YES	
319846	Alpha-HCH (alpha-BHC)	YES	YES	
62533	Aniline	YES	NO	NA
120127	Anthracene	NO	YES	NA
56553	Benz(a)anthracene	YES	NO	NA
100527	Benzaldehyde	YES	YES	
71432	Benzene	YES	YES	
50328	Benzo(a)pyrene	YES	NO	NA
205992	Benzo(b)fluoranthene	YES	YES	
207089	Benzo(k)fluoranthene	NO	NO	NA
65850	Benzoic Acid	NO	NO	NA
100516	Benzyl alcohol	YES	NO	NA
100447	Benzylchloride	YES	YES	
91587	Beta-Chloronaphthalene [3]	YES	YES	
319857	Beta-HCH(beta-BHC)	YES	NO	NA
92524	Biphenyl	YES	YES	
111444	Bis(2-chloroethyl)ether	YES	YES	
108601	Bis(2-chloroisopropyl)ether [3]	YES	YES	
117817	Bis(2-ethylhexyl)phthalate	NO	NO	NA
542881	Bis(chloromethyl)ether [3]	YES	YES	
75274	Bromodichloromethane	YES	YES	
75252	Bromoform	YES	YES	
106990	1,3-Butadiene	YES	YES	
71363	Butanol	YES	NO	NA
85687	Butyl benzyl phthalate	NO	NO	NA
86748	Carbazole	YES	NO	NA
75150	Carbon disulfide	YES	YES	
56235	Carbon tetrachloride	YES	YES	
57749	Chlordane	YES	YES	

(continued)

CAS No.	Chemical	Is Chemical Sufficiently Toxic?[1]	Is Chemical Sufficiently Volatile?[2]	Check Here if Known or Reasonably Suspected to be Present [3]
126998	2-Chloro-1,3-butadiene(chloroprene)	YES	YES	
108907	Chlorobenzend	YES	YES	
109693	1-Chlorobutane	YES	YES	
124481	Chlorodibromomethane	YES	YES	
75456	Chlorodifluoromethane	YES	YES	
75003	Chloroethane (ethyl chloride)	YES	YES	
67663	Chloroform	YES	YES	
95578	2-Chlorophenol	YES	YES	
75296	2-Chloropropane	YES	YES	
218019	Chrysene	YES	YES	
156592	Cis-1,2-Dichloroethylene	YES	YES	
123739	Crotonaldehyde(2-butenal)	YES	YES	
998828	Cumene	YES	YES	
72548	DDD	YES	NO	NA
72559	DDE	YES	YES	
50293	DDT	YES	NO	NA
53703	Dibenz(a,h)anthracene	YES	NO	NA
132649	Dibenzofuran	YES	YES	
96128	1,2-Dibromo-3-chloropropane [3]	YES	YES	
106934	1,2-Dibromoethane(ethylene dibromide)	YES	YES	
541731	1,3-Dichlorobenzene	YES	YES	
95501	1,2-Dichlorobenzene	YES	YES	
106467	1,4-Dichlorobenzene	YES	YES	
91941	3,3-Dichlorobenzidine	YES	NO	NA
75718	Dichlorodifluoromethane	YES	YES	
75343	1,1-Dichloroethane	YES	YES	
107062	1,2-dichloroethane	YES	YES	
75354	1,1-Dichloroethylene	YES	YES	
120832	2,4-Dichloroephenol	YES	NO	NA
78875	1,2-Dichloropropane	YES	YES	
542756	1,3-Dichloropropene	YES	YES	
60571	Dieldrin	YES	YES	
84662	Diethylphthalate	YES	NO	NA
105679	2,4-Dimethylphenol	YES	NO	NA
131113	Dimethylphthalate	NA	NO	NA
84742	Di-n-butyl phthalate	NO	NO	NA

(continued)

CAS No.	Chemical	Is Chemical Sufficiently Toxic?[1]	Is Chemical Sufficiently Volatile?[2]	Check Here if Known or Reasonably Suspected to be Present [3]
534521	4,6 Dinitro-2methylphenol (4, 6-dinitro-o-cresol)	YES	NO	NA
51285	2,4-Dinitrophenol	YES	NO	NA
121142	2,4-Dinitrotoluene	YES	NO	NA
606202	2,6-Dinitrotoluene	YES	NO	NA
117840	Di-n-octyl phthalate	NO	YES	NA
115297	Endosulfan	YES	YES	
72208	Endrin	YES	NO	NA
106898	Epichlorohydrin [3]	YES	YES	
60297	Ethyl ether	YES	YES	
141786	Ethylacetate	YES	YES	
100414	Ethylbenzene	YES	YES	
75218	Ethylene oxide	YES	YES	
97632	Ethylmethacrylate	YES	YES	
206440	Fluoranthene	NO	YES	NA
86737	Fluorene	YES	YES	
110009	Furane	YES	YES	
58899	Gamma-HCH(Lindane)	YES	YES	
76448	Heptachlor	YES	YES	
1024573	Heptachlor epoxide	YES	NO	NA
87683	Hexachloro-1,3-butadiene	YES	YES	
118741	Hexachlorobenzene	YES	YES	
77474	Hexachlorocyclopentadiene	YES	YES	
67721	Hexachloroethane	YES	YES	
110543	Hexane	YES	YES	
74908	Hydrogene cyanide	YES	YES	
193395	Indeno (1,2,3-cd)pyrene	NO	NO	NA
78831	Isobutanol	YES	YES	
78591	Isophorone	YES	NO	NA
7439976	Mercury (elemental)	YES	YES	
126987	Methacrylonitrile	YES	YES	
72435	Methoxychlor	YES	YES	
79209	Methy acetate	YES	YES	
96333	Methyl acrylate	YES	YES	
74839	Methyl bromide	YES	YES	
74873	Methyl chloride (chloromethane)	YES	YES	
108872	Methylcyclohexane	YES	YES	

(continued)

CAS No.	Chemical	Is Chemical Sufficiently Toxic?[1]	Is Chemical Sufficiently Volatile?[2]	Check Here if Known or Reasonably Suspected to be Present [3]
74953	Methylene bromide	YES	YES	
75092	Methylene chloride	YES	YES	
78933	Methylethylketone (2-butanone)	YES	YES	
108101	Methylisobutylketone (4-methyl-2-pentanone)	YES	YES	
80626	Methylmethacrylate	YES	YES	
91576	2-Methylnaphthalene	YES	YES	
108394	3-Methylphenol(m-cresol)	YES	NO	NA
95487	2-Methylphenol(o-cresol)	YES	NO	NA
106455	4-Methylphenol (p-cresol)	YES	NO	NA
99081	m-Nitrotoluene	YES	NO	NA
1634044	MTBE	YES	YES	
108383	m-Xylene	YES	YES	
91203	Naphthalene	YES	YES	
104518	n-Butylbenzene	YES	YES	
98953	Nitrobenzene	YES	YES	
100027	4-Nitrophenol	YES	NO	NA
79469	2-Nitropropane	YES	YES	
924163	N-nitroso-di-n-butylamine [3]	YES	YES	
621647	N-Nitroso-di-n-propylamine	YES	NO	NA
86306	N-Nitrosodiphenylamine	YES	NO	NA
103651	n-Propylbenzene	YES	YES	
88722	o-Nitrotoluene	YES	YES	
95476	o-Xylene	YES	YES	
106478	p-Chloroaniline	YES	NO	NA
87865	Pentachlorophenol	YES	NO	NA
108952	Phenol	YES	NO	NA
99990	p-Nitrotoluene	YES	NO	NA
106423	p-Xylene	YES	YES	
129000	Pyrene	YES	YES	
110861	Pyridine	YES	NO	NA
135988	Sec-Butylbenzene	YES	YES	
100425	Styrene	YES	YES	
98066	Tert-Butylbenzene	YES	YES	
630206	1,1,1,2-Tetrachloroethane	YES	YES	
79345	1,1,2,2,-Tetrachloroethane	YES	YES	
127184	Tetrachloroethylene	YES	YES	

(continued)

CAS No.	Chemical	Is Chemical Sufficiently Toxic?[1]	Is Chemical Sufficiently Volatile?[2]	Check Here if Known or Reasonably Suspected to be Present [3]
108883	Toluene	YES	YES	
8001352	Toxaphen	YES	NO	NA
156605	Trans-1,2-Dichloroethylene	YES	YES	
76131	1,1,2-Trichloro-1,2,2-trifluoroethane	YES	YES	
120821	1,2,4-Trichlorobenzene	YES	YES	
79005	1,1,2-Trichloroethane	YES	YES	
71556	1,1,1-Trichloroethane	YES	YES	
79016	Trichloroethylene	YES	YES	
75694	Trichlorofluoromethane	YES	YES	
95954	2,4,5-Trichlorophenol	YES	NO	NA
88062	2,4,6-Trichlorophenol	YES	NO	NA
96184	1,2,3-Trichloropropane	YES	YES	
95636	1,2,4-Trimethylbenzene	YES	YES	
108678	1,3,5-Trimethylbenzene	YES	YES	
108054	Vinyl acetate	YES	YES	
75014	Vinyl chloride (chloroethene)	YES	YES	

[1] A chemical is considered sufficiently toxic if the vapor concentration of the pure component poses an incremental lifetime cancer risk greater than 10^{-6} or a non-cancer hazard index greater than 1.

[2] A chemical is considered sufficiently volatile if its Henry's law constant is 1×10^{-5} atm-m^3/mol or greater.

[3] One or more of the physical chemical properties required to run the indoor air vapor intrusion models was not found during a literature search conducted March 2003.

C_R = Initial soil concentration, g/g

ρ_b = Soil dry bulk density, g/cm^3

θ_w = Soil water-filled porosity, cm^3/cm^3

K_d = Soil-water partition coefficient, cm^3/g (= K_{oc} x f_{oc})

θ_a = Soil air-filled porosity, cm^3/cm^3

K_{oc} = Soil organic carbon partition coefficient, cm^3/g

f_{oc} = Soil organic carbon weight fraction.

If the initial soil concentration includes a residual phase, the user is referred to the NAPL-SCREEN or NAPL-ADV models as discussed in Appendix A. These models estimate indoor air concentrations and associated risks for up to 10 user-defined contaminants that comprise a residual phase mixture in soils.

C_{source} for groundwater contamination is estimated assuming that the vapor and aqueous-phases are in local equilibrium according to Henry's law such that:

$$C_{source} = H'_{TS} C_w \qquad (2)$$

where C_{source} = Vapor concentration at the source of contamination, g/cm^3-v

H'_{TS} = Henry's law constant at the system (groundwater) temperature, dimensionless

C_w = Groundwater concentration, g/cm^3-w.

The dimensionless form of the Henry's law constant at the system temperature (i.e., at the average soil/groundwater temperature) may be estimated using the Clapeyron equation by:

$$H'_{TS} = \frac{\exp\left[-\frac{\Delta H_{v,TS}}{R_c}\left(\frac{1}{T_S} - \frac{1}{T_R}\right)\right] H_R}{R T_S} \qquad (3)$$

where H'_{TS} = Henry's law constant at the system temperature, dimensionless

$\Delta H_{v,TS}$ = Enthalpy of vaporization at the system temperature, cal/mol

T_S = System temperature, °K

T_R = Henry's law constant reference temperature, ^oK

H_R = Henry's law constant at the reference temperature, atm-m^3/mol

R_C = Gas constant (= 1.9872 cal/mol - ^oK)

R = Gas constant (= 8.205 E-05 atm-m^3/mol-^oK).

The enthalpy of vaporization at the system temperature can be calculated from Lyman et al. (1990) as:

$$\Delta H_{v,TS} = \Delta H_{v,b}\left[\frac{(1-T_S/T_C)}{(1-T_B/T_C)}\right]^n \qquad (4)$$

where $\Delta H_{v,TS}$ = Enthalpy of vaporization at the system temperature, cal/mol

$\Delta H_{v,b}$ = Enthalpy of vaporization at the normal boiling point, cal/mol

T_S = System temperature, ^oK

T_C = Critical temperature, ^oK

T_B = Normal boiling point, ^oK

n = Constant, unitless.

Table 2 gives the value of n as a function of the ratio T_B/T_C.

TABLE 2. VALUES OF EXPONENT n AS A FUNCTION OF T_B/T_C

T_B/T_C	N
< 0.57	0.30
0.57 - 0.71	0.74 (T_B/T_C) - 0.116
> 0.71	0.41

2.3 DIFFUSION THROUGH THE CAPILLARY ZONE

Directly above the water table, a saturated capillary zone exists whereby groundwater is held within the soil pores at less than atmospheric pressure (Freeze and Cherry, 1979). Between drainage and wetting conditions, the saturated water content varies but is always less than the fully saturated water content which is equal to the soil total porosity. This is the result of air entrapment in the pores during the wetting process (Gillham, 1984). Upon rewetting, the air content of the capillary zone will be higher than after main drainage. Therefore, the air content will vary as a function of groundwater recharge and discharge. At the saturated water content, Freijer (1994) found that the relative vapor-phase diffusion coefficient was almost zero. This implies that all remaining air-filled soil pores are disconnected and thus blocked for gas diffusion. As the air-filled porosity increased, however, the relative diffusion coefficient indicated the presence of connected air-filled pores that corresponded to the air-entry pressure head. The air-entry pressure head corresponds with the top of the saturated capillary zone. Therefore, to allow for the calculation of the effective diffusion coefficient by lumping the gas-phase and aqueous-phase together, the water-filled soil porosity in the capillary zone ($\theta_{w,cz}$) is calculated at the air-entry pressure head (h) according to the procedures of Waitz et al. (1996) and the van Genuchten equation (van Genuchten, 1980) for the water retention curve:

$$\theta_{w,cz} = \theta_r + \frac{\theta_s - \theta_r}{\left[1 + (\alpha_1 h)^N\right]^M} \tag{5}$$

where $\theta_{w,cz}$ = Water-filled porosity in the capillary zone, cm^3/cm^3

θ_r = Residual soil water content, cm^3/cm^3

θ_s = Saturated soil water content, cm^3/cm^3

α_1 = Point of inflection in the water retention curve where d θ_w/dh is maximal, cm^{-1}

h = Air-entry pressure head, cm (= $1/\alpha_1$ and assumed to be positive)

N = van Genuchten curve shape parameter, dimensionless

M = 1 - (1/N).

With a calculated value of $\theta_{w,cz}$ within the capillary zone at the air-entry pressure head, the air-filled porosity within the capillary zone ($\theta_{a,cz}$) corresponding to the minimum value at which gas diffusion is relevant is calculated as the total porosity (n) minus $\theta_{w,cz}$.

Hers (2002) computed the SCS class average values of the water filled porosity and the height of the capillary zone SCS soil textural classifications. Table 3 provides the class average values for each of the SCS soil types. These data replace the mean values developed by Schaap and

Leij (1998) included in the previous U.S. Environmental Protection Agency (EPA) version of the J&E Models. With the class average values presented in Table 3, a general estimate can be made of the values of $\theta_{w,cz}$ and $\theta_{a,cz}$ for each soil textural classification.

The total concentration effective diffusion coefficient across the capillary zone (D_{cz}^{eff}) may then be calculated using the Millington and Quirk (1961) model as:

$$D_{cz}^{eff} = D_a\left(\theta_{a,cz}^{3.33} / n_{cz}^2\right) + \left(D_w / H'_{TS}\right)\left(\theta_{w,cz}^{3.33} / n_{cz}^2\right) \tag{6}$$

where D_{cz}^{eff} = Effective diffusion coefficient across the capillary zone, cm^2/s

D_a = Diffusivity in air, cm^2/s

$\theta_{a,cz}$ = Soil air-filled porosity in the capillary zone, cm^3/cm^3

n_{cz} = Soil total porosity in the capillary zone, cm^3/cm^3

D_w = Diffusivity in water, cm^2/s

H'_{TS} = Henry's law constant at the system temperature, dimensionless

$\theta_{w,cz}$ = Soil water-filled porosity in the capillary zone, cm^3/cm^3.

According to Fick's law of diffusion, the rate of mass transfer across the capillary zone can be approximated by the expression:

$$E = A\left(C_{source} - C_{g0}\right)D_{cz}^{eff} / L_{cz} \tag{7}$$

where E = Rate of mass transfer, g/s

A = Cross-sectional area through which vapors pass, cm^2

C_{source} = Vapor concentration within the capillary zone, g/cm^3-v

C_{g0} = A known vapor concentration at the top of the capillary zone, g/cm^3-v (C_{g0} is assumed to be zero as diffusion proceeds upward)

D_{cz}^{eff} = Effective diffusion coefficient across the capillary zone, cm^2/s

L_{cz} = Thickness of capillary zone, cm.

TABLE 3. CLASS AVERAGE VALUES OF THE VAN GENUCHTEN SOIL WATER RETENTION PARAMETERS FOR THE 12 SCS SOIL TEXTURAL CLASSIFICATIONS

Soil texture (USDA)	Saturated water content, θ_s	Residual water Content, θ_r	van Genuchten parameters		
			α_1 (1/cm)	N	M
Clay	0.459	0.098	0.01496	1.253	0.2019
Clay loam	0.442	0.079	0.01581	1.416	0.2938
Loam	0.399	0.061	0.01112	1.472	0.3207
Loamy sand	0.390	0.049	0.03475	1.746	0.4273
Silt	0.489	0.050	0.00658	1.679	0.4044
Silty loam	0.439	0.065	0.00506	1.663	0.3987
Silty clay	0.481	0.111	0.01622	1.321	0.2430
Silty clay loam	0.482	0.090	0.00839	1.521	0.3425
Sand	0.375	0.053	0.03524	3.177	0.6852
Sandy clay	0.385	0.117	0.03342	1.208	0.1722
Sandy clay loam	0.384	0.063	0.02109	1.330	0.2481
Sandy loam	0.387	0.039	0.02667	1.449	0.3099

The value of C_{source} is calculated using Equation 2; the value of A is assumed to be 1 cm^2; and the value of D_{cz}^{eff} is calculated by Equation 6. What remains is a way to estimate a value for L_{cz}.

Lohman (1972) and Fetter (1994) estimated the rise of the capillary zone above the water table using the phenomenon of capillary such that water molecules are subject to an upward attractive force due to surface tension at the air-water interface and the molecular attraction of the liquid and solid phases. The rise of the capillary zone can thus be estimated using the equation for the height of capillary rise in a bundle of tubes of various diameters equivalent to the diameters between varying soil grain sizes. Fetter (1994) estimated the mean rise of the capillary zone as:

$$L_{cz} = \frac{2 \ \alpha_2 \ COS \ \lambda}{\rho_w \ g \ R} \qquad (8)$$

where L_{cz} = Mean rise of the capillary zone, cm

α_2 = Surface tension of water, g/s (= 73)

λ = Angle of the water meniscus with the capillary tube, degrees (assumed to be zero)

ρ_w = Density of water, g/cm^3 (= 0.999)

g = Acceleration due to gravity, cm/s^2 (= 980)

R = Mean interparticle pore radius, cm

and;

$$R = 0.2D \qquad (9)$$

where R = Mean interparticle pore radius, cm

D = Mean particle diameter, cm.

Assuming that the default values of the parameters given in Equation 8 are for groundwater between 5^o and 25^{o}C, Equation 8 reduces to:

$$L_{cz} = \frac{0.15}{R} \quad . \qquad (10)$$

Nielson and Rogers (1990) estimated the arithmetic mean particle diameter for each of the 12 SCS soil textural classifications at the mathematical centroid calculated from its classification area (Figure 3). Table 4 shows the centroid compositions and mean particle sizes of the 12 SCS soil textural classes.

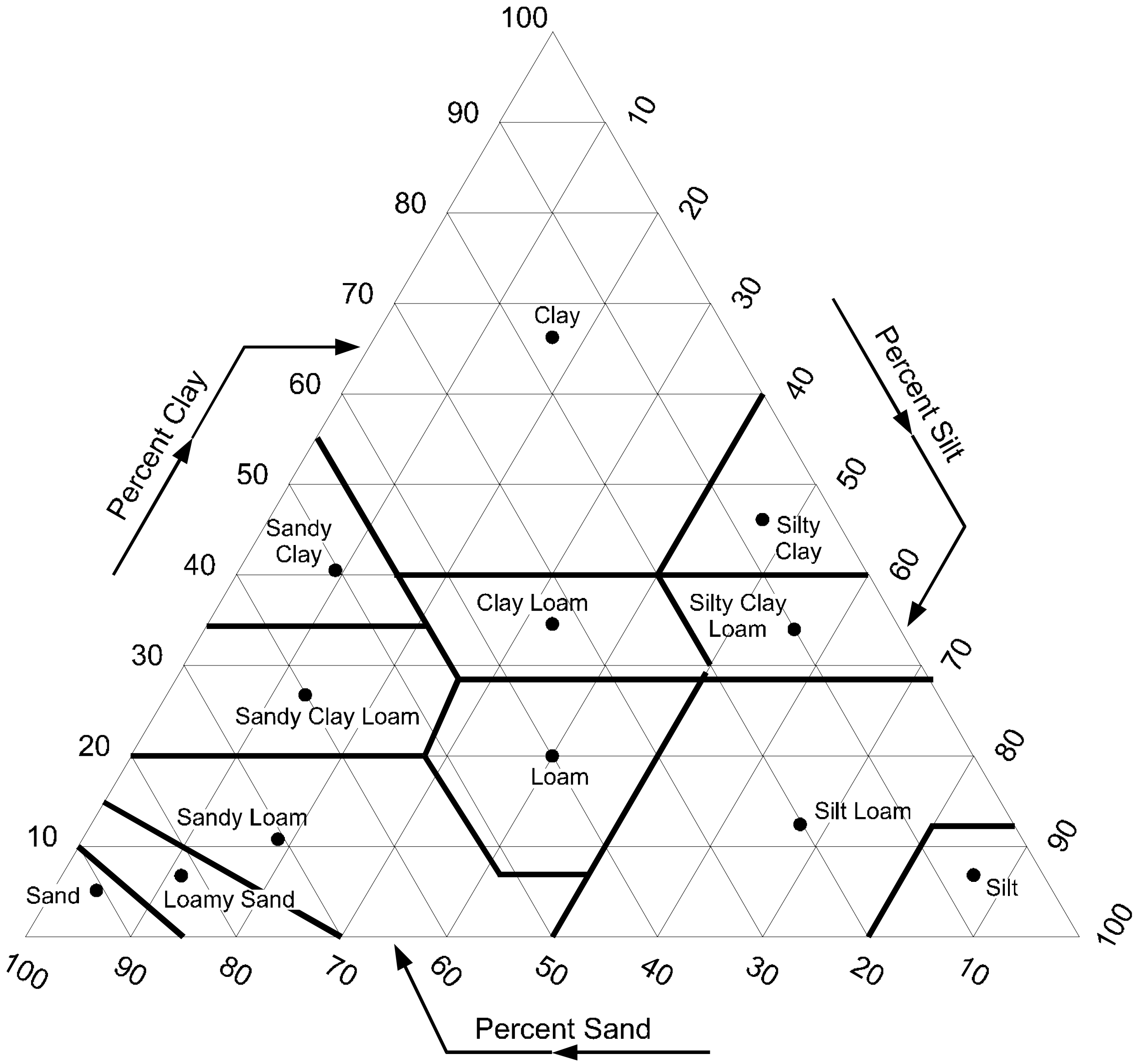


Figure 3. U.S. Soil Conservation Service Classification Chart Showing Centroid Compositions (Solid Circles)

TABLE 4. CENTROID COMPOSITIONS, MEAN PARTICLE DIAMETERS AND DRY BULK DENSITY OF THE 12 SCS SOIL TEXTURAL CLASSIFICATIONS

Textural class	% clay	% silt	% sand	Arithmetic mean particle diameter, cm	Dry Bulk Density g/cm^3
Sand	3.33	5.00	91.67	0.044	1.66
Loamy sand	6.25	11.25	82.50	0.040	1.62
Sandy loam	10.81	27.22	61.97	0.030	1.62
Sandy clay loam	26.73	12.56	60.71	0.029	1.63
Sandy clay	41.67	6.67	51.66	0.025	1.63
Loam	18.83	41.01	40.16	0.020	1.59
Clay loam	33.50	34.00	32.50	0.016	1.48
Silt loam	12.57	65.69	21.74	0.011	1.49
Clay	64.83	16.55	18.62	0.0092	1.43
Silty clay loam	33.50	56.50	10.00	0.0056	1.63
Silt	6.00	87.00	7.00	0.0046	1.35
Silty clay	46.67	46.67	6.66	0.0039	1.38

Given the mean particle diameter data in Table 4, the mean thickness of the capillary zone may then be estimated using Equations 9 and 10.

2.4 DIFFUSION THROUGH THE UNSATURATED ZONE

The effective diffusion coefficient within the unsaturated zone may also be estimated using the same form as Equation 6:

$$D_i^{eff} = D_a\left(\theta_{a,i}^{3.33} / n_i^2\right) + \left(D_w / H'_{TS}\right)\left(\theta_{w,i}^{3.33} / n_i^2\right) \qquad (11)$$

where D_i^{eff} = Effective diffusion coefficient across soil layer i, cm^2/s

D_a = Diffusivity in air, cm^2/s

$\theta_{a,i}$ = Soil air-filled porosity of layer i, cm^3/cm^3

n_i = Soil total porosity of layer i, cm^3/cm^3

D_w = Diffusivity in water, cm^2/s

$\theta_{w,i}$ = Soil water-filled porosity of layer i, cm^3/cm^3

H'_{TS} = Henry's law constant at the system temperature, dimensionless

The overall effective diffusion coefficient for systems composed of n distinct soil layers between the source of contamination and the enclosed space floor is:

$$D_T^{eff} = \frac{L_T}{\sum_{i=0}^{n} L_i / D_i^{eff}} \tag{12}$$

where D_T^{eff} = Total overall effective diffusion coefficient, cm^2/s

L_i = Thickness of soil layer i, cm

D_i^{eff} = Effective diffusion coefficient across soil layer i, cm^2/s

L_T = Distance between the source of contamination and the bottom of the enclosed space floor, cm.

Note that in the case of cracks in the floor of the enclosed space, the value of L_T does not include the thickness of the floor, nor does the denominator of Equation 12 include the thickness of the floor and the associated effective diffusion coefficient across the crack(s). An unlimited number of soil layers, including the capillary zone, may be included in Equation 12, but all layers must be located between the source of contamination and the enclosed space floor.

2.5 THE INFINITE SOURCE SOLUTION TO CONVECTIVE AND DIFFUSIVE TRANSPORT

Under the assumption that mass transfer is steady-state, J&E (1991) give the solution for the attenuation coefficient (α) as:

$$\alpha = \frac{\left[\left(\frac{D_T^{eff}\ A_B}{Q_{building}\ L_T}\right) x \ \exp\left(\frac{Q_{soil}\ L_{crack}}{D^{crack}\ A_{crack}}\right)\right]}{\left[\exp\left(\frac{Q_{soil}\ L_{crack}}{D_{crack}\ A_{crack}}\right)+\left(\frac{D_T^{eff}\ A_B}{Q_{building}\ L_T}\right)+\left(\frac{D_T^{eff}\ A_B}{Q_{soil}\ L_T}\right)\left[\exp\left(\frac{Q_{soil}\ L_{crack}}{D^{crack}\ A_{crack}}\right)-1\right]\right]} \qquad (13)$$

where α = Steady-state attenuation coefficient, unitless

D_T^{eff} = Total overall effective diffusion coefficient, cm^2/s

A_B = Area of the enclosed space below grade, cm^2

$Q_{building}$ = Building ventilation rate, cm^3/s

L_T = Source-building separation, cm

Q_{soil} = Volumetric flow rate of soil gas into the enclosed space, cm^3/s

L_{crack} = Enclosed space foundation or slab thickness, cm

A_{crack} = Area of total cracks, cm^2

D_{crack} = Effective diffusion coefficient through the cracks, cm^2/s (assumed equivalent to D_i^{eff} of soil layer i in contact with the floor).

The total overall effective diffusion coefficient is calculated by Equation 12. The value of A_B includes the area of the floor in contact with the underlying soil and the total wall area below grade. The building ventilation rate ($Q_{building}$) may be calculated as:

$$Q_{building} = \left(L_B\ W_B\ H_B\ ER\right)/\,3{,}600\ s/h \qquad (14)$$

where $Q_{building}$ = Building ventilation rate, cm^3/s

L_B = Length of building, cm

W_B = Width of building, cm

H_B = Height of building, cm

ER = Air exchange rate, (1/h).

The building dimensions in Equation 14 are those dimensions representing the total "living" space of the building; this assumes that the total air volume within the structure is well mixed and that any vapor contaminant entering the structure is instantaneously and homogeneously distributed.

The volumetric flow rate of soil gas entering the building (Q_{soil}) is calculated by the analytical solution of Nazaroff (1988) such that:

$$Q_{soil} = \frac{2\,\pi \Delta P\; k_v\; X_{crack}}{\mu\,\ln\left(2\,Z_{crack} / r_{crack}\right)} \tag{15}$$

where Q_{soil} = Volumetric flow rate of soil gas entering the building, cm^3/s

π = 3.14159

ΔP = Pressure differential between the soil surface and the enclosed space, $g/cm\text{-}s^2$

k_v = Soil vapor permeability, cm^2

X_{crack} = Floor-wall seam perimeter, cm

μ = Viscosity of air, g/cm-s

Z_{crack} = Crack depth below grade, cm

r_{crack} = Equivalent crack radius, cm.

Equation 15 is an analytical solution to vapor transport solely by pressure-driven air flow to an idealized cylinder buried some distance (Z_{crack}) below grade; the length of the cylinder is taken to be equal to the building floor-wall seam perimeter (X_{crack}). The cylinder, therefore, represents that portion of the building below grade through which vapors pass. The equivalent radius of the floor-wall seam crack (r_{crack}) is given in J&E (1991) as:

$$r_{crack} = \eta\left(A_B / X_{crack}\right) \tag{16}$$

where r_{crack} = Equivalent crack radius, cm

η = A_{crack}/A_B, $(0 \lneq \eta \lneq 1)$

A_B = Area of the enclosed space below grade, cm^2

X_{crack} = Floor-wall seam perimeter, cm.

The variable r_{crack} is actually the product of the fixed crack-to-total area ratio (η) and the hydraulic radius of the idealized cylinder, which is equal to the total area (A_B) divided by that portion of the cylinder perimeter in contact with the soil gas (X_{crack}). Therefore, if the dimensions of the enclosed space below grade (A_B) and/or the floor-wall seam perimeter (X_{crack}) vary, and the crack-to-total area ratio (η) remains constant, the value of r_{crack} must also vary. The total area of cracks (A_{crack}) is the product of η and A_B.

Equation 15 requires that the soil column properties within the zone of influence of the building (e.g., porosities, bulk density, etc.) be homogeneous, that the soil be isotropic with respect to vapor permeability, and that the pressure within the building be less than atmospheric.

Equation 13 contains the exponent of the following dimensionless group:

$$\left(\frac{Q_{soil}\ L_{crack}}{D^{crack}\ A_{crack}}\right) \quad . \tag{17}$$

This dimensionless group represents the equivalent Peclet number for transport through the building foundation. As the value of this group approaches infinity, the value of α approaches:

$$\frac{\left(\dfrac{D_T^{eff}\ A_B}{Q_{building}\ L_T}\right)}{\left(\dfrac{D_T^{eff}\ A_B}{Q_{soil}\ L_T}\right)+1} \quad . \tag{18}$$

In the accompanying spreadsheets, if the exponent of Equation 17 is too great to be calculated, the value of α is set equal to Equation 18.

With a calculated value of α, the steady-state vapor-phase concentration of the contaminant in the building ($C_{building}$) is calculated as:

$$C_{building} = \alpha C_{source} \quad . \tag{19}$$

2.6 THE FINITE SOURCE SOLUTION TO CONVECTIVE AND DIFFUSIVE TRANSPORT

If the thickness of soil contamination is known, the finite source solution of J&E (1991) can be employed such that the time-averaged attenuation coefficient (<α>) may be calculated as:

$$\langle\alpha\rangle = \frac{\rho_b\, C_R\, \Delta H_c\, A_B}{Q_{building}\, C_{source}\, \tau}\left(\frac{L_T^0}{\Delta H_c}\right)\left[\left(\beta^2 + 2\,\Psi\,\tau\right)^{1/2} - \beta\right] \tag{20}$$

where $<\alpha>$ = Time-averaged finite source attenuation coefficient, unitless

ρ_b = Soil dry bulk density at the source of contamination, g/cm^3

C_R = Initial soil concentration, g/g

ΔH_c = Initial thickness of contamination, cm

A_B = Area of enclosed space below grade, cm^2

$Q_{building}$ = Building ventilation rate, cm^3/s

C_{source} = Vapor concentration at the source of contamination, g/cm^3-v

τ = Exposure interval, s

L_T^0 = Source-building separation at time = 0, cm

and;

$$\beta = \left(\frac{D_T^{eff}\ A_B}{L_T^O\ Q_{soil}}\right)\left[1 - \exp\left(-\frac{Q_{soil}\ L_{crack}}{D^{crack}\ A_{crack}}\right)\right] + 1 \tag{21}$$

and;

$$\Psi = \frac{D_T^{eff}\ C_{source}}{\left(L_T^O\right)^2\ \rho_b\, C_R} \quad . \tag{22}$$

Implicit in Equation 20 is the assumption that source depletion occurs from the top boundary of the contaminated zone as contaminant volatilizes and moves upward toward the soil surface. This creates a hypothetical "dry zone" (δ) that grows with time; conversely, the "wet zone" of contamination retreats proportionally. When the thickness of the depletion zone (δ) is equal to the initial thickness of contamination (ΔH_c), the source is totally depleted. The unitless expression $(L_T^0/\Delta H_c)[(\beta^2 + 2\,\Psi\tau)^{1/2} - \beta]$ in Equation 20 represents the cumulative fraction of the depletion zone at the end of the exposure interval τ. Multiplying this expression by the remainder of Equation 20 results in the time-averaged finite source attenuation coefficient ($<\alpha>$).

With a calculated value for $<\alpha>$, the time-averaged vapor concentration in the building ($C_{building}$) is:

$$C_{building} = \langle \alpha \rangle C_{source} \quad . \tag{23}$$

For extended exposure intervals (e.g., 30 years), the time for source depletion may be less than the exposure interval. The time for source depletion τ_D) may be calculated by:

$$\tau_D = \frac{\left[\Delta H_c / L_T^O + \beta\right]^2 - \beta^2}{2\,\Psi} \quad . \tag{24}$$

If the exposure interval (τ) is greater than the time for source depletion τ_D), the time-averaged building vapor concentration may be calculated by a mass balance such that:

$$C_{building} = \frac{\rho_b\, C_R\, \Delta H_c\, A_B}{Q_{building}\ \tau} \tag{25}$$

where $C_{building}$ = Time-averaged vapor concentration in the building, g/cm^3-v

ρ_b = Soil dry bulk density at the source of contamination, g/cm^3

C_R = Initial soil concentration, g/g

ΔH_c = Initial thickness of contamination, cm

A_B = Area of enclosed space below grade, cm^2

$Q_{building}$ = Building ventilation rate, cm^3/s

τ = Exposure interval, s.

2.7 THE SOIL GAS MODELS

Use of the J&E Model has typically relied on a theoretical partitioning of the total volume soil concentration into the sorbed, aqueous, and vapor phases. The model has also relied on a theoretical approximation of vapor transport by diffusion and convection from the source of emissions to the building floor in contact with the soil. Use of measured soil gas concentrations directly beneath the building floor instead of theoretical vapor concentrations and vapor transport has obvious advantages that would help to reduce the uncertainty in the indoor air concentration estimates made by the model.

The soil gas models (SG-SCREEN and SG-ADV) are designed to allow the user to input measured soil gas concentration and sampling depth information directly into the spreadsheets. In the new models, the value of the user-defined soil gas concentration is assigned as the value of C_{source} in Equation 19. The steady-state (infinite source) attenuation coefficient (α) in Equation 19 is calculated using Equation 13. The steady-state solution for the attenuation coefficient is used because no evaluation has been made regarding the size and total mass of the source of emissions. The source of emissions, therefore, cannot be depleted over time. The soil gas models estimate the steady-state indoor air concentration over the exposure duration. For a detailed discussion of using the soil gas models as well as soil gas sampling, see Section 4 of this document.

2.8 SOIL VAPOR PERMEABILITY

Soil vapor permeability (k_v) is one of the most sensitive model parameters associated with convective transport of vapors within the zone of influence of the building. Soil vapor permeability is typically measured from field pneumatic tests. If field data are lacking, however, an estimate of the value of k_v can be made with limited data.

Soil intrinsic permeability is a property of the medium alone that varies with the size and shape of connected soil pore openings. Intrinsic permeability (k_i) can be estimated from the soil saturated hydraulic conductivity:

$$k_i = \frac{K_s\,\mu_w}{\rho_w\,g} \qquad (26)$$

where k_i = Soil intrinsic permeability, cm^2

K_s = Soil saturated hydraulic conductivity, cm/s

μ_w = Dynamic viscosity of water, g/cm-s (= 0.01307 at 10^{o}C)

ρ_w = Density of water, g/cm^3 (= 0.999)

g = Acceleration due to gravity, cm/s^2 (= 980.665).

Schaap and Leij (1998) computed the SCS class average values of the saturated hydraulic conductivity (K_s) for each of the 12 SCS soil textural classifications (Table 5). With these values, a general estimate of the value of k_i can be made by soil type. As an alternative, in situ measurements of the site-specific saturated hydraulic conductivity can be made and the results input into Equation 26 to compute the value of the soil intrinsic permeability.

Effective permeability is the permeability of the porous medium to a fluid when more than one fluid is present; it is a function of the degree of saturation. The relative air permeability of soil (k_{rg}) is the effective air permeability divided by the intrinsic permeability and therefore takes into account the effects of the degree of water saturation on air permeability.

TABLE 5. CLASS AVERAGE VALUES OF SATURATED HYDRAULIC CONDUCTIVITY FOR THE 12 SCS SOIL TEXTURAL CLASSIFICATIONS

Soil texture , USDA	Class average saturated hydraulic conductivity, cm/h
Sand	26.78
Loamy sand	4.38
Sandy loam	1.60
Sandy clay loam	0.55
Sandy clay	0.47
Loam	0.50
Clay loam	0.34
Silt loam	0.76
Clay	0.61
Silty clay loam	0.46
Silt	1.82
Silty clay	0.40

Parker et al. (1987) extended the relative air permeability model of van Genuchten (1980) to allow estimation of the relative permeabilities of air and water in a two- or three-phase system:

$$k_{rg} = (1 - S_{te})^{1/2} \left(1 - S_{te}^{1/M}\right)^{2M} \tag{27}$$

where k_{rg} = Relative air permeability, unitless ($0 \le k_{rg} \le 1$)

S_{te} = Effective total fluid saturation, unitless

M = van Genuchten shape parameter, unitless.

Given a two-phase system (i.e., air and water), the effective total fluid saturation (S_{te}) is calculated as:

$$S_{te} = \frac{(\theta_w - \theta_r)}{(n - \theta_r)} \tag{28}$$

where S_{te} = Effective total fluid saturation, unitless

θ_w = Soil water-filled porosity, cm^3/cm^3

θ_r = Residual soil water content, cm^3/cm^3

n = Soil total porosity, cm^3/cm^3.

Class average values for the parameters θ_r and M by SCS soil type may be obtained from Table 3.

The effective air permeability (k_v) is then the product of the intrinsic permeability (k_i) and the relative air permeability (k_{rg}) at the soil water-filled porosity θ_w.

2.9 CALCULATION OF A RISK-BASED SOIL OR GROUNDWATER CONCENTRATION

Both the infinite source model estimate of the steady-state building concentration and the finite source model estimate of the time-averaged building concentration represent the exposure point concentration used to assess potential risks. Calculation of a risk-based media concentration for a carcinogenic contaminant takes the form:

$$C_C = \frac{TR\,x\,AT_C\,x\,365\,days/yr}{URF\,x\,EF\,x\,ED\,x\,C_{building}} \tag{29}$$

where C_C = Risk-based media concentration for carcinogens, µg/kg-soil, or µg/L-water

TR = Target risk level, unitless

AT_C = Averaging time for carcinogens, yr

URF = Unit risk factor, $\mu g/m^3)^{-1}$

EF = Exposure frequency, days/yr

ED = Exposure duration, yr

$C_{building}$ = Vapor concentration in the building, µg/m^3 per µg/kg-soil, or µg/m^3 per µg/L-water.

In the case of a noncarcinogenic contaminant, the risk-based media concentration is calculated by:

$$C_{NC} = \frac{THQ \; x \; AT_{NC} \; x \, 365 \, days / yr}{EF \; x \, ED \, x \, \frac{1}{RfC} \, x \, C_{building}} \qquad (30)$$

where C_{NC} = Risk-based media concentration for noncarcinogens, µg/kg-soil, or µg/L-water

THQ = Target hazard quotient, unitless

AT_{NC} = Averaging time for noncarcinogens, yr

EF = Exposure frequency, days/yr

ED = Exposure duration, yr

RfC = Reference concentration, mg/m^3

$C_{building}$ = Vapor concentration in the building, mg/m^3 per µg/kg-soil, or mg/m^3 per µg/L-water.

The spreadsheets calculate risk-based media concentrations based on a unity initial concentration. That is, soil risk-based concentrations are calculated with an initial hypothetical soil concentration of 1 µg/kg-soil, while for groundwater the initial hypothetical concentration is 1 µg/L-water.

For this reason, the values of C_{source} and $C_{building}$ shown on the INTERCALCS worksheet when reverse-calculating a risk-based media concentration do not represent actual values. For these calculations, the following message will appear on the RESULTS worksheet:

> "MESSAGE: The values of C_{source} and $C_{building}$ on the INTERCALCS worksheet are based on unity and do not represent actual values."

When forward-calculating risks from a user-defined initial soil or groundwater concentration, the values of C_{source} and $C_{building}$ on the INTERCALCS worksheet are correct.

2.10 CALCULATION OF INCREMENTAL RISKS

Forward-calculation of incremental risks begins with an actual initial media concentration (i.e., µg/kg-soil or µg/L-water). For carcinogenic contaminants, the risk level is calculated as:

$$Risk = \frac{URF\ x\ EF\ x\ ED\ x\ C_{building}}{AT_C\ x\ 365\ days/yr} \tag{31}$$

For noncarcinogenic contaminants, the hazard quotient (HQ) is calculated as:

$$HQ = \frac{EF\ x\ ED\ x\ \frac{1}{RfC}\ x\ C_{building}}{AT_{NC}\ x\ 365\ \ days/yr}\quad . \tag{32}$$

2.11 MAJOR MODEL ASSUMPTIONS/LIMITATIONS

The following represent the major assumptions/limitations of the J&E Model.

1. Contaminant vapors enter the structure primarily through cracks and openings in the walls and foundation.

2. Convective transport occurs primarily within the building zone of influence and vapor velocities decrease rapidly with increasing distance from the structure.

3. Diffusion dominates vapor transport between the source of contamination and the building zone of influence.

4. All vapors originating from below the building will enter the building unless the floors and walls are perfect vapor barriers.

5. All soil properties in any horizontal plane are homogeneous.

6. The contaminant is homogeneously distributed within the zone of contamination.

7. The areal extent of contamination is greater than that of the building floor in contact with the soil.

8. Vapor transport occurs in the absence of convective water movement within the soil column (i.e., evaporation or infiltration), and in the absence of mechanical dispersion.

9. The model does not account for transformation processes (e.g., biodegradation, hydrolysis, etc.).

10. The soil layer in contact with the structure floor and walls is isotropic with respect to permeability.

11. Both the building ventilation rate and the difference in dynamic pressure between the interior of the structure and the soil surface are constant values.

Use of the J&E Model as a first-tier screening tool to identify sites needing further assessment requires careful evaluation of the assumptions listed in the previous section to determine whether any conditions exist that would render the J&E Model inappropriate for the site. If the model is deemed applicable at the site, care must be taken to ensure reasonably conservative and self-consistent model parameters are used as input to the model. Considering the limited site data typically available in preliminary site assessments, the J&E Model can be expected to predict only whether or not a risk-based exposure level will be exceeded at the site. Precise prediction of concentration levels is not possible with this approach.

The suggested minimum site characterization information for a first tier evaluation of the vapor intrusion pathway includes: site conceptual model, nature and extent of contamination distribution, soil lithologic descriptions, groundwater concentrations, and/or possibly near source soil vapor concentrations. The number of samples and measurements needed to establish this information varies by site and it's not possible to provide a hard and fast rule. Bulk soil concentrations should not be used unless appropriately preserved during sampling.

Based on the conceptual site model (CSM), the user can select the appropriate spreadsheet corresponding to the vapor source at the site and determine whether to use the screening level spreadsheet (which allows only one soil type above the capillary fringe) or the more advanced version (which allows up to three layers above the capillary fringe). Because most of the inputs to the J&E Model are not collected during a typical site characterization, conservative inputs have to be estimated or inferred from available data and other non-site-specific sources of information.

The uncertainty in determining key model parameters and sensitivity of the J&E Model to those key model parameters is qualitatively described in Table 6. As shown in the table, building-related parameters will moderate to high uncertainty and model sensitivity include: Qsoil, building crack ratio, building air-exchange rate, and building mixing height. Building-related parameters with low uncertainty and sensitivity include: foundation area, depth to base of foundation, and foundation slab thickness. Of the soil-dependent properties, the soil moisture parameters clearly are of critical importance for the attenuation value calculations.

TABLE 6. UNCERTAINTY AND SENSITIVITY OF KEY PARAMETERS FOR THE VAPOR INTRUSION MODEL

			Parameter Sensitivity		
Input Parameter	Parameter Uncertainty Or Variability	Shallower Contamination Building Underpressurized	Deeper Contamination Building Underpressurized	Shallower Contamination Building Not Underpressurized	Deeper Contamination Building Not Underpressurized
Soil Total Porosity (n)	Low	Low	Low	Low	Low
Soil Water-filled Porosity (θ_w)	Moderate to High	Low to Moderate	Moderate to High	Moderate to High	Moderate to High
Capillary Zone Water-filled Porosity ($\theta_{n, cz}$)	Moderate to High	Moderate to High	Moderate to High	Moderate to High	Moderate to High
Thickness of Capillary Zone (L_{cz})	Moderate to High	Moderate to High	Moderate to High	Moderate to High	Moderate to High
Soft Dry Bulk Density (ρ_b)	Low	Low	Low	Low	Low
Average Vapor Flowrate into a Building (Q_{soil})	High	Moderate to High	Low to Moderate	N/A	N/A
Soil Vapor Permeability(K_v)	High	Moderate to High	Low to Moderate	N/A	N/A
Soil to Building Pressure Differential (ΔP)	Moderate	Moderate	Low to Moderate	N/A	N/A
Henry's Law Constant (for single chemical) (H)	Low to Moderate	Low to Moderate	Low to Moderate	Low to Moderate	Low to Moderate
Diffusivity in Air (D_A)	Low	Low	Low	Low	Low
Indoor Air Exchange Rate (ER)	Moderate	Moderate	Moderate	Moderate	Moderate
Enclosed Space Height (H_B)	Moderate	Moderate	Moderate	Moderate	Moderate
Area of Enclosed Space Below Grade (A_B)	Low to Moderate	Low to Moderate	Low to Moderate	Low to Moderate	Low to Moderate
Depth Below Grade to Bottom of Enclosed Space (L_F)	Low	Low	Low	Low	Low
Crack-to-Total Area Ratio (η)	High	Low	Low	Moderate to High	Low to Moderate
Enclosed Space Floor Thickness (L_{crack})	Low	Low	Low	Low	Low

SECTION 3

SOIL AND GROUNDWATER MODEL APPLICATION

This section provides step-by-step instructions on how to implement the soil and groundwater contamination versions of the J&E Model using the spreadsheets. This section also discusses application of the soil gas versions of the model. The user provides data and selects certain input options, and views model results via a series of worksheets. Error messages are provided within both the data entry worksheet and the results worksheet to warn the user that entered data are missing or outside of permitted limits.

The J&E Model as constructed within the accompanying spreadsheets requires a range of input variables depending on whether a screening-level or advanced model is chosen. Table 7 provides a list of all major input variables, the range of practical values for each variable, the default value for each variable, and the relative model sensitivity and uncertainty of each variable. Table 7 also includes references for each value or range of values.

Table 8 indicates the results of an increase in the value of each input parameter. The results are shown as either an increase or a decrease in the building concentration ($C_{building}$) of the pollutant. An increase in the building concentration will result in an increase in the risk when forward-calculating from an initial soil or groundwater concentration. When reverse-calculating to a risk-based "acceptable" soil or groundwater concentration, an increase in the hypothetical unit building concentration will result in a lower "acceptable" soil or groundwater concentration.

A list of reasonably conservative model input parameters for building-related parameters is provided in Table 9, which also provides the practical range, typical or mean value (if applicable), and most conservative value for these parameters. For building parameters with low uncertainty and sensitivity, only a single "fixed" value corresponding to the mean or typical value is provided in Table 9. Soil-dependent properties are provided in Table 10 for soils classified according to the US SCS system. If site soils are not classified according to the US SCS, Table 11 can be used to assist in selecting an appropriate SCS soil type corresponding to the available site lithologic information. Note that the selection of the soil texture class should be biased towards the coarsest soil type of significance, as determined by the site characterization program.

TABLE 7. RANGE OF VALUES FOR SELECTED INPUT PARAMETERS

Input parameter	Practical range of values	Default value
Soil water-filled porosity (θ_w)	0.04 – 0.33 cm^3/cm^{3a}	Soil dependent see Table 10
Soil vapor permeability (k_v)	10^{-6} – 10^{-12} $cm^{2b,c}$	10^{-8} cm^{2d}
Soil-building pressure differential (ΔP)	0 – 20 Pa^3	4 Pa^f
Media initial concentration (C_R, C_w)	User-defined	NA
Depth to bottom of soil contamination (L_b)	User-defined	NA
Depth to top of concentration (L_T)	User-defined	NA
Floor-wall seam gap (w)	0.05 – 1.0 cm^e	0.1 cm^e
Soil organic carbon fraction (f_{oc})	0.001 – 0.006^a	0.002^a
Indoor air exchange rate (ER)	0.18 – 1.26 $(H^{-1})^g$	0.25 $(h^{-1})^{g,h}$
Soil total porosity (n)	0.34 – 0.53 cm^3/cm^{3a}	0.43 cm^3/cm^{3a}
Soil dry bulk density (ρ_b)	1.25 – 1.75 g/cm^{3a}	1.5 g/cm^{3a}

[a] U.S. EPA (1996a and b).

[b] Johnson and Ettinger (1991).

[c] Nazaroff (1988).

[d] Based on transition point between diffusion and convection dominated transport from Johnson and Ettinger (1991).

[e] Eaton and Scott (1984); Loureiro et al. (1990).

[f] Loureiro et al. (1990); Grimsrud et al. (1983).

[g] Koontz and Rector (1995).

[h] Parker et al. (1990).

[i] U.S. DOE (1995).

TABLE 8. EFFECT ON BUILDING CONCENTRATION FROM AN INCREASE IN INPUT PARAMETER VALUES

Input parameter	Change in parameter value	Effect on building concentration
Soil water-filled porosity (θ_w)	Increase	Decrease
Soil vapor permeability (k_v)	Increase	Increase
Soil-building pressure differential (ΔP)	Increase	Increase
Media initial concentration (C_R, C_w)[a]	Increase	Increase
Depth to bottom of soil contamination (L_b)[b]	Increase	Increase
Depth to top of concentration (L_T)	Increase	Decrease
Floor-wall seam gap (w)	Increase	Increase
Soil organic carbon fraction (f_{oc})	Increase	Decrease
Indoor air exchange rate (ER)	Increase	Decrease
Building volume[c] (L_B x W_B x H_B)	Increase	Decrease
Soil total porosity (n)	Increase	Increase
Soil dry bulk density (ρ_b)	Increase	Decrease

[a] This parameter is applicable only when forward-calculating risk.

[b] Applicable only to advanced model for soil contamination.

[c] Used with building air exchange rate to calculate building ventilation rate.

TABLE 9. BUILDING-RELATED PARAMETERS FOR THE VAPOR INTRUSION MODEL

Input Parameter	Units	Fixed or Variable	Typical or Mean Value	Range	Conservative Value	Default Value
Total Porosity	cm^3/cm^3	Fixed	Specific to soil texture, see Table 10			
Unsaturated Zone Water-filled Porosity	cm^3/cm^3	Variable	Specific to soil texture, see Table 10			
Capillary Transition zone Water-filled Porosity	cm^3/cm^3	Fixed	Specific to soil texture, see Table 10			
Capillary Transition Zone height	cm^3/cm^3	Fixed	Specific to soil texture, see Table 10			
Q_{soil}	L/min	Variable	Specific to soil texture, see Table 10			
Soil air permeability	m^2	Variable	Specific to soil texture, see Table 10			
Building Depressurization	Pa	Variable	4	0-15	15	N/A
Henry's law constant (for single chemical)	-	Fixed	Specific to chemical, see Appendix B			
Free-Air Diffusion Coefficient (single chemical)	-	Fixed	Specific to chemical, see Appendix B			
Building Air exchange Rate	hr^{-1}	Variable	0.5	0.1-1.5	0.1	0.25
Building Mixing height – Basement scenario	m	Variable	3.66	2.44-4.88	2.44	3.66
Building Mixing height – Slab-on-grade scenario	m	Variable	2.44	2.13-3.05	2.13	2.44
Building Footprint Area – Basement Scenario	m^2	Variable	120	80-200+	80	100
Building Footprint Area – Slab-on-Grade Scenario	m^2	Variable	120	80-200+	80	100
Subsurface Foundation area – Basement Scenario	m^2	Variable	208	152-313+	152	180
Subsurface Foundation area – Slab-on-Grade Scenario	m^2	Fixed	127	85-208+	85	106
Depth to Base of Foundation – Basement Scenario	m	Fixed	2	N/A	N/A	2
Depth to Base of Foundation – Slab-on-Grade Scenario	m	Fixed	0.15	N/A	N/A	0.15
Perimeter Crack Width	mm	Variable	1	0.5-5	5	1
Building Crack ratio – Slab-on-Grade Scenario	dimensionless	Variable	0.00038	0.00019-0.0019	0.0019	3.77×10^{-4}
Building Crack ratio – Basement Scenario	dimensionless	Variable	0.0002	0.0001-0.001	0.001	2.2×10^{-4}
Crack Dust Water-Filled Porosity	cm^3/cm^3	Fixed	Dry	N/A	N/A	Dry
Building Foundation Slab Thickness	m	Fixed	0.1	N/A	N/A	0.1

TABLE 10. SOIL-DEPENDENT PROPERTIES FOR THE VAPOR INTRUSION MODEL - FIRST TIER ASSESSMENT

			Unsaturated Zone				Capillary Transition Zone		
			Water-Filled Porosity						
U.S. Soil Conservation Service (SCS) Soil Texture	Saturated Water Content Total Porosity θ_s (cm^3/cm^3)	Residual Water Content θ_r (cm^3/cm^3)	Mean or Typical ($FC_{1/3bar}+\theta_r$)/2 $\theta_{w,unsat}$ (cm^3/cm^3)	Range $\theta_{w,unsat}$ (cm^3/cm^3)	Conservative $\theta_{w,unsat}$ (cm^3/cm^3)	Modeled $\theta_{w,unsat}$ (cm^3/cm^3)	Saturated Water Content Total Porosity θ_s (cm^3/cm^3)	$\theta_{w,cap}$ Cap @ air-entry	Height Cap Zone Fetter (94) (cm)
Clay	0.459	0.098	0.215	0.098-0.33	0.098	0.215	0.459	0.412	81.5
Clay Loam	0.442	0.079	0.168	0.079-0.26	0.079	0.168	0.442	0.375	46.9
Loam	0.399	0.061	0.148	0.061-0.24	0.061	0.148	0.399	0.332	37.5
Loamy Sand	0.39	0.049	0.076	0.049-0.1	0.049	0.076	0.39	0.303	18.8
Silt	0.489	0.05	0.167	0.05-0.28	0.050	0.167	0.489	0.382	163.0
Silt Loam	0.439	0.065	0.180	0.065-0.3	0.065	0.180	0.439	0.349	68.2
Silty Clay	0.481	0.111	0.216	0.11-0.32	0.111	0.216	0.481	0.424	192.0
Silty Clay Loam	0.482	0.09	0.198	0.09-0.31	0.090	0.198	0.482	0.399	133.9
Sand	0.375	0.053	0.054	0.053-0.055	0.053	0.054	0.375	0.253	17.0
Sandy Clay	0.385	0.117	0.197	0.117-0.28	0.117	0.197	0.385	0.355	30.0
Sandy Clay Loam	0.384	0.063	0.146	0.063-0.23	0.063	0.146	0.384	0.333	25.9
Sandy Loam	0.387	0.039	0.103	0.039-0.17	0.039	0.103	0.387	0.320	25.0
Loamy Sand	0.39	0.049	0.076	0.049-0.1	0.049	0.076	0.39	0.303	18.8

TABLE 11. GUIDANCE FOR SELECTION OF SOIL TYPE

If your boring log indicates that the following materials are the predominant soil types …	**Then you should use the following texture classification when obtaining the attenuation factor**
Sand or Gravel or **Sand and Gravel**, with less than about 12 % fines, where "fines" are smaller than 0.075 mm in size.	Sand
Sand or Silty Sand, with about 12 % to 25 % fines	Loamy Sand
Silty Sand, with about 20 % to 50 % fines	Sandy Loam
Silt and Sand or Silty Sand or Clayey, Silty Sand or Sandy Silt or Clayey, Sandy Silt, with about 45 to 75 % fines	Loam
Sandy Silt or Silt, with about 50 to 85 % fines	Silt Loam

These input parameters were developed from the best available soil-physics science, available studies of building characteristics, and international-expert opinion. Consequently, the input parameters listed in Tables 9 and 10 are considered default parameters for a first-tier assessment, which should in most cases provide a reasonably (but not overly) conservative estimate of the vapor intrusion attenuation factor for a site. Justification for the building-related and soil-dependent parameters values selected as default values for the J&E Model is described below.

3.1 JUSTIFICATION OF DEFAULT SOIL-DEPENDENT PROPERTIES

The default soil-dependent parameters recommended for a first tier assessment (Table 10) represent mean or typical values, rather than the most conservative value, in order to avoid overly conservative estimates of attenuation factors. Note, however, that the range of values for some soil properties can be very large, particularly in the case of moisture content and hydraulic conductivity. Consequently, selecting a soil type and corresponding typical soil property value may not accurately or conservatively represent a given site. Note also that Table 9 does not provide estimates of soil properties for very coarse soil types, such as gravel, gravelly sand, and sandy gravel, etc., which also may be present in the vadose zone. Consequently, in cases where the vadose zone is characterized by very coarse materials, the J&E Model may not provide a conservative estimate of attenuation factor.

As discussed above, the J&E Model is sensitive to the value of soil moisture content. Unfortunately, there is little information available on measured moisture contents below buildings. Therefore, the typical approach is to use a water retention model (e.g., van Genuchten model) to approximate moisture contents. For the unsaturated zone, the selected default value for soil moisture is a value equal to halfway between the residual saturation value and field capacity, using the van Genuchten model-predicted values for U.S. SCS soil types. For the capillary transition zone, a moisture content corresponding to the air entry pressure head is calculated by using the van Genuchten model. When compared to other available water retention models, the van Genuchten model yields somewhat lower water contents, which results in more conservative estimates of attenuation factor. The soil moisture contents listed in Table 10 are based on agricultural samples, which are likely to have higher water contents than soils below building foundations and, consequently result in less-conservative estimates of the attenuation factor.

3.2 JUSTIFICATION OF DEFAULT BUILDING-RELATED PROPERTIES

Building Air Exchange Rate (Default Value = 0.25 AEH)

The results of 22 studies for which building air exchange rates are reported in Hers et al. (2001). Ventilation rates vary widely from approximately 0.1 AEH for energy efficient “air-tight” houses (built in cold climates) (Fellin and Otson, 1996) to over 2 AEH (AHRAE (1985); upper range). In general, ventilation rates will be higher in summer months when natural ventilation rates are highest. Murray and Burmaster (1995) conducted one of the most comprehensive studies of U.S. residential air exchange rates (sample size of 2844 houses). The data set was analyzed on a seasonal basis and according to climatic region. When all the data were analyzed, the 10th, 50th and 90th percentile values were 0.21, 0.51 and 1.48 AEH. Air exchange rates varied depending on season and climatic region. For example, for the winter season and coldest climatic area (Region 1, e.g., Great Lakes area and extreme northeast U.S.), the 10th, 50th , and 90th percentile values were 0.11, 0.27 and 0.71 AEH, respectively.. In contrast, for the winter season and warmest climatic area [Region 4 (southern California, Texas, Florida, Georgia)], the 10th, 50th, and 90th percentile values were 0.24, 0.48 and 1.13 AEH, respectively. Although building air exchange rates would be higher during the summer months, vapor intrusion during winter months (when house depressurization is expected to be most significant) would be of greatest concern. For this guidance, a default value of 0.25 for air exchange rate was selected to represent the lower end of these distributions.

Crack Width and Crack Ratio (Default Value = 0.0002 for basement house; = 0.0038 for slab-on-grade house)

The crack width and crack ratio are related. Assuming a square house and that the only crack is a continuous edge crack between the foundation slab and wall ("perimeter crack"), the crack ratio and crack width are related as follows:

Crack Ratio = Crack Width x 4 x (Subsurface Foundation Area)^0.5/Subsurface Foundation Area

Little information is available on crack width or crack ratio. One approach used by radon researchers is to back-calculate crack ratios using a model for soil gas flow through cracks and the results of measured soil gas flow rates into a building. For example, the back-calculated values for a slab/wall edge crack based on soil gas-entry rates reported in Nazaroff (1992), Revzan *et al.* (1991), and Nazaroff *et al.* (1985) range from about 0.0001 to 0.001. Another possible approach is to measure crack openings although this, in practice, is difficult to do. Figley and Snodgrass (1992) present data from 10 houses where edge crack measurements were made. At the eight houses where cracks were observed, the crack widths ranged from hairline cracks up to 5 mm wide, while the total crack length per house ranged from 2.5 m to 17.3 m. Most crack widths were less than 1 mm. The suggested defaults for crack ratio in regulatory guidance, literature, and models also vary. In ASTM E1739-95, a default crack ratio of 0.01 is used. The crack ratios suggested in the VOLASOIL model (developed by the Dutch Ministry of Environment) range from 0.0001 to 0.000001. The VOLASOIL model values correspond to values for a "good" and "bad" foundation, respectively. The crack ratio used by J&E (1991) for illustrative purposes ranged from 0.001 to 0.01. The selected default values fall within the ranges observed.

Building Area and Subsurface Foundation Area (Default Value = 10 m by 10 m)

The default building area is based on the following information:

- Default values used in the Superfund User's Guide (9.61 m by 9.61 m or 92.4 m^2)
- Default values used by the State of Michigan, as documented in Part 201, Generic Groundwater and Soil Volatilization to Indoor Air Inhalation Criteria: Technical Support Document (10.5 m by 10.5 m of 111.5 m^2).

The Michigan guidance document indicates that the 111.5 m^2 area approximately corresponds to the 10th percentile floor space area for a residential single-family dwelling, based on statistics compiled by the U.S. Department of Commerce (DOC) and U.S. Housing and Urban Development (HUD). The typical, upper, and lower ranges presented in Table 9 are subjectively chosen values. The subsurface foundation area is a function of the building area, and depth to the base of the foundation, which is fixed.

Building Mixing Height (Default Value = 2.44 m for slab-on-grade scenario; = 3.66 m for basement scenario)

The J&E Model assumes that subsurface volatiles migrating into the building are completely mixed within the building volume, which is determined by the building area and mixing height. The building mixing height will depend on a number of factors including building height; heating, ventilation, and air conditioning (HVAC) system operation, environmental factors such as indoor-outdoor pressure differentials and wind loading, and seasonal factors. For a single-story house, the variation in mixing height can be approximated by using the room height. For a multi-story house or apartment building, the mixing height will be greatest for houses with HVAC systems that result in significant air circulation (e.g., forced-air heating systems). Mixing heights would likely be less for houses with electrical baseboard heaters. It is likely that mixing height is, to some degree, correlated to the building air exchange rate.

Little data are available that provides for direct inference of mixing height. There are few sites, with a small number of houses where indoor air concentrations were above background, and where both measurements at ground level and the second floor were made Colorado Department of Transportation (CDOT), Redfields, Eau Claire). Persons familiar with the data sets for these sites indicate that in most cases a fairly significant reduction in concentrations (factor of two or greater) was observed, although at one site (Eau Claire, “S” residence), the indoor trichloroethylene (TCE) concentrations were similar in both the basement and second floor of the house. For the CDOT site apartments, there was an approximate five-fold reduction between the concentrations measured for the first floor and second floor units (Mr. Jeff Kurtz, EMSI, personal communication, June 2002). Less mixing would be expected for an apartment because there are less cross-floor connections than for a house. The value chosen for a basement house scenario (3.66 m) would be representative of a two-fold reduction or attenuation in vapor concentrations between floors.

Q_{soil} (Default Value = 5 L/min)

The method often used with the J&E Model for estimating the soil gas advection rate (Q_{soil}) through the building envelope is an analytical solution for two-dimensional soil gas flow to a small horizontal drain (Nazaroff 1992) (“Perimeter Crack Model”). Use of this model can be problematic in that Q_{soil} values are sensitive to soil-air permeability and consequently a wide range in flows can be predicted.

An alternate empirical approach is to select a Q_{soil} value on the basis of tracer tests (i.e., mass balance approach). When soil gas advection is the primary mechanism for tracer intrusion into a building, the Q_{soil} can be estimated by measuring the concentrations of a chemical tracer in indoor air, in outdoor air, and in soil vapor below a building, and by measuring the building ventilation rate (Hers et al. 2000a; Fischer et al. 1996; Garbesi et al. 1993; Rezvan et al. 1991; Garbesi and Sextro, 1989). For sites with coarse-grained soils (Table 10). The Q_{soil} values measured using this technique are compared to predicted rates using the Perimeter Crack model. The Perimeter Crack model predictions are both higher and lower than the measured values, but overall are within one order of magnitude of the measured values. Although the Q_{soil} values predicted by the models and measured using field tracer tests are uncertain, the results suggest that a "typical" range for houses on coarse-grained soils is on the order of 1 to 10 L/min. A disadvantage with the tracer test approach is that only limited data are available and there do not appear to be any tracer studies for field sites with fine-grained soils.

It is also important to recognize that the advective zone of influence for soil gas flow is limited to soil immediately adjacent to the building foundation. Some data on pressure coupling provide insight on the extent of the advective flow zone. For example, Garbesi *et al.* (1993) report a pressure coupling between the soil and experimental basement (*i.e.*, relative to that between the basement and atmosphere) equal to 96 percent directly below the slab, between 29 percent and 44 percent at 1 m below the basement floor slab, and between 0.7 percent and 27 percent at a horizontal distance of 2 m from the basement wall. At the Chatterton site (research site investigated by the author), the pressure coupling immediately below the building floor slab ranged from 90 to 95 percent and at a depth of 0.5 m was on the order of 50 percent. These results indicate that the advective zone of influence will likely be limited to a zone within 1 to 2 m of the building foundation.

Because the advective flow zone is relatively limited in extent, the soil type adjacent to the building foundation is of importance. In many cases, coarse-grained imported fill is placed below foundations, and either coarse-grained fill, or disturbed, loose fill is placed adjacent to the foundation walls. Therefore, a conservative approach for the purposes of this guidance is to assume that soil gas flow will be controlled by coarse-grained soil, and not rely on the possible reduction in flow that would be caused by fine-grained soils near to the house foundation. For these reasons, a soil gas flow rate of 5 L/min (midpoint between 1 and 10 L/min) was chosen as the input value.

3.3 RUNNING THE MODELS

Eight different models are provided in MICROSOFT EXCEL formats.

1. Models for Soil Contamination:
   SL-SCREEN-Feb 04.XLS
   SL-ADV-Feb 04.XLS

2. Models for Groundwater Contamination:
   GW-SCREEN-Feb 04.XLS
   GW-ADV-Feb 04.XLS

3. Model for Soil Gas Contamination
   SG-SCREEN-Feb 04.xls
   SG-ADV-Feb 04.xls

4. Models for Non Aqueous Phase Liquids
   NAPL-SCREEN-Feb 04.xls

NAPL-ADV-Feb 04.xls

Both the screening-level models and the advanced models allow the user to calculate a risk-based media concentration or incremental risks from an actual starting concentration in soil or in groundwater. Data entry within the screening-level models is limited to the most sensitive model parameters and incorporates only one soil stratum above the contamination. The advanced models provide the user with the ability to enter data for all of the model parameters and also incorporate up to three individual soil strata above the contamination for which soil properties may be varied.

To run any of the models, simply open the appropriate model file within MICROSOFT EXCEL. Each model is constructed of the following worksheets:

1. DATENTER (Data Entry Sheet)
2. CHEMPROPS (Chemical Properties Sheet)
3. INTERCALCS (Intermediate Calculations Sheet)
4. RESULTS (Results Sheet)
5. VLOOKUP (Lookup Tables).

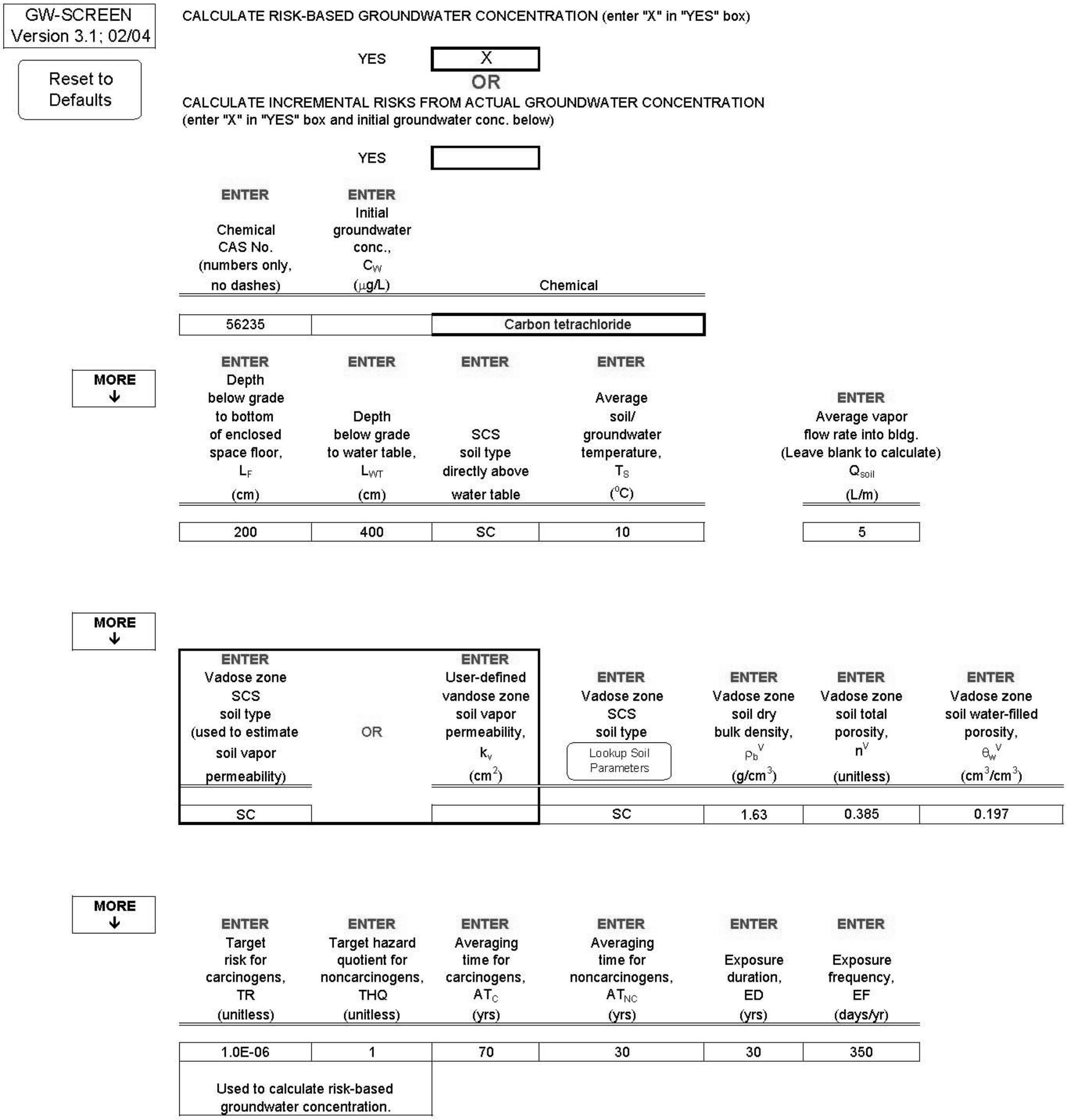
The following is an explanation of what is contained in each worksheet, how to enter data, how to interpret model results, and how to add/revise the chemical properties data found in the VLOOKUP Tables. As examples, Appendix C contains all the worksheets for the advanced soil contamination model SL-ADV.

3.4 THE DATA ENTRY SHEET (DATENTER)

Figure 4 is an example of a data entry sheet. In this case, it shows the data entry sheet for the screening-level model for contaminated groundwater (GW-SCREEN). Figure 5 is an example of an advanced model data entry sheet (GW-ADV). Note that the screening-level model sheet requires entry of considerably less data than does the advanced sheet. To enter data, simply position the cursor within the appropriate box and type the value; all other cells are protected.

Error Messages

In the case of the screening-level models, all error messages will appear in red type below the applicable row of data entry boxes. For the advanced models, error messages may appear on the data entry sheet or in the lower portion of the results sheet. Error messages will occur if required entry data are missing or if data are out of range or do not conform to model conventions. The error message will tell the user what kind of error has occurred.



CALCULATE RISK-BASED GROUNDWATER CONCENTRATION (enter "X" in "YES" box)

YES ☒ X

OR

CALCULATE INCREMENTAL RISKS FROM ACTUAL GROUNDWATER CONCENTRATION
(enter "X" in "YES" box and initial groundwater conc. below)

YES ☐

ENTER Chemical CAS No. (numbers only, no dashes)	ENTER Initial groundwater conc., C_W (μg/L)	Chemical
56235		Carbon tetrachloride

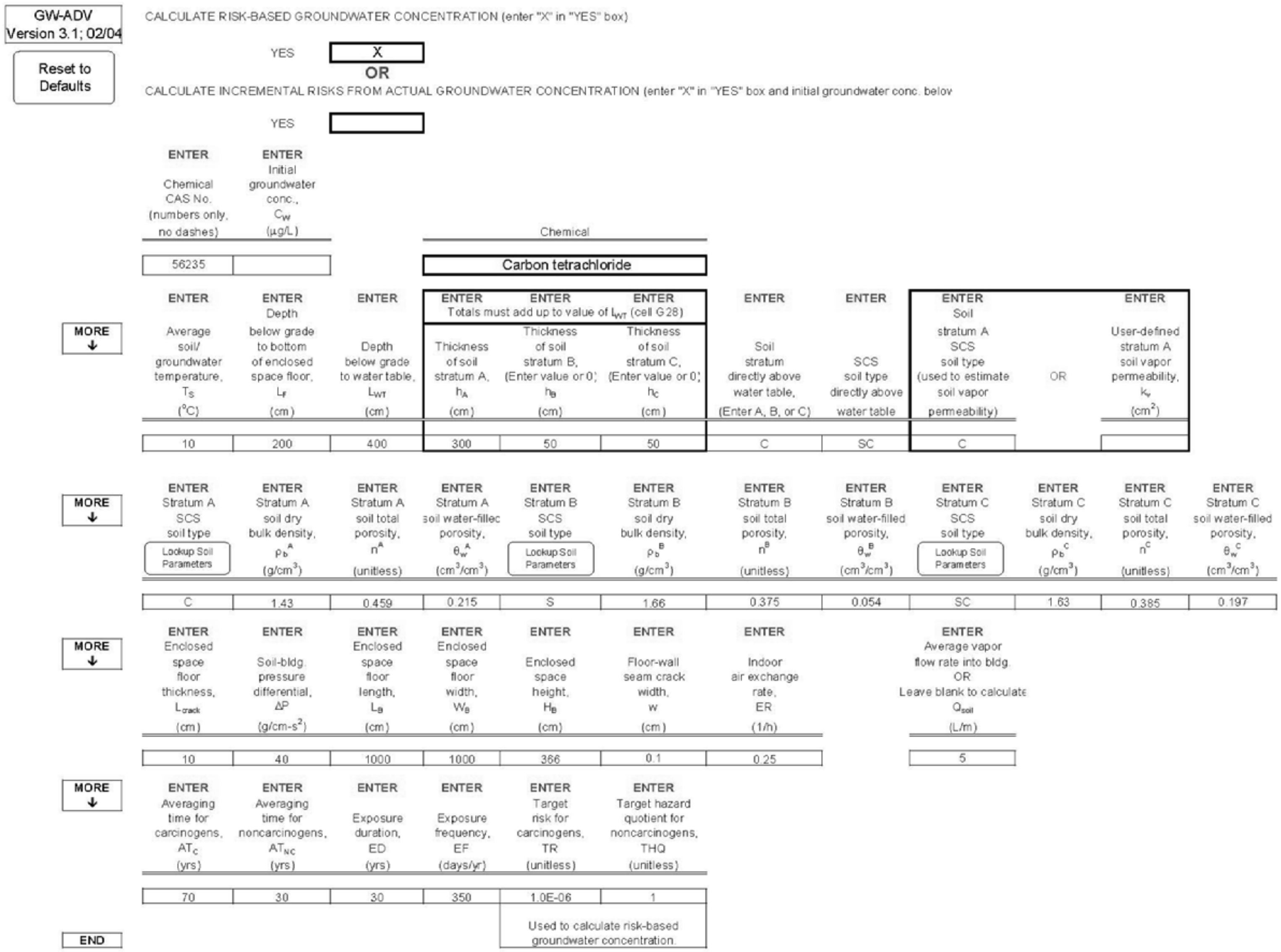
ENTER Depth below grade to bottom of enclosed space floor, L_F (cm)	ENTER Depth below grade to water table, L_{WT} (cm)	ENTER SCS soil type directly above water table	ENTER Average soil/ groundwater temperature, T_S (^oC)	ENTER Average vapor flow rate into bldg. (Leave blank to calculate) Q_{soil} (L/m)
200	400	SC	10	5

ENTER Vadose zone SCS soil type (used to estimate soil vapor permeability)	OR	ENTER User-defined vandose zone soil vapor permeability, k_v (cm^2)	ENTER Vadose zone SCS soil type	ENTER Vadose zone soil dry bulk density, ρ_b^V (g/cm^3)	ENTER Vadose zone soil total porosity, n^V (unitless)	ENTER Vadose zone soil water-filled porosity, θ_w^V (cm^3/cm^3)
SC			SC	1.63	0.385	0.197

ENTER Target risk for carcinogens, TR (unitless)	ENTER Target hazard quotient for noncarcinogens, THQ (unitless)	ENTER Averaging time for carcinogens, AT_C (yrs)	ENTER Averaging time for noncarcinogens, AT_{NC} (yrs)	ENTER Exposure duration, ED (yrs)	ENTER Exposure frequency, EF (days/yr)
1.0E-06	1	70	30	30	350

Used to calculate risk-based groundwater concentration.

Figure 4. GW-SCREEN Data Entry Sheet



CALCULATE RISK-BASED GROUNDWATER CONCENTRATION (enter "X" in "YES" box)

YES X

OR

CALCULATE INCREMENTAL RISKS FROM ACTUAL GROUNDWATER CONCENTRATION (enter "X" in "YES" box and initial groundwater conc. belov

YES

ENTER Chemical CAS No. (numbers only, no dashes)	ENTER Initial groundwater conc., C_W (µg/L)	Chemical
56235		Carbon tetrachloride

ENTER Average soil/ groundwater temperature, T_S (°C)	ENTER Depth below grade to bottom of enclosed space floor, L_F (cm)	ENTER Depth below grade to water table, L_{WT} (cm)	ENTER Thickness of soil stratum A, h_A (cm)	ENTER Thickness of soil stratum B, (Enter value or 0) h_B (cm)	ENTER Thickness of soil stratum C, (Enter value or 0) h_C (cm)	ENTER Soil stratum directly above water table, (Enter A, B, or C)	ENTER SCS soil type directly above water table	ENTER Soil stratum A SCS soil type (used to estimate soil vapor permeability)		ENTER User-defined stratum A soil vapor permeability, k_v (cm^2)
10	200	400	300	50	50	C	SC	C	OR	

Totals must add up to value of L_{WT} (cell G28)

ENTER Stratum A SCS soil type	ENTER Stratum A soil dry bulk density, ρ_b^A (g/cm^3)	ENTER Stratum A soil total porosity, n^A (unitless)	ENTER Stratum A soil water-fillec porosity, θ_w^A (cm^3/cm^3)	ENTER Stratum B SCS soil type	ENTER Stratum B soil dry bulk density, ρ_b^B (g/cm^3)	ENTER Stratum B soil total porosity, n^B (unitless)	ENTER Stratum B soil water-filled porosity, θ_w^B (cm^3/cm^3)	ENTER Stratum C SCS soil type	ENTER Stratum C soil dry bulk density, ρ_b^C (g/cm^3)	ENTER Stratum C soil total porosity, n^C (unitless)	ENTER Stratum C soil water-filled porosity, θ_w^C (cm^3/cm^3)
C	1.43	0.459	0.215	S	1.66	0.375	0.054	SC	1.63	0.385	0.197

ENTER Enclosed space floor thickness, L_{crack} (cm)	ENTER Soil-bldg. pressure differential, ΔP (g/cm-s^2)	ENTER Enclosed space floor length, L_B (cm)	ENTER Enclosed space floor width, W_B (cm)	ENTER Enclosed space height, H_B (cm)	ENTER Floor-wall seam crack width, w (cm)	ENTER Indoor air exchange rate, ER (1/h)	ENTER Average vapor flow rate into bldg. OR Leave blank to calculate Q_{soil} (L/m)
10	40	1000	1000	366	0.1	0.25	5

ENTER Averaging time for carcinogens, AT_C (yrs)	ENTER Averaging time for noncarcinogens, AT_{NC} (yrs)	ENTER Exposure duration, ED (yrs)	ENTER Exposure frequency, EF (days/yr)	ENTER Target risk for carcinogens, TR (unitless)	ENTER Target hazard quotient for noncarcinogens, THQ (unitless)
70	30	30	350	1.0E-06	1

Used to calculate risk-based groundwater concentration.

Figure 5. GW-ADV Data Entry Sheet

Figure 6 is an example of an error message appearing on the data entry sheet. Figure 7 illustrates error messages appearing within the message and error summary section on the results sheet (advanced models only).

Entering Data

Each data entry sheet requires the user to input values for model variables. Data required for the soil contamination scenario will differ from that required for the groundwater contamination scenario. In addition, data required for the screening-level models will differ from that required for the advanced models.

Model Variables--

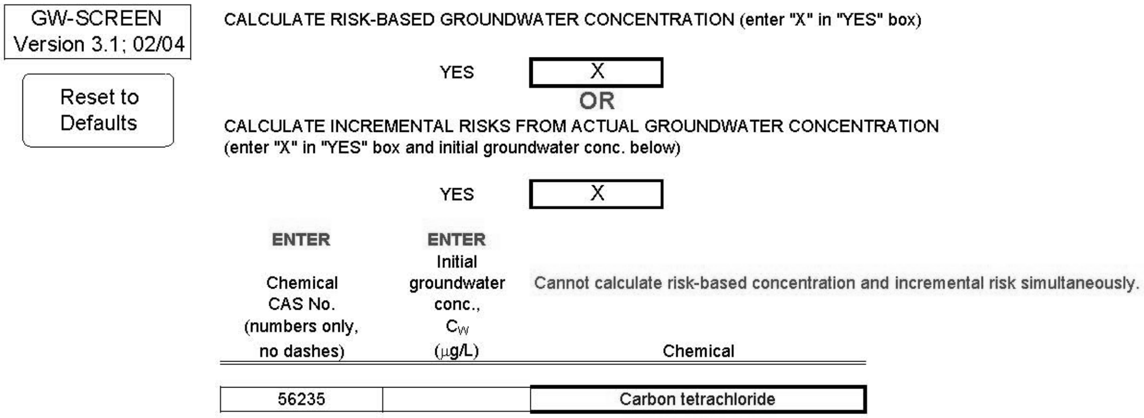
The following is a list of all data entry variables required for evaluating either a risk-based media concentration or the incremental risks due to actual contamination. A description for which model(s) the variable is appropriate is given in parenthesis after the name of the variable. In addition, notes on how the variable is used in the calculations and how to determine appropriate values of the variable are given below the variable name. A quick determination of which variables are required for a specific model can be made by reviewing the data entry sheet for the model chosen. Example data entry sheets for each model can be found in Appendix D.

1. *Calculate Risk-Based Concentration* or *Calculate Incremental Risks from Actual Concentration* (All Soil and Groundwater Models)

   The model will calculate either a risk-based soil or groundwater concentration or incremental risks but cannot calculate both simultaneously. Enter an "X" in only one box.

2. *Chemical CAS No.* (All Models)

   Enter the appropriate CAS number for the chemical you wish to evaluate; do not enter dashes. The CAS number entered must exactly match that of the chemical, or the error message "CAS No. not found" will appear in the "Chemical" box. Once the correct CAS number is entered, the name of the chemical will automatically appear in the "Chemical" box. A total of 108 chemicals and their associated properties are included with each model; see Section 3.7 for instructions on adding/revising chemicals.


GW-SCREEN
Version 3.1; 02/04

CALCULATE RISK-BASED GROUNDWATER CONCENTRATION (enter "X" in "YES" box)

YES ☒ X

OR

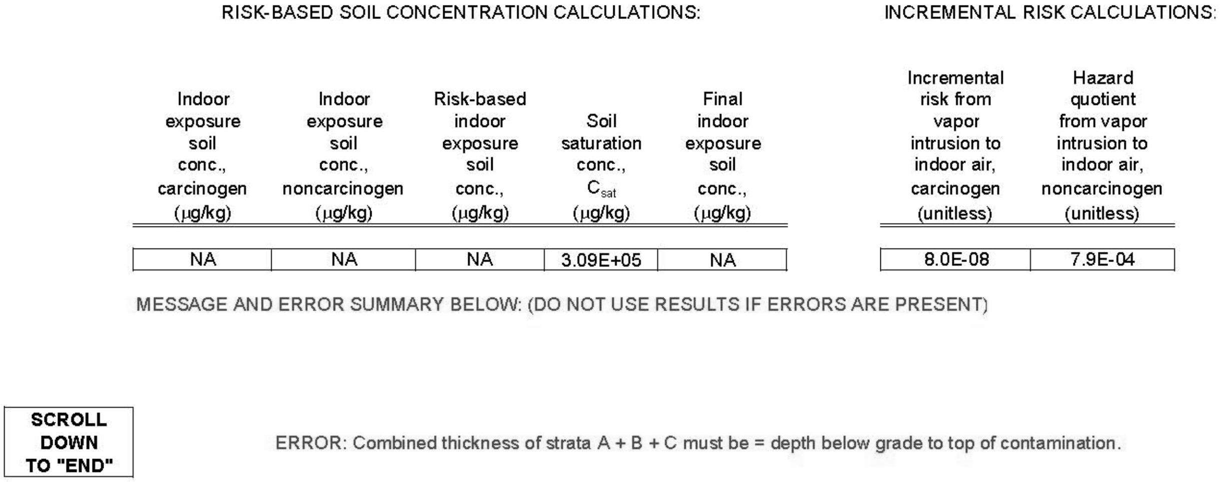
CALCULATE INCREMENTAL RISKS FROM ACTUAL GROUNDWATER CONCENTRATION
(enter "X" in "YES" box and initial groundwater conc. below)

YES ☒ X

Cannot calculate risk-based concentration and incremental risk simultaneously.

ENTER Chemical CAS No. (numbers only, no dashes)	ENTER Initial groundwater conc., C_W (μg/L)	Chemical
56235		Carbon tetrachloride

Figure 6. Example Error Message on Data Entry Sheet


RISK-BASED SOIL CONCENTRATION CALCULATIONS:

Indoor exposure soil conc., carcinogen (μg/kg)	Indoor exposure soil conc., noncarcinogen (μg/kg)	Risk-based indoor exposure soil conc., (μg/kg)	Soil saturation conc., C_{sat} (μg/kg)	Final indoor exposure soil conc., (μg/kg)
NA	NA	NA	3.09E+05	NA

INCREMENTAL RISK CALCULATIONS:

Incremental risk from vapor intrusion to indoor air, carcinogen (unitless)	Hazard quotient from vapor intrusion to indoor air, noncarcinogen (unitless)
8.0E-08	7.9E-04

MESSAGE AND ERROR SUMMARY BELOW: (DO NOT USE RESULTS IF ERRORS ARE PRESENT)

ERROR: Combined thickness of strata A + B + C must be = depth below grade to top of contamination.

Figure 7. Example Error Message on Results Sheet

3. *Initial Soil or Groundwater Concentration* (All Soil and Groundwater Models) (L_w)

   Enter a value only if incremental risks are to be calculated. Be sure to enter the concentration in units of µg/kg (wet weight basis soil) or µg/L (groundwater). Typically, this value represents the average concentration within the zone of contamination. If descriptive statistics are not available to quantify the uncertainty in the average value, the maximum value may be used as an upper bound estimate.

4. *Average Soil/Groundwater Temperature* (All Models) (T_s)

   The soil/groundwater temperature is used to correct the Henry's law constant to the specified temperature. Figure 8 from U.S. EPA (1995) shows the average temperature of shallow groundwater in the continental United States. Shallow groundwater temperatures may be used to approximate subsurface soil temperatures greater than 1 to 2 meters below the ground surface. Another source of information may be your State groundwater protection regulatory agency.

5. *Depth Below Grade to Bottom of Enclosed Space Floor* (All Models) (L_F)

   Enter the depth to the bottom of the floor in contact with the soil. The default value for slab-on-grade and basement construction is 15 cm and 200 cm, respectively.

6. *Depth Below Grade to Top of Contamination* (Soil Models Only) (L_T)

   Enter the depth to the top of soil contamination. If the contamination begins at the soil surface, enter the depth below grade to the bottom of the enclosed space floor. The depth to the top of contamination must be greater than or equal to the depth to the bottom of the floor.

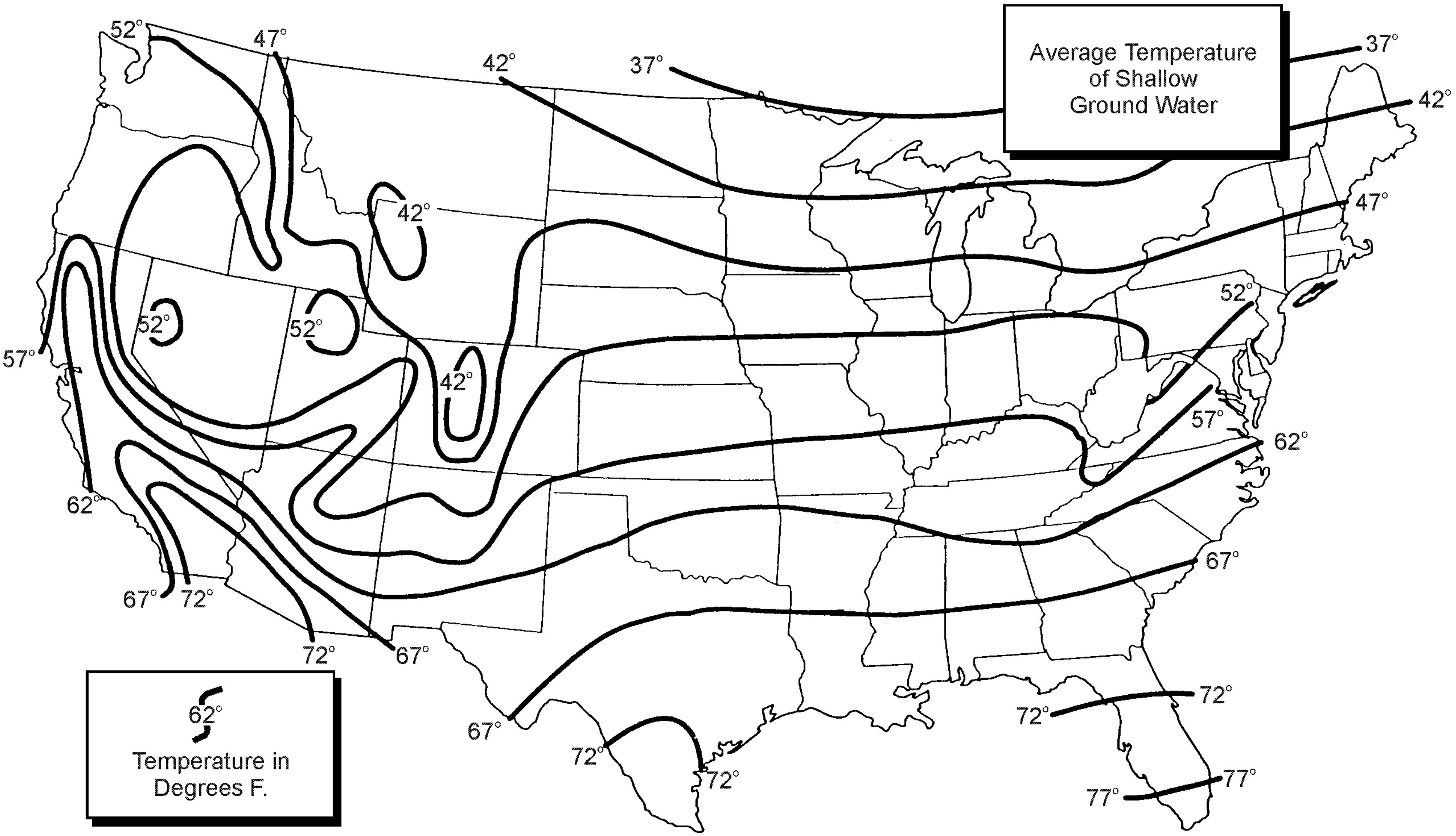


Figure 8. Average Shallow Groundwater Temperature in the United States

7. *Depth Below Grade to Water Table* (Groundwater Models Only) (L_{wt})

Enter the depth to the top of the water table (i.e., where the pressure head is equal to zero and the pressure is atmospheric).

Note: The thickness of the capillary zone is calculated based on the SCS soil textural classification above the top of the water table. The depth below grade to the top of the water table minus the thickness of the capillary zone must be greater than the depth below grade to the bottom of the enclosed space floor. This means that the top of the capillary zone is always below the floor.

8. *Depth Below Grade to Bottom of Contamination* (Advanced Soil Model Only) (L_B)

This value is used to calculate the thickness of soil contamination. A value greater than zero and greater than the depth to the top of contamination will automatically invoke the finite source model. If the thickness of contamination is unknown, two options are available:

1. Entering a value of zero will automatically invoke the infinite source model.

2. Enter the depth to the top of the water table. This will invoke the finite source model under the assumption that contamination extends from the top of contamination previously entered down to the top of the water table.

9. *Thickness of Soil Stratum "X"* (Advanced Models Only) (h_x, x = A, B, or C)

In the advanced models, the user can define up to three soil strata between the soil surface and the top of contamination or to the soil gas sampling depth, as appropriate. These strata are listed as A, B, and C. Stratum A extends down from the soil surface, Stratum B is below Stratum A, and Stratum C is the deepest stratum. The thickness of Stratum A must be at least as thick as the depth below grade to the bottom of the enclosed space floor. The combined thickness of all strata must be equal to the depth to the top of contamination, or to the soil gas sampling depth, as appropriate. If soil strata B and/or C are not to be considered, a value of zero must be entered for each stratum not included in the analysis.

10. *Soil Stratum A SCS Soil Type* (Advanced Models Only) (SES – soil)

Enter one of the following SCS soil type abbreviations:

Abbreviation	SCS Soil Type
C	Clay
CL	Clay loam
L	Loam
LS	Loamy sand
S	Sand
SC	Sandy clay
SCL	Sandy clay loam
SI	Silt
SIC	Silty clay
SICL	Silty clay loam
SIL	Silty loam
SL	Sandy loam

The SCS soil textural classification can be determined by using either the ATSM Standard Test Method for Particle-Size Analysis of Soils (D422-63) or by using the analytical procedures found in the U.S. Natural Resources Conservation Service (NRCS) Soil Survey Laboratory Methods Manual, Soil Survey Laboratory Investigations Report No. 42. After determining the particle size distribution of a soil sample, the SCS soil textural classification can be determined using the SCS classification chart in Figure 7.

The SCS soil type along with the Stratum A soil water-filled porosity is used to estimate the soil vapor permeability of Stratum A which is in contact with the floor and walls of the enclosed space below grade. Alternatively, the user may define a soil vapor permeability (see Variable No. 11).

11. *User-Defined Stratum A Soil Vapor Permeability* (Advanced Models Only)(K_v)

As an alternative to estimating the soil vapor permeability of soil Stratum A, the user may define the soil vapor permeability. As a general guide, the following represent the practical range of vapor permeabilities:

Soil type	Soil vapor permeability, cm^2
Medium sand	1.0×10^{-7} to 1.0×10^{-6}
Fine sand	1.0×10^{-8} to 1.0×10^{-7}
Silty sand	1.0×10^{-9} to 1.0×10^{-8}
Clayey silts	1.0×10^{-10} to 1.0×10^{-9}

12. *Vadose Zone SCS Soil Type* (Screening Models Only) (SCS – soil)

Because the screening-level models accommodate only one soil stratum above the top of contamination or soil gas sampling depth, enter the SCS soil type from the list given in Variable No. 10.

13. *User-Defined Vadose Zone Soil Vapor Permeability* (Screening Models Only) (K_v)

For the same reason cited in No. 12 above, the user may alternatively define a soil vapor permeability. Use the list of values given in Variable No. 11 as a general guide.

14. *Soil Stratum Directly Above the Water Table* (Advanced Groundwater Models Only) (A, B, or C)

Enter either A, B, or C as the soil stratum directly above the water table. This value <u>must</u> be the letter of the <u>deepest</u> stratum for which a thickness value has been specified under Variable No. 9.

15. *SCS Soil Type Directly Above Water Table* (Groundwater Models Only) (SCS – soil)

Enter the correct SCS soil type from the list given in Variable No. 10 for the soil type directly above the water table. The soil type entered is used to estimate the rise (thickness) of the capillary zone.

16. *Stratum "X" Soil Dry Bulk Density* (Advanced Models Only) (P_x, x = A, B, or C)

    Identify the soil type for each strata and accept the default value or enter a site-specific value for the average soil dry bulk density. Dry bulk density is used in a number of intermediate calculations and is normally determined by field measurements (ASTM D 2937 Method).

17. *Stratum "X" Soil Total Porosity* (Advanced Models Only) (n^x, x = A, B, or C)

    Total soil porosity (n) is determined as:

$$n = 1\ \rho_b/\rho_s$$

    where ρ_b is the soil dry bulk density (g/cm^3) and ρ_s is the soil particle density (usually 2.65 g/cm^3).

18. *Stratum "X" Soil Water-Filled Porosity* (Advanced Models Only) (θ_w^x, X = a, b, or c)

    Enter the average long-term volumetric soil moisture content; this is typically a depth-averaged value for the appropriate soil stratum. A long-term average value is typically not readily available. Do not use values based on episodic measurements unless they are representative of long-term conditions. Table 10 provides a soil-specific range of typical value for specified soils. The user must define soil type or input site-specific values.

    One option is to use a model to estimate the long-term average soil water-filled porosities of each soil stratum between the enclosed space floor and the top of contamination. The HYDRUS model version 5.0 (Vogel et al., 1996) is a public domain code for simulating one-dimensional water flow, solute transport, and heat movement in variably-saturated soils. The water flow simulation module of HYDRUS will generate soil water content as a function of depth and time given actual daily precipitation data. Model input requirements include either the soil hydraulic properties of van Genuchten (1980) or those of Brooks and Corey (1966). The van Genuchten soil hydraulic properties required are the same as those given in Tables 3 and 4 (i.e., θ_s, θ_r, N, α_1, and K_s). The HYDRUS model is available from the U.S. Department of Agriculture (USDA) - Agricultural Research Service in Riverside, California via their internet website at http://www.ussl.ars.usda.gov/MODELS/HYDRUS.HTM. One and two-dimensional commercial versions of HYDRUS (Windows versions) are available at the International Ground Water Modeling Center website at http://www.mines.edu/research/igwmc/software/. Schaap and Leij (1998) have recently developed a Windows program entitled ROSETTA for estimating the van Genuchten soil hydraulic properties based on a limited or more extended set of input data. The ROSETTA program can be found at the USDA website: http://www.ussl.ars.usda.gov/MODELS/rosetta/rosetta.htm. The van Genuchten hydraulic properties can then be input into HYDRUS to estimate soil moisture content.

19. *Stratum "X" Soil Organic Carbon Fraction* (Advanced Soil Models Only) (f_{oc}^{x}, X = A, B, or c)

    Enter the depth-averaged soil organic carbon fraction for the stratum specified. Soil organic carbon is measured by burning off soil carbon in a controlled-temperature oven. This parameter, along with the chemical's organic carbon partition coefficient (K_{oc}), is used to determine the soil-water partition coefficient (K_d).

20. *Vadose Zone Soil Dry Bulk Density* (Screening Models Only) (ρ^A)

    Because the screening-level models accommodate only one soil stratum above the top of contamination, identify the soil type and accept the default values or enter the depth-averaged soil dry bulk density. The universal default value is 1.5 g/cm^3, which is consistent with U.S. EPA (1996a and b) for subsurface soils.

21. *Vadose Zone Soil Total Porosity* (Screening Models Only) (m^A)

    Because the screening-level models accommodate only one soil stratum above the top of contamination, enter the depth-averaged soil total porosity. The default value is 0.43, which is consistent with U.S. EPA (1996a and b) for subsurface soils.

22. *Vadose Zone Soil Water-Filled Porosity* (Screening Models Only) (θ_w^A)

    Because the screening-level models accommodate only one soil stratum above the top of contamination, enter the depth-averaged soil water-filled porosity. The default value is 0.30, which is consistent with U.S. EPA (1996a and b) for subsurface soils.

23. *Vadose Zone Soil Organic Carbon Fraction* (Soil Screening Model Only) (f_{oc}^A)

    Because the screening-level models accommodate only one soil stratum above the top of contamination, enter the depth-averaged soil organic carbon fraction. The default value is 0.002, which is consistent with U.S. EPA (1996a and b) for subsurface soils.

24. *Enclosed Space Floor Thickness* (Advanced Models Only) (L_{crack})

    Enter the thickness of the floor slab. All models operate under the assumption that the floor in contact with the underlying soil is composed of impermeable concrete whether constructed as a basement floor or slab-on-grade. The default value is 10 cm, which is consistent with J&E (1991).

25. *Soil-Building Pressure Differential* (Advanced Models Only) (ΔP)

Because of wind effects on the structure, stack effects due to heating of the interior air, and unbalanced mechanical ventilation, a negative pressure with respect to the soil surface is generated within the structure. This pressure differential (ΔP) induces a flow of soil gas through the soil matrix and into the structure through cracks, gaps, and openings in the foundation. The effective range of values of ΔP is 0-20 pascals (Pa) (Loureiro et al., 1990; Eaton and Scott, 1984). Individual average values for wind effects and stack effects are approximately 2 Pa (Nazaroff et al., 1985; Put and Meijer, 1989). Typical values for the combined effects of wind pressures and heating are 4 to 5 Pa (Loureiro et al., 1990; Grimsrud et al., 1983). A conservative default value of ΔP was therefore chosen to be 4 Pa (40 g/cm-s^2).

For more information on estimating site-specific values of ΔP, the user is referred to Nazaroff et al. (1987) and Grimsrud et al. (1983).

26. *Enclosed Space Floor Length* (Advanced Models Only) (L_B)

The default value is 1000 cm (see Variable No. 28).

27. *Enclosed Space Floor Width* (Advanced Models Only) (W_B)

The default value is 1000 cm (see Variable No. 28).

28. *Enclosed Space Height* (Advanced Models Only) (H_B)

For a single story home, the variation in mixing height will be the greatest for houses with HVAC systems that result in significant air circulation (e.g., forced air heat pump). Mixing heights would be less for houses with electrical baseboard heaters. The mixing height is approximated by the room height. The default value is 2.44 meters for a single story house without a basement.

For a single story house with a basement less mixing would be expected because of the cross floor connections. The default values for a house with a basement is 3.66 m. This value represents a two-fold reduction in vapor concentrations between the floors.

29. *Floor-Wall Seam Crack Width* (Advanced Models Only) (W)

The conceptual model used in the spreadsheets follows that of Loureiro et al. (1990) and Nazaroff (1988) and is illustrated in Figure 9. The model is based on a single-

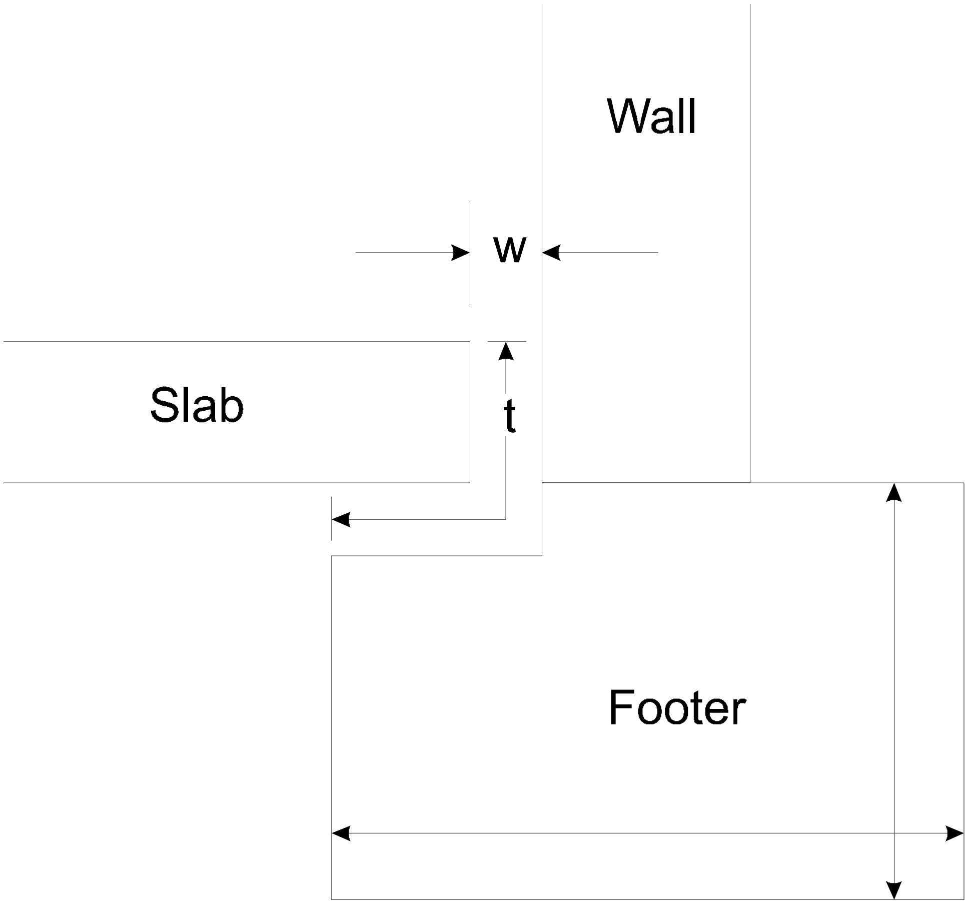


Figure 9. Floor Slab and Foundation

family house with a poured concrete basement floor and wall foundations, or constructed slab-on-grade in similar fashion. A gap is assumed to exist at the junction between the floor and the foundation along the perimeter of the floor. The gap exists as a result of building design or concrete shrinkage. This gap is assumed to be the only opening in the understructure of the house and therefore the only route for soil gas entry.

Eaton and Scott (1984) reported typical open areas of approximately 300 cm^2 for the joints between walls and floor slabs of residential structures in Canada. Therefore, given the default floor length and width of 1000 cm, a gap width (w) of 0.1 cm equates to a total gap area of 900 cm^2, which is reasonable given the findings of Eaton and Scott. This value of the gap width is also consistent with the typical value reported in Loureiro et al. (1990). The default value of the floor-wall seam crack width was therefore set equal to 0.1 cm.

30. *Indoor Air Exchange Rate* (Advanced Models Only) (ER)

The indoor air exchange rate is used along with the building dimensions to calculate the building ventilation rate. The default value of the indoor air exchange rate is 0.25/h. This value is consistent with the 10th percentile of houses in all regions of the U.S., as reported in Koontz and Rector (1995). This value is also consistent with the range of the control group of 331 houses in a study conducted by Parker et al. (1990) to compare data with that of 292 houses with energy-efficient features in the Pacific Northwest.

31. *Averaging Time for Carcinogens* (All Models) (AT_c)

Enter the averaging time in units of years. The default value is 70 years.

32. *Averaging Time for Noncarcinogens* (All Models) (AT_{nc})

Enter the averaging time in units of years. The averaging time for noncarcinogens is set equal to the exposure duration. The default value for residential exposure from U.S. EPA (1996a and b) is 30 years.

33. *Exposure Duration* (All Models) (ED)

Enter the exposure duration in units of years. The default value for residential exposure from U.S. EPA (1996a and b) is 30 years.

34. *Exposure Frequency* (All Models) (EF)

Enter the exposure frequency in units of days/yr. The default value for residential exposure from U.S. EPA (1996a and b) is 350 days/yr.

35. *Target Risk for Carcinogens* (All Soil and Groundwater Models) (TR)

If a risk-based media concentration is to be calculated, enter the target risk-level. The default value is 1×10^{-6}.

36. *Target Hazard quotient for Noncarcinogens* (All Soil and Groundwater Models) (THQ)

If a risk-based media concentration is to be calculated, enter the target hazard quotient. The default value is 1.

The remaining four worksheets include the results sheet (RESULTS) and three ancillary sheets. The ancillary sheets include the chemical properties sheet (CHEMPROPS), the intermediate calculations sheet (INTERCALCS), and the lookup tables (VLOOKUP).

3.5 THE RESULTS SHEET (RESULTS)

Once all data are entered in the data entry sheet, the model results may be viewed on the RESULTS sheet. For the soil and groundwater models, calculations are presented as either a risk-based soil or groundwater concentration, or the incremental risks associated with an initial soil or groundwater concentration. In the case of the advanced models, the user should check the message and error summary below the results section to ensure that no error messages appear. If one or more error messages appear, re-enter the appropriate data.

The RESULTS worksheet shows the indoor exposure soil or groundwater concentration for either a carcinogen or noncarcinogen as appropriate. When a contaminant is both a carcinogen and a noncarcinogen, the risk-based indoor exposure concentration is set equal to the lower of these two values. In addition, the soil saturation concentration (C_{sat}) or the aqueous solubility limit (S) is also displayed for the soil and groundwater models, respectively.

The equilibrium vapor concentration at the source of contamination is limited by the value of C_{sat} for soil contamination and by the value of S for groundwater contamination, as appropriate. For a single contaminant, the vapor concentration directly above the source of soil contamination cannot be greater than that associated with the soil saturation concentration; for groundwater contamination, the vapor concentration cannot be greater than that associated with the solubility limit. As a result, subsurface soil concentrations greater than C_{sat} and groundwater concentrations greater than S will not produce higher vapor concentrations. Therefore, if the indoor vapor concentration predicted from a soil concentration greater than or equal to the value of C_{sat} and it does not exceed the health-based limit in indoor air (target risk or target hazard quotient), the vapor intrusion pathway will not be of concern for that particular chemical. The same is true for an indoor vapor concentration predicted from a groundwater concentration greater than or equal to the value of S. That does not necessarily mean, however, that the subsurface contamination will not be of concern from a groundwater protection standpoint, (ingestion) and the potential for free-phase contamination (e.g., NAPL) must also be addressed.

For subsurface soils, the physical state of a contaminant at the soil temperature plays a significant role. When a contaminant is a liquid (or gas) at the soil temperature, the upper limit of the soil screening level is set at C_{sat}. This tends to reduce the potential for NAPL to exist within the vadose zone. The case is different for a subsurface contaminant that is a solid at the soil temperature. In this case, the screening level is not limited by C_{sat} because of the reduced possibility of leaching to the water table. If the model estimates a risk-based screening level greater than C_{sat} for a solid in soils, the model will display the final soil concentration as "NOC" or Not of Concern for the vapor intrusion pathway.

In the case of groundwater contamination, the physical state of the contaminant is not an issue in that the contamination has already reached the water table. Because the equilibrium vapor concentration at the source of emissions cannot be higher than that associated with the solubility limit, the vapor concentration is calculated at the solubility limit if the user enters a groundwater concentration greater than the value of S when forward-calculating risk. When reverse-calculating a risk-based groundwater concentration, the model will display the final groundwater concentration as "NOC" for the vapor intrusion pathway if the model calculates a risk-based level greater than or equal to the value of S. It should be noted, however, that if the soil properties or other conditions specified in the DATENTER worksheet are changed, the final risk-based soil or groundwater concentration must be remodeled.

It should also be understood that if a contaminant is labeled "Not of Concern" for the vapor intrusion pathway, all other relevant exposure pathways must be considered for both contaminated soils and groundwater.

3.6 THE CHEMICAL PROPERTIES SHEET (CHEMPROPS)

The chemical properties sheet provides a summary of the chemical and toxicological properties of the chemical selected for analysis. These data are retrieved from the VLOOKUP sheet by CAS number. All data in the chemical properties sheet are protected.

3.7 THE INTERMEDIATE CALCULATIONS SHEET (INTERCALS)

The intermediate calculations sheet provides solutions to intermediate variables. Review of the values of the intermediate variables may be helpful in an analysis of the cause-and-effect relationships between input values and model results. All data in the intermediate calculations sheet are protected.

3.8 THE LOOKUP TABLES (VLOOKUP)

The VLOOKUP sheet contains two lookup tables from which individual data are retrieved for a number of model calculations. The first table is the Soil Properties Lookup Table. This table contains the average soil water retention curve data of Hers (2002) and Schaap and Leij (1998) and the mean grain diameter data of Nielson and Rogers (1990) by SCS soil type, and the mean dry bulk density from Leij, Stevens, et al (1994).

3.9 ADDING, DELETING, OR REVISING CHEMICALS

Data for any chemical may be edited, new chemicals added, or existing chemicals deleted from the Chemical Properties Lookup Table within the VLOOKUP worksheet. To begin an editing session, the user must unprotect (unseal) the worksheet (the password is "ABC" in capital letters); editing of individual elements or addition and deletion of chemicals may then proceed. Space has been allocated for up to 260 chemicals in the lookup table. Row number 284 is the last row that may be used to add new chemicals. After the editing session is complete, the user must sort all the data in the lookup table (except the column headers) in ascending order by CAS number. After sorting is complete, the worksheet should again be protected (sealed).

SECTION 4

SOIL GAS MODEL APPLICATION

Two additional models have been added to allow the user to input measured soil gas concentration and sampling depth data directly into the spreadsheet. These models eliminate the need for theoretical partitioning of a total volume soil concentration or a groundwater concentration into discrete phases. This section provides instructions for using the soil gas models.

4.1 RUNNING THE MODELS

Two models are provided as MICROSOFT EXCEL spreadsheets. The screening-level model is titled SG-SCREEN.xls (EXCEL). The advanced model is titled SG-ADV.xls.

Both the screening-level and advanced models allow the user to calculate steady-state indoor air concentrations and incremental risks from user-defined soil gas concentration data. The models do not allow for reverse-calculation of a risk-based soil or groundwater concentration. As with the soil and groundwater screening-level models, the SG-SCREEN model operates under the assumption that the soil column properties are homogeneous and isotropic from the soil surface to an infinite depth. In addition, the SG-SCREEN model uses the same default values for the building properties as the SL-SCREEN and GW-SCREEN models. The advanced model allows the user to specify up to three different soil strata from the bottom of the building floor in contact with the soil to the soil gas sampling depth. Finally, the advanced model allows the user to specify values for all of the model variables.

To run the models, simply open the appropriate file within either MICROSOFT EXCEL worksheet. Each model is constructed of the following worksheets:

1. DATENTER (Data Entry Sheet)
2. CHEMPROPS (Chemical Properties Sheet)
3. INTERCALCS (Intermediate Calculations Sheet)
4. RESULTS (Results Sheet)
5. VLOOKUP (Lookup Tables)

Each worksheet follows the form of the worksheets in the soil and groundwater models. See Section 4.2 for a description of each worksheet.

The DATENTER worksheet of each of the soil gas models is different than those of the soil and groundwater models. Figure 10 shows the DATA ENTER worksheet of the SG-ADV model. Note that there is no option for running the model to calculate a risk-based media concentration. As with the other models, the user enters the CAS number of the chemical of interest. This automatically retrieves the chemical and toxicological data for that chemical. The CAS number must match one of the chemicals listed in the VLOOKUP worksheet, or the message "CAS No. not found" will appear in the "Chemical" box. The user also has the opportunity to add new chemicals to the data base. Next, the user must enter a value for the soil gas concentration of the chemical of interest. The user may enter this value in units of $\mu g/m^3$ or parts-per-million by volume (ppmv). If the soil gas concentration is entered in units of ppmv, the concentration is converted to units of $\mu g/m^3$ by:

$$C_g' = \frac{C_g \times MW}{R \times T_S} \tag{33}$$

where C_g' = Soil gas concentration, $\mu g/m^3$

C_g = Soil gas concentration, ppmv

MW = Molecular weight, g/mol

R = Gas constant (= 8.205 E-05 atm-m^3/mol-^oK)

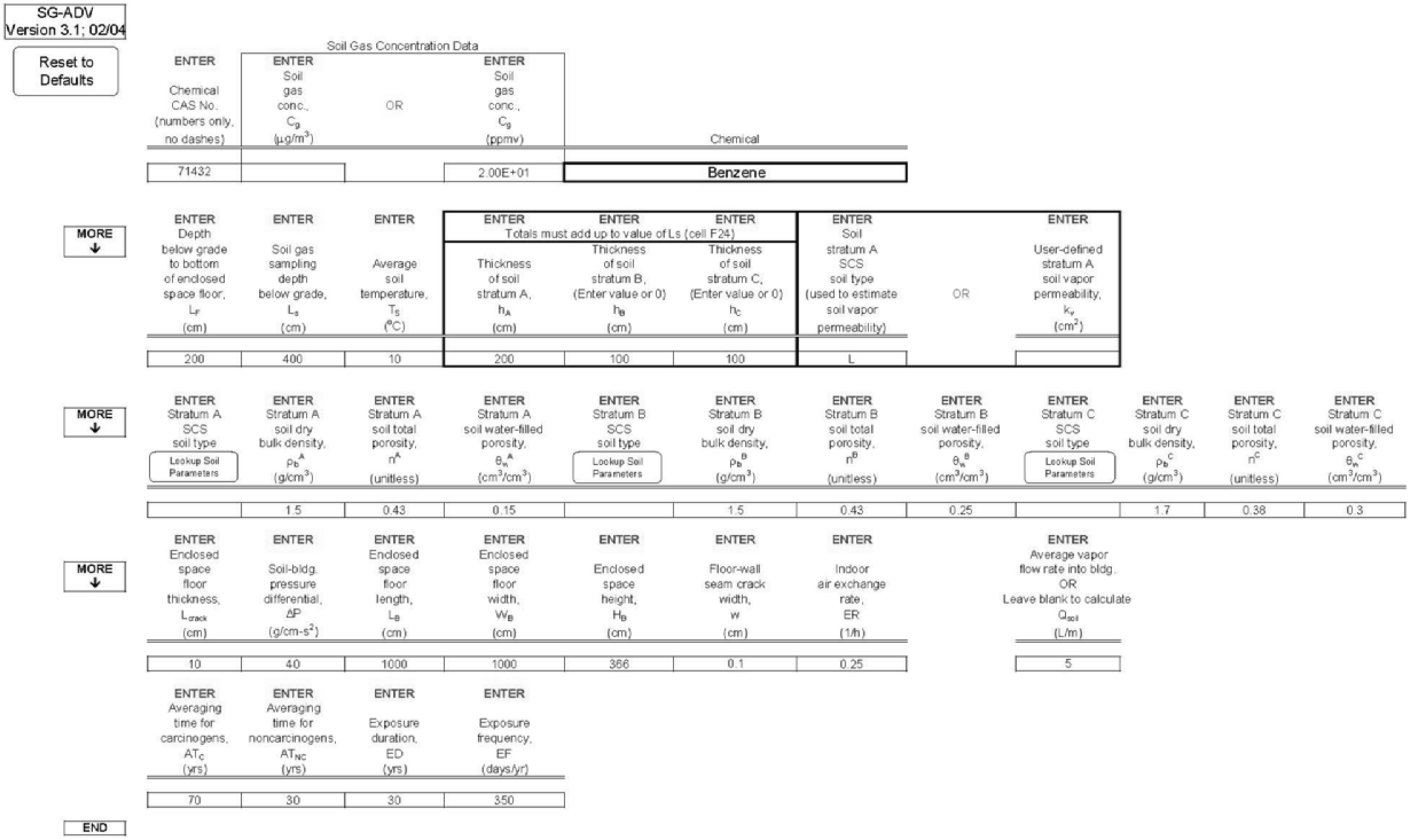
T_S = System (soil) temperature, ^oK.

In the soil gas models, the steady-state indoor air concentration is calculated by Equation 19 (i.e., $C_{building} = \alpha\ C_{source}$). The value of the vapor concentration at the source of emissions (C_{source}) is assigned the value of the user-defined soil gas concentration. The value of the steady-state attenuation coefficient (α) in Equation 19 is calculated by Equation 13. Because no evaluation has been made of the extent of the source of emissions, steady-state conditions (i.e., a non-diminishing source) must be assumed.

The SG-SCREEN model operates under the assumption of homogeneously distributed soil properties and isotropic conditions with respect to soil vapor permeability from the soil surface to an infinite depth. The SG-ADV model, on the other hand, allows the user to specify up to three different soil strata between the building floor in contact with the soil and the soil gas sampling depth. Soil properties within these three strata may be varied to allow for different diffusion resistances to vapor transport.

4.2 SOIL GAS SAMPLING

In order to use the soil gas models, soil gas concentrations must be measured at one or more depths below ground surface (bgs). The user is advised to take samples directly under building slabs


SG-ADV
Version 3.1; 02/04

Soil Gas Concentration Data

ENTER Chemical CAS No. (numbers only, no dashes)	ENTER Soil gas conc., C_g ($\mu g/m^3$)	OR	ENTER Soil gas conc., C_g (ppmv)	Chemical
71432			2.00E+01	**Benzene**

			Totals must add up to value of Ls (cell F24)					
ENTER Depth below grade to bottom of enclosed space floor, L_F (cm)	ENTER Soil gas sampling depth below grade, L_s (cm)	ENTER Average soil temperature, T_S (°C)	ENTER Thickness of soil stratum A, h_A (cm)	ENTER Thickness of soil stratum B, (Enter value or 0) h_B (cm)	ENTER Thickness of soil stratum C, (Enter value or 0) h_C (cm)	ENTER Soil stratum A SCS soil type (used to estimate soil vapor permeability)	OR	ENTER User-defined stratum A soil vapor permeability, k_v (cm^2)
200	400	10	200	100	100	L		

ENTER Stratum A SCS soil type Lookup Soil Parameters	ENTER Stratum A soil dry bulk density, ρ_b^A (g/cm^3)	ENTER Stratum A soil total porosity, n^A (unitless)	ENTER Stratum A soil water-filled porosity, θ_w^A (cm^3/cm^3)	ENTER Stratum B SCS soil type Lookup Soil Parameters	ENTER Stratum B soil dry bulk density, ρ_b^B (g/cm^3)	ENTER Stratum B soil total porosity, n^B (unitless)	ENTER Stratum B soil water-filled porosity, θ_w^B (cm^3/cm^3)	ENTER Stratum C SCS soil type Lookup Soil Parameters	ENTER Stratum C soil dry bulk density, ρ_b^C (g/cm^3)	ENTER Stratum C soil total porosity, n^C (unitless)	ENTER Stratum C soil water-filled porosity, θ_w^C (cm^3/cm^3)
	1.5	0.43	0.15		1.5	0.43	0.25		1.7	0.38	0.3

ENTER Enclosed space floor thickness, L_{crack} (cm)	ENTER Soil-bldg. pressure differential, ΔP ($g/cm\text{-}s^2$)	ENTER Enclosed space floor length, L_B (cm)	ENTER Enclosed space floor width, W_B (cm)	ENTER Enclosed space height, H_B (cm)	ENTER Floor-wall seam crack width, w (cm)	ENTER Indoor air exchange rate, ER (1/h)		ENTER Average vapor flow rate into bldg. OR Leave blank to calculate Q_{soil} (L/m)
10	40	1000	1000	366	0.1	0.25		5

ENTER Averaging time for carcinogens, AT_C (yrs)	ENTER Averaging time for noncarcinogens, AT_{NC} (yrs)	ENTER Exposure duration, ED (yrs)	ENTER Exposure frequency, EF (days/yr)
70	30	30	350

Figure 10. SG-ADV Data Entry Worksheet

or basement floors when possible. This can be accomplished by drilling through the floor and sampling through the drilled hole. Alternatively, an angle-boring rig can be used to sample beneath the floor from outside the footprint of the building. When sampling directly beneath the floor is not possible, enough samples adjacent to the structure should be taken to adequately estimate an average concentration based on reasonable spatial and temporal scales.

Soil gas measurements can be made using several techniques; however, active whole-air sampling methods and active or passive sorbent sampling methods are usually employed. Typically, a whole-air sampling method is used whereby a non-reactive sampling probe is inserted into the soil to a prescribed depth. This can be accomplished manually using a "slam bar," or a percussion power drill, or the probe can be inserted into the ground using a device such as a Geoprobe.® The Geoprobe® device is attached to the rear of a specially customized vehicle. In the field, the rear of the vehicle is placed over the sample location and hydraulically raised on its base. The weight of the vehicle is then used to push the sampling probe into the soil. A built-in hammer mechanism allows the probe to be driven to predetermined depths up to 50 feet depending on the type of soil encountered. Soil gas samples can be withdrawn directly from the probe rods, or flexible tubing can be connected to the probe tips at depth for sample withdrawal.

Whole-air sampling is typically accomplished using an evacuated Summa or equivalent canister, or by evacuation to a Tedlar bag. Normal operation includes the use of an in-line flow controller and a sintered stainless steel filter to minimize particles becoming entrained in the sample atmosphere. For a 6-liter Summa canister, a normal sampling flow rate for a 24-hr integrated sample might be on the order of 1.5 ml/min; however, higher sampling rates can be used for grab samples. The sampling rate chosen, however, must not be so high as to allow for ambient air inleakage between the annulus of the probe and the surrounding soils. Depending on the target compounds, excessive air inleakage can dilute the sample (in some cases below the analytical detection limits).

One way to check for inleakage is to test an aliquot of the sample gas for either nitrogen or oxygen content before the sample is routed to the canister or Tedlar bag. To test for nitrogen in real- or near real-time requires a portable gas chromatograph/mass spectrometer (GC/MS). A portable oxygen meter, however, can be used to test for sample oxygen content in real-time with a typical accuracy of one-half of one percent. If air inleakage is detected by the presence of excessive nitrogen or oxygen, the seal around the sample probe at the soil surface as well as all sampling equipment connections and fittings should be checked. Finally, the flow rate may need to be reduced to decrease or eliminate the air inleakage.

The collection and concentration of soil gas contaminants can be greatly affected by the components of the sampling system. It is imperative to use materials that are inert to the contaminants of concern. Areas of sample collection that need particular attention are:

- The seal at the soil surface around the sample probe
- Use of a probe constructed of stainless steel or other inert material
- Minimization of the use of porous or synthetic materials (i.e., PTFE, rubber, or most plastics) that may adsorb soil gas and cause cross-contamination

- Purging of the sample probe and collection system before sampling
- Leak-check of sampling equipment to reduce air infiltration
- Keeping the length of all sample transfer lines as short as possible to minimize condensation of extracted gas in the lines.

The choice of analytical methods for whole-air soil gas sampling depends on the contaminants of concern. Concentrations of volatile organic compounds (VOCs) in the soil gas are typically determined using EPA Method TO-14 or TO-15. In the case of semi-volatile compounds, an active sorbent sampling methodology can be used. In this case, a low-volume sampling pump is normally used to withdraw the soil gas, which is then routed to a polyurethane foam (PUF) plug. Vapor concentrations of semi-volatile contaminants sorbed to the PUF are then determined using EPA Method TO-10. The active soil gas sampling equipment can be assembled to allow for both canister sampling for volatiles and PUF sampling for semi-volatiles.

Passive sorbent sampling involves burial of solid sorbent sampling devices called cartridges or cassettes to a depth of normally 5 feet or less. The cassettes may be configured with one or more sorbents depending on the list of target analytes, and are typically left in-ground for 72 to 120 hours or longer. During this time period, the vapor-phase soil gas contaminants pass through the cassette and are adsorbed as the soil gas moves toward the soil surface by diffusion and/or convection. Analytical methods for sorbent sampling depend on the target analytes and the sorbent used and may include EPA Method TO-10 or a modified EPA Method TO-1. Vapor-phase concentrations for some solid sorbent sampling systems are determined using the total mass of each contaminant recovered, the time in-ground, the cross-sectional area of the cassette, the diffusivity of the compound in air, and a quasi-empirical adsorption rate constant.

Recent EPA technology verification reports produced by the EPA National Exposure Research Laboratory (EPA 1998, 1998a) concluded, at least for two such systems, that the sorbent methodologies accurately accounted for the presence of most of the soil gas contaminants in the studies. Further, the reports concluded that the sorbent systems showed detection of contaminants at low concentrations not reported using an active whole-air sampling system. For one system, however, it was noted that as the vapor concentrations reported for the whole-air sampling system increased by 1 to 4 orders-of-magnitude, the associated concentrations reported for the sorbent system increased only marginally. Perhaps the best use of such passive sorbent sampling methods is to help confirm which contaminants are present in the soil gas and not necessarily contaminant concentrations.

An excellent discussion of soil gas measurement methods and limitations can be found in the ASTM Standard Guide for Soil Gas Monitoring in the Vadose Zone D5314-92e1. ASTM Standard Guides are available from the ASTM website at:

http://www.astm.org.

In addition, soil gas measurement method summaries can be found in the EPA Standard Operating Procedures for Soil Gas Sampling (SOP No. 2042) developed by the EPA Environmental Response

Team (ERT) in Edison, New Jersey. This document can be downloaded from the ERT Compendium of Standard Operating Procedures at the following website:

http://www.ert.org/media_resrcs/media_resrcs.asp.

Data Quality and Data Quality Objectives

The results of soil gas sampling must meet the applicable requirements for data quality and satisfy the data quality objectives of the study for which they are intended. Data quality objectives are qualitative and quantitative statements derived from the data quality objectives process that clarify study objectives, define the appropriate type of data, and specify the tolerable levels of potential decision errors that will be used to support site decisions. Data quality objectives are formulated in the first phase of a sampling project.

In the second phase of the project, a Quality Assurance Project Plan (QAPP) translates these requirements into measurement performance specifications and quality assurance/quality control procedures to provide the data necessary to satisfy the user's needs. The QAPP is the critical planning document for any environmental data collection operation because it documents how quality assurance and quality control activities will be implemented during the life of the project. Development of the data quality objectives and the QAPP for soil gas sampling should follow the guidance provided by EPA's Quality Assurance Division of the Office of Research and Development. Guidance documents concerning the development and integration of the data quality objectives and the QAPP can be obtained from the EPA website at:

http://epa.gov/ncerqa/qa/qa_docs.html.

In addition to the above guidance, the EPA Regional Office and/or other appropriate regulatory agency should be consulted concerning specific sampling requirements.

4.3 ASSUMPTIONS AND LIMITATIONS OF THE SOIL GAS MODEL

As discussed previously, the soil gas models operate under the assumption of steady-state conditions. This means that enough time has passed for the vapor plume to have reached the building of interest directly above the source of contamination and that the vapor concentrations have reached their maximum values. Depending on the depth at which the soil gas is sampled, diffusion of the soil gas toward the building is a function of the soil properties between the building floor in contact with the soil and the sampling depth. Convection of the soil gas into the structure is a function of the building properties and the effective soil vapor permeability. Assumptions and limitations of the soil gas models are the same as those in Section 2.11 with the exception of the source vapor concentration that is determined empirically through soil gas sampling.

The user should also recognize the inherent limitations of soil gas sampling. First, the geologic variability of the subsurface may be considerable. This may be especially problematic for shallow soil gas sampling because soil moisture content can vary widely as a function of precipitation events and surface runoff. The soil moisture content has an exponential effect on the rate of vapor diffusion. Transformation processes such as biodegradation can also occur in shallow subsurface soils. In some cases, only a relatively thin stratum of bioactive soil can greatly reduce the emission flux toward the soil surface. Finally, subsurface phase equilibria is a dynamic process resulting in varying vapor-phase concentrations over time at the same sampling location and depth. These factors can result in significant differences in measured soil gas concentrations over relatively small spatial and temporal scales.

For these reasons, the planning phase of the soil gas-sampling program should carefully consider the inherent uncertainties in site-specific sampling and analytical data. In the final analysis, the extent of soil gas sampling is a trade-off between sampling costs and the degree of certainty required in the soil gas concentration data.

SECTION 5

ASSUMPTIONS AND LIMITATIONS OF THE J&E MODEL

The J&E Model is a one-dimensional analytical solution to diffusive and convective transport of vapors into indoor spaces. The model is formulated as an attenuation factor that relates the vapor concentration in the indoor space to the vapor concentration at the source. It was developed for use as a screening level model and consequently is based on a number of simplifying assumptions regarding contaminant distribution and occurrence, subsurface characteristics, transport mechanisms, and building construction.

EPA is suggesting that the J&E Model be used at Resource Conservation and Recovery Act (RCRA) Corrective Action Sites, Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA)/Superfund Sites, and voluntary cleanup sites. EPA is not recommending that the J&E Model be used for sites contaminated with petroleum products if the products were derived from Underground Storage Tanks. The J&E Model does not account for contaminant attenuation (biodegradation, hydrolysis, sorption, and oxidation/reduction). Attenuation is potentially a significant concern for these type of sites. EPA is recommending that investigators use OSWER Directive 9610.17: Use of Risk Based Decision-Making in UST Corrective Action Programs to evaluate these types of sites.

The J&E Model as implemented by EPA assumes homogeneous soil layers with isotropic properties that characterize the subsurface. The first tier spreadsheet versions allow only one layer; the advanced spreadsheet versions allow up to three layers. Sources of contaminants that can be modeled include dissolved, sorbed, or vapor sources where the concentrations are below the aqueous solubility limit, the soil saturation concentration, and/or the pure component vapor concentration. The contaminants are assumed to be homogeneously distributed at the source. All but one of the spreadsheets assumes an infinite source. The exception is the advanced model for a bulk soil source, which allows for a finite source. For the groundwater and bulk soil models, the vapor concentration at the source is calculated assuming equilibrium partitioning. Vapor from the source is assumed to diffuse directly upward (one-dimensional transport) through uncontaminated soil (including an uncontaminated capillary fringe if groundwater is the vapor source) to the base of a building foundation, where convection carries the vapor through cracks and openings in the foundation into the building. Both diffusive and convective transport processes are assumed to be at steady state. Neither sorption nor biodegradation is accounted for in the transport of vapor from the source to the base of the building.

The assumptions described above and in Table 12 suggest a number of conditions that preclude the use of the Non-NAPL Models as implemented by EPA. These conditions include:

TABLE 12. ASSUMPTIONS AND LIMITATIONS OF THE VAPOR INTRUSION MODEL

Assumption	Implication	Field Evaluation
Contaminant		
No contaminant free-liquid/precipitate phase present	J&E Model not representative of NAPL partitioning from source	NAPL or not at site–easier to evaluation for floating product or soil contamination sites. Most DNAPL sites with DNAPL below the water table defy easy characterization.
Contaminant is homogeneously distributed within the zone of contamination		
No contaminant sources or sinks in the building.	Indoor sources of contaminants and/or sorption of vapors on materials may confound interpretation of results.	Survey building for sources, assessment of sinks unlikely
Equilibrium partitioning at contaminant source.	Groundwater flow rates are low enough so that there are no mass transfer limitations at the source.	Not likely
Chemical or biological transformations are not significant (model will predict more intrusion)	Tendency to over predict vapor intrusion for degradable compounds	From literature
Subsurface Characteristics		
Soil is homogeneous within any horizontal plane	Stratigraphy can be described by horizontal layers (not tilted layers)	Observe pattern of layers and unconformities Note: In simplified J&E Model layering is not considered
All soil properties in any horizontal plane are homogeneous		
The top of the capillary fringe must be below the bottom of the building floor in contact with the soil.		
EPA version of JE Model assumes the capillary fringe is uncontaminated.		
Transport Mechanisms		
One-dimensional transport	Source is directly below building, stratigraphy does not influence flow direction, no effect of two- or three-dimensional flow patterns.	Observe location of source, observe stratigraphy, pipeline conduits, not likely to assess two- and three-dimensional pattern.
Two separate flow zones, one diffusive one convective.	No diffusion (dispersion) in the convective flow zone. Plug flow in convective zone	Not likely
Vapor-phase diffusion is the dominant mechanism for transporting contaminant vapors from contaminant sources located away from the foundation to the soil region near the foundation	Neglects atmospheric pressure variation effects, others?	Not likely

(continued)

Assumption	Implication	Field Evaluation
Straight-line gradient in diffusive flow zone.	Inaccuracy in flux estimate at match point between diffusive and convective sections of the model.	Not likely
Diffusion through soil moisture will be insignificant (except for compounds with very low Henry's Law Constant	Transport through air phase only. Good for volatiles. Only low volatility compounds would fail this and they are probably not the compounds of concern for vapor intrusion	From literature value of Henry's Law Constant.
Convective transport is likely to be most significant in the region very close to a basement, or a foundation, and vapor velocities decrease rapidly with increasing distance from a structure		Not likely
Vapor flow described by Darcy's law	Porous media flow assumption.	Observations of fractured rock, fractured clay, karst, macropores, preferential flow channels.
Steady State convection	Flow not affected by barometric pressure, infiltration, etc.	Not likely
Uniform convective flow near the foundation	Flow rate does not vary by location	Not likely
Uniform convective velocity through crack or porous medium	No variation within cracks and openings and constant pressure field between interior spaces and the soil surface	Not likely
Significant convective transport only occurs in the vapor phase	Movement of soil water not included in vapor impact	Not likely
All contaminant vapors originating from directly below the basement will enter the basement, unless the floor and walls are perfect vapor barriers. (Makes model over est. vapors as none can flow around the building)	Model does not allow vapors to flow around the structure and not enter the building	Not likely
Contaminant vapors enter structures primarily through cracks and openings in the walls and foundation	Flow through the wall and foundation material itself neglected	Observe numbers of cracks and openings. Assessment of contribution from construction materials themselves not likely

- The presence or suspected presence of residual or free-product non-aqueous phase liquids (LNAPL, DNAPL, fuels, solvents, etc.) in the subsurface.
- The presence of heterogeneous geologic materials (other than the three layers allowed in the advanced spreadsheets) between the vapor source and building. The J&E Model does not apply to geologic materials that are fractured, contain macropores or other preferential pathways, or are composed of karst.

- Sites where significant lateral flow of vapors occurs. These can include geologic layers that deflect contaminants from a strictly upward motion and buried pipelines or conduits that form preferential paths. Significantly different permeability contrasts between layers are likely to cause lateral flow of vapors. The model assumes the source of contaminants is directly below the potential receptors.
- Very shallow groundwater where the building foundation is wetted by the groundwater.
- Very small building air exchange rates (e.g., < 0.25/h)
- Buildings with crawlspace structures or other significant openings to the subsurface (e.g., earthen floors, stone buildings, etc.). The EPA spreadsheet only allows for either slab on grade or basement construction.
- Contaminated groundwater sites with large fluctuations in the water table elevation. In these cases, the capillary fringe is likely to be contaminated; whereas in the groundwater source spreadsheets, the capillary fringe is assumed to be uncontaminated.

In theory the above limitations are readily conceptualized, but in practice the presence of these limiting conditions may be difficult to verify even when extensive site characterization data are available. Conditions that are particularly difficult to verify in the field include the presence of residual non-aqueous phase liquids (NAPLs) in the unsaturated zone and the presence and influence of macropores, fractures and other preferential pathways in the subsurface. Additionally, in the initial stages of evaluation, especially at the screening level, information about building construction and water table fluctuations may not be available. Even the conceptually simple assumptions (e.g., one-dimensional flow, lack of preferential pathways) may be difficult to assess when there are little site data available.

The vapor equilibrium models employed to estimate the vapor concentration at the source of soil contamination is applicable only if "low" concentrations of the compound(s) are sorbed to organic carbon in the soil, dissolved in soil moisture, and present as vapor within the air-filled soil pores (i.e., a three-phase system). The vapor equilibrium models do not account for a residual phase NAPLs. If residual phase contaminants are present in the soil column, the user is referred to either the NAPL-SCREEN or NAPL-ADV model (Appendix A), as appropriate.

In the case of contaminated groundwater, the vapor equilibrium model operates under the assumption that the contaminant is present at levels below the water solubility limit. If the user-defined soil concentration is greater than the soil saturation concentration (C_{sat}) or if the groundwater concentration is greater than the solubility limit (S), the equilibrium vapor concentration will be calculated at the value of C_{sat} or S as appropriate.

The user is also reminded that when estimating a risk-based soil concentration, the model will compare the calculated soil concentration with the soil saturation concentration above which a residual phase is likely to occur. The soil saturation concentration (C_{sat}) is calculated as in U.S. EPA (1996a and b). If the risk-based concentration is greater than the saturation concentration and the contaminant is a liquid or gas at the soil temperature, the final soil concentration will be set equal to the soil saturation concentration. This tends to eliminate the possibility of allowing a liquid residual phase to exist within the soil column, which may leach to the water table. If the risk-based soil concentration is greater than C_{sat} and the contaminant is a solid, the contaminant is not of concern for the vapor intrusion pathway.

Likewise, the groundwater models will compare the calculated risk-based groundwater concentration to the aqueous solubility limit of the compound. If the risk-based groundwater concentration is greater than the solubility limit, the contaminant is not of concern for the vapor intrusion pathway.

Finally, it should be recognized that the procedures used to estimate both the soil saturation concentration and the aqueous solubility limit do not consider the effects of multiple contaminants. The estimated values, therefore, may be artificially high such that a residual phase may actually exist at somewhat lower concentrations.

The procedures used to estimate the soil vapor permeability of the soil stratum in contact with the building floor and walls assume isotropic soils and steady-state soil moisture content. In addition, the calculations do not account for preferential vapor pathways due to soil fractures, vegetation root pathways, or the effects of a gravel layer below the floor slab or backfill. These items may act to increase the vapor permeability of in situ soils.

If in situ pneumatic tests are used to measure site vapor permeability, care must be taken to ensure adequate sampling to reduce the possibility of missing important soil structure effects due to anisotropy.

Single-point in situ pneumatic tests are typically conducted by measuring the pressure in a probe as a metered flow of air is passed through the probe and into the soil. Garbesi et al. (1996), however, demonstrated that soil vapor permeability increases with the sampling length scale. Using a dual-probe dynamic pressure sampling apparatus, Garbesi et al. (1996) demonstrated that the average soil vapor permeability typically increases up to a constant value as the distance between the source probe and detector probe increases. On a length scale typical of a house (3 to 10 m), use of the dual-probe sampling technique found that the soil permeability was approximately 10 to 20 times higher than that measured by the single-point method. Although arguably the most accurate means of determining in situ soil vapor permeability, the techniques of Garbesi et al. (1996) are complex and require specialized equipment.

Another method for determining the intrinsic permeability of soil is to conduct empirical measurements of the saturated hydraulic conductivity (K_s). These data are then input into Equation

26. The resulting value of k_i is then multiplied by the relative air permeability (k_{rg}) calculated by Equation 27 to yield the effective air permeability of the soil.

Estimation of the rise of the capillary zone is based on the equation for the rise of a liquid in a capillary tube. The procedure assumes that the interstitial space between the soil particles is equivalent to the capillary tube diameter and that the resulting rise of water occurs under steady-state soil column drainage conditions. In actuality, the height of the capillary zone is uneven or fingered due to the variation in the actual in situ particle size distribution. In addition, the groundwater models do not account for the episodic rise and fall of the water table or the capillary zone due to aquifer recharge and discharge. As constructed, the groundwater models do not allow the top of the capillary zone to be above the bottom of the building floor in contact with the soil. The user should be aware, however, that in reality the top of the capillary zone may rise to levels above the floor in some cases.

Diffusion across the capillary zone is estimated based on lumping vapor and aqueous-phase diffusion together within the calculation of the effective diffusion coefficient. To allow for vapor-phase diffusion within the capillary zone, the air-filled soil pores must be connected. In reality, the capillary zone may be comprised of a tension-saturated zone immediately above the water table and the deep portion of the vadose zone within which the soil water content is strongly dependent on the pressure head. Diffusion across the tension-saturated zone is dominated by liquid-phase diffusion, which is typically four orders of magnitude less than vapor-phase diffusion. Therefore, a large concentration gradient may exist between the top of the water table and the top of the tension-saturated zone (McCarthy and Johnson, 1993).

Lumping vapor and aqueous-phase diffusion together is a less-intensive, although less-rigorous, method for estimating the effective diffusion coefficient. The result is typically a higher effective diffusion coefficient relative to separate solutions for aqueous diffusion across the tension-saturated zone and both vapor and aqueous diffusion across the unsaturated portion of the vadose zone.

To minimize the possible overestimation of the effective diffusion coefficient, the soil air-filled porosity within the capillary zone is estimated based on the air-entry pressure head, which corresponds with the water-filled porosity at which the interstitial air-filled pores first become connected. The user should be aware that this procedure is inherently conservative if a significant concentration gradient exists across the tension-saturated zone. This conservatism may be somewhat offset in that the model does not consider any episodic rise in the level of the water table. During such events, water that had previously been part of the saturated zone (and hence contain higher contaminant concentrations) is redistributed in the vadose zone resulting in temporary elevations in soil gas concentrations.

The model assumes that all vapors from underlying soils will enter the building through gaps and openings in the walls, floor, and foundation. This implies that a constant pressure field is generated between the interior spaces and the soil surface and that the vapors are intercepted within the pressure field and transported into the building. This assumption is inherently conservative in that it neglects periods of near zero pressure differentials (e.g., during mild weather when windows are left open).

As with the estimation procedure for soil vapor permeability, the model assumes isotropic soils in the horizontal direction; vertical anisotropy is accounted for by a series of isotropic soil strata above the top of contamination. Soil properties within the zone of soil contamination are assumed to be identical to those of the soil stratum directly above the contamination and extend downward to an infinite depth. Solute transports by convection (e.g., water infiltration) and by mechanical dispersion are neglected. Transformation processes (e.g., biodegradation, hydrolysis, etc.) are also neglected.

The J&E Model treats the entire building as a single chamber with instantaneous and homogeneous vapor dispersion. It therefore neglects contaminant sinks and the room-to-room variation in vapor concentration due to unbalanced mechanical and/or natural ventilation.

5.1 SOURCE VAPOR CONCENTRATION

As applied in the accompanying spreadsheets, the vapor equilibrium model employed to estimate the vapor concentration at the source of soil contamination is applicable in the limit of "low" concentrations where compounds are sorbed to organic carbon in the soil, dissolved is soil moisture, and present as vapor within the air-filled soil pores (i.e., a three-phase system). The model does not account for a residual phase (e.g., NAPL). If residual phase contaminants are present in the soil column, the user is referred to either the NAPL-SCREEN or NAPL-ADV model, as appropriate.

In the case of contaminated groundwater, the vapor equilibrium model operates under the assumption that the contaminant is present at levels below the water solubility limit. If the user-defined soil concentration is greater than the soil saturation concentration (C_{sat}) or if the groundwater concentration is greater than the solubility limit (S), the equilibrium vapor concentration will be calculated at the value of C_{sat} or S as appropriate.

The user is also reminded that when estimating a risk-based soil concentration, the model will compare the calculated soil concentration with the soil saturation concentration above which a residual phase is likely to occur. The soil saturation concentration (C_{sat}) is calculated as in U.S. EPA (1996a and b). If the risk-based concentration is greater than the saturation concentration and the contaminant is a liquid or gas at the soil temperature, the final soil concentration will be set equal to the soil saturation concentration. This tends to eliminate the possibility of allowing a liquid residual phase to exist within the soil column, which may leach to the water table. If the risk-based soil concentration is greater than C_{sat} and the contaminant is a solid, the contaminant is not of concern for the vapor intrusion pathway.

Likewise, the groundwater models will compare the calculated risk-based groundwater concentration to the aqueous solubility limit of the compound. If the risk-based groundwater concentration is greater than the solubility limit, the contaminant is not of concern for the vapor intrusion pathway.

Finally, it should be recognized that the procedures used to estimate both the soil saturation concentration and the aqueous solubility limit do not consider the effects of multiple contaminants. The estimated values, therefore, may be artificially high such that a residual phase may actually exist at somewhat lower concentrations.

5.2 SOIL VAPOR PERMEABILITY

The procedures used to estimate the soil vapor permeability of the soil stratum in contact with the building floor and walls assumes isotropic soils and steady-state soil moisture content. In addition, the calculations do not account for preferential vapor pathways due to soil fractures, vegetation root pathways, or the effects of a gravel layer below the floor slab or backfill which may act to increase the vapor permeability with respect to in situ soils.

If in situ pneumatic tests are used to measure site vapor permeability, care must be taken to ensure adequate sampling to reduce the possibility of missing important soil structure effects due to anisotropy.

Single point in situ pneumatic tests are typically conducted by measuring the pressure in a probe as a metered flow of air is passed through the probe and into the soil. Garbesi et al. (1996), however, demonstrated that soil vapor permeability increases with the sampling length scale. Using a dual-probe dynamic pressure sampling apparatus, Garbesi et al. (1996) demonstrated that the average soil vapor permeability typically increases up to a constant value as the distance between the source probe and detector probe increases. On a length scale typical of a house (3 to 10 m) use of the dual-probe sampling technique found that the soil permeability was approximately 10 to 20 times higher than that measured by the single point method. Although arguably the most accurate means of determining in situ soil vapor permeability, the techniques of Garbesi et al. (1996) are complex and require specialized equipment.

Another method for determining the intrinsic permeability of soil is to conduct empirical measurements of the saturated hydraulic conductivity (K_s). These data are then input into Equation 26. The resulting value of k_i is then multiplied by the relative air permeability (k_{rg}) calculated by Equation 27 to yield the effective air permeability of the soil.

5.3 RISE OF AND DIFFUSION ACROSS THE CAPILLARY ZONE

Estimation of the rise of the capillary zone is based on the equation for the rise of a liquid in a capillary tube. The procedure assumes that the interstitial space between the soil particles is equivalent to the capillary tube diameter and that the resulting rise of water occurs under steady-state soil column drainage conditions. In actuality, the height of the capillary zone is uneven or fingered due to the variation in the actual in situ particle size distribution. In addition, the groundwater models do not account for the episodic rise and fall of the water table or the capillary zone due to aquifer recharge and discharge. As constructed, the groundwater models do not allow the top of the capillary zone to be above the bottom of the building floor in contact with the soil. The user should be aware, however, that in reality the top of the capillary zone might rise to levels above the floor in some cases.

Diffusion across the capillary zone is estimated based on lumping vapor and aqueous-phase diffusion together within the calculation of the effective diffusion coefficient. To allow for vapor-phase diffusion within the capillary zone, the air-filled soil pores must be connected. In reality, the capillary zone may be comprised of a tension-saturated zone immediately above the water table and the deep portion of the vadose zone within which the soil water content is a strongly dependent on the pressure head. Diffusion across the tension-saturated zone is dominated by liquid-phase diffusion which is typically four orders of magnitude less than vapor-phase diffusion. Therefore, a large concentration gradient may exist between the top of the water table and the top of the tension-saturated zone (McCarthy and Johnson, 1993).

Lumping vapor and aqueous-phase diffusion together is a less intensive, although less rigorous, method for estimating the effective diffusion coefficient. The result is typically a higher effective diffusion coefficient relative to separate solutions for aqueous diffusion across the tension-saturated zone and both vapor and aqueous diffusion across the unsaturated portion of the vadose zone.

To minimize the possible over estimation of the effective diffusion coefficient, the soil air-filled porosity within the capillary zone is estimated based on the air-entry pressure head, which corresponds with the water-filled porosity at which the interstitial air-filled pores first become connected. The user should be aware that this procedure is inherently conservative if a significant concentration gradient exists across the tension-saturated zone. This conservatism may be somewhat offset in that the model does not consider any episodic rise in the level of the water table. During such events, water which had previously been part of the saturated zone (and hence contain higher contaminant concentrations) is redistributed in the vadose zone resulting in temporary elevations in soil gas concentrations.

5.4 DIFFUSIVE AND CONVECTIVE TRANSPORT INTO THE STRUCTURE

The following is a discussion of the major assumptions and limitations of the J&E Model for diffusive and convective vapor transport into buildings.

The model assumes that all vapors from underlying soils will enter the building through gaps and openings in the walls, floor, and foundation. This implies that a constant pressure field is generated between the interior spaces and the soil surface and that the vapors are intercepted within the pressure field and transported into the building. This assumption is inherently conservative in that it neglects periods of near zero pressure differentials (e.g., during mild weather when windows are left open).

As with the estimation procedure for soil vapor permeability, the model assumes isotropic soils in the horizontal direction; vertical anisotropy is accounted for by a series of isotropic soil strata above the top of contamination. Soil properties within the zone of soil contamination are assumed to be identical to those of the soil stratum directly above the contamination and extend downward to an infinite depth. Solute transports by convection (e.g., water infiltration) and by mechanical dispersion are neglected. Transformation processes (e.g., biodegradation, hydrolysis, etc.) are also neglected.

An empirical field study (Fitzpatrick and Fitzgerald, 1997) indicated that the model may be overly conservative for nonchlorinated species (e.g., benzene, toluene, ethylbenzene and xylene) but in some cases, may underpredict indoor concentrations for chlorinated species. The authors contribute the likely cause for this discrepancy to the significant biodegradation of the nonchlorinated compounds.

The J&E Model treats the entire building as a single chamber with instantaneous and homogeneous vapor dispersion. It therefore neglects contaminant sinks and the room-to-room variation in vapor concentration due to unbalanced mechanical and/or natural ventilation.

Finally, convective vapor flow from the soil matrix into the building is represented as an idealized cylinder buried below grade. This cylinder represents the total area of the structure below the soil surface (walls and floor). The total crack or gap area is assumed to be a fixed fraction of this area. Because of the presence of basement walls, the actual vapor entry rate is expected to be 50 to 100 percent of that provided by the idealized geometry (Johnson and Ettinger, 1991).

SECTION 6

INTERPRETATION OF RESULTS

The models described herein are theoretical approximations of complex physical and chemical processes and as such should not be used in a deterministic fashion (i.e., to generate a single outcome). At the least, a range of outcomes should be explored focusing on the most sensitive model input variables. In general, using the default values for input variables will result in higher indoor air concentrations and thus higher incremental risks or lower risk-based media concentrations. With a realistic range of outcomes, the risk manager may assess the uncertainty in the model predictions.

From a conceptual point of view, the vapor intrusion model provides a theoretical description of the processes involved in vapor intrusion from subsurface soils or groundwater into indoor structures. A combination of modeling and sampling methods is also possible to reduce the uncertainty of the calculated indoor air concentrations. Typically this involves field methods for measuring soil gas very near or below an actual structure. It should be understood, however, that soil gas sampling results outside the footprint of the building may or may not be representative of the soil gas concentrations directly below the structure. For solid building floors in contact with the soil (e.g., concrete slabs), the soil gas directly beneath the floor may be considerably higher than that adjacent to the structure. This is typically due to a vapor pooling effect underneath the near impermeable floor. Once a representative average concentration is determined, all vapor directly below the areal extent of the building is presumed to enter the structure. The soil gas concentration, along with the building ventilation rate and the soil gas flow rate into the building, will determine the indoor concentration. When using the soil gas models, it must be remembered that no analysis has been made concerning the source of contamination. Therefore, the calculated indoor concentration is assumed to be steady-state. The procedures described in API (1998) can be used to calibrate the diffusion transport considerations of the J&E Model as well as for calibrating the Model for transformation processes (e.g., biodegradation). The reader is also referred to U.S. EPA (1992) for a more detailed discussion of applying soil gas measurements to indoor vapor intrusion.

Finally, calibration and verification of the model have been limited due to the paucity of suitable data. Research is needed to provide spatially and temporally correlated measurements during different seasons, at different locations, with different buildings, and over a range of different contaminants such that the accuracy of the model may be determined. Appendix E contains bibliography and references.

APPENDIX A

USER'S GUIDE FOR NON-AQUEOUS PHASE LIQUIDS

Purpose

The NAPL-SCREEN and NAPL-ADV models are designed to forward calculate incremental cancer risks or noncarcinogenic hazard quotients due to subsurface soil vapor intrusion into buildings. The models are specifically designed to handle nonaqueous phase liquids or solids in soils. The user may specify up to 10 soil contaminants, the concentrations of which form a residual phase mixture. A residual phase mixture occurs when the sorbed phase, aqueous phase, and vapor phase of each chemical have reached saturation in soil. Concentrations above this saturation limit for all of the specified chemicals of a mixture will result in a fourth or residual phase (i.e., nonaqueous phase liquid or solid).

Other vapor intrusion models (SL-SCREEN, SL-ADV, SG-SCREEN, SG-ADV, GW-SCREEN, and GW-ADV) handled only a single contaminant and only when the soil concentration was at or below the soil saturation limit (i.e., a three-phase system). Use of these models when a residual phase is present, results in an overprediction of the soil vapor concentration and subsequently the building vapor concentration.

Residual Phase Theory

The three-phase system models estimate the equilibrium soil vapor concentration at the emission source (C_{source}) using the procedures from Johnson et al. (1990):

$$C_{source} = \frac{H'_{TS} C_R \rho_b}{\theta_w + K_d \rho_b + H'_{TS} \theta_a} \qquad (1)$$

where:
C_{source} = Vapor concentration at the source of contamination, g/cm^3
H'_{TS} = Henry's law constant at the soil temperature, dimensionless
C_R = Initial soil concentration, g/g
ρ_b = Soil dry bulk density, g/cm^3
θ_w = Soil water-filled porosity, cm^3/cm^3
K_d = Soil-water partition coefficient, cm^3/g (= $K_{oc} \times f_{oc}$)
θ_a = Soil air-filled porosity, cm^3/cm^3
K_{oc} = Soil organic carbon partition coefficient, cm^3/g
f_{oc} = Soil organic carbon weight fraction.

In Equation 1, the equilibrium vapor concentration is proportional to the soil concentration up to the soil saturation limit. When a residual phase is present, however, the vapor concentration is independent of the soil concentration but proportional to the mole fraction of the individual component of the residual phase mixture. In this case, the equilibrium vapor concentration must be calculated numerically for a series of time-steps. For each time-step, the mass of each constituent that is volatilized is calculated using Raoult's law and the appropriate mole fraction. At the end of each time-step, the total mass lost is subtracted from the initial mass and the mole fractions are recomputed for the next time-step.

The NAPL-SCREEN and NAPL-ADV models use the procedures of Johnson et al. (2001) to calculate the equilibrium vapor concentration at the source of emissions for each time-step. Within each model, the user-defined initial soil concentration of each component in the mixture is checked to see if a residual phase is present. This is done by calculating the product of the activity coefficient of component *i* in water (α_i) and the mole fraction of *i* dissolved in soil moisture (y_i) such that:

$$\alpha_i y_i = \frac{M_i}{\left[\left(P_i^v(T_S)\theta_a V / RT_S\right) + \left(M^{H2O}/\alpha_i\right) + \left(K_{d,i}M_{soil}/\alpha_i MW_{H2O}\right)\delta\left(M^{H2O}\right)\right]} \quad (2)$$

where:
M_i = Initial moles of component *i* in soil, moles
$P_i^v(T_S)$ = Vapor pressure of *i* at the average soil temperature, atm
θ_a = Soil air-filled porosity, cm^3/cm^3
V = Volume of contaminated soil, cm^3
R = Ideal gas constant, 82.05 atm-cm^3/mol-^{o}K
T_S = Average soil temperature, ^{o}K
M^{H_2O} = Total moles in soil moisture dissolved phase, moles
α_i = Activity coefficient of *i* in water, unitless
$K_{d,i}$ = Soil-water partition coefficient of *i*, cm^3/g
M_{soil} = Total mass of contaminated soil, g
MW_{H2O} = Molecular weight of water, 18 g/mol
$\delta(M^{H_2O})$ = 1 if $M^{H_2O} > 0$, and
$\delta(M^{H_2O})$ = 0 if $M^{H_2O} = 0$.

If the sum of all the values of $\alpha_i y_i$ for all of the components of the mixture is less than 1, the mixture does not contain a residual phase and the models are not applicable. In such cases, the SL-SCREEN or SL-ADV model can be used to estimate the building concentration.

Once it has been determined that a residual phase does exists, the mole fraction of each component (x_i) is determined by iteratively solving Equations 3 and 4 subject to the constraint that the sum of all the mole fractions equals unity ($\Sigma x_i = 1$):

$$x_i = \frac{M_i}{\left[\left(P_i^v(T_S)\theta_a V / RT_S\right) + M^{HC} + \left(M^{H2O}/\alpha_i\right) + \left(K_{d,i}M_{soil}/\alpha_i MW_{H2O}\right)\delta\left(M^{H2O}\right)\right]} \quad (3)$$

and,

$$x_i = \frac{M_i^{HC}}{M^{HC}} \quad (4)$$

where M_i^{HC} is the number of moles of component *i* in residual phase and M^{HC} is the total number of moles of all components in residual phase. The solution is simplified by assuming that M^{H_2O} is approximately equal to the number of moles of water in the soil moisture. With the mole fraction of each component at the initial time-step, the equilibrium vapor concentration at the source of emissions is calculated by Raoult's law:

$$C_{source} = \frac{x_i P_i^v(T_S) MW_i}{RT_S} \qquad (5)$$

where MW_i is the molecular weight of component *i* (g/mol).

At the beginning of each succeeding time-step, the number of moles of each chemical remaining in the soil from the previous time-step are again checked to see if a residual phase is present using Equation 2. When a residual phase is no longer present, the equilibrium vapor concentration at the source of emissions is calculated by:

$$C_{source} = \frac{\alpha_i y_i P_i^v(T_S) MW_i}{RT_S}. \qquad (6)$$

Ancillary Calculations

The activity coefficient of component *i* in water (α_i) is estimated from its solubility. Because hydrocarbons are typically sparingly soluble in water, the following generalization has been applied to compounds that are liquid or solid at the average soil temperature:

$$\alpha_i = (1/y_i) = (55.55\ \text{moles/L}) MW_i / S_i \qquad (7)$$

where S_i is the solubility of component *i* (g/L). For gases at the average soil temperature, the corresponding relationship is:

$$\alpha_i = (1/y_i)(1 atm / P_i^v(T_S)) = (55.55\ \text{moles}/L)(MW_i(1\ atm)/S_i P_i^v(T_S)) . \qquad (8)$$

Assuming that the vapor behaves as an ideal gas with a relatively constant enthalpy of vaporization between 70°F and the average soil temperature, the Claussius-Clapeyron equation can be used to estimate the vapor pressure at the desired temperature:

$$P^v(T_S) = P^v(T_R) \times \exp\left[\left(\frac{T_B \times T_R}{(T_B - T_R)}\right)\left(\frac{1}{T_S} - \frac{1}{T_R}\right)\ln\left(\frac{P^v(T_R)}{P_B}\right)\right] \qquad (9)$$

where: $P^v(T_S)$ = Vapor pressure at the desired temperature T_S, atm

$P^v(T_R)$ = Vapor pressure at the reference temperature T_R, atm

T_B = Normal boiling point, ^{o}K
T_R = Vapor pressure reference temperature, ^{o}K
T_S = The desired temperature, ^{o}K
P_B = Normal boiling point pressure = 1 atm.

Building Concentration

The vapor concentration within the building or enclosed space ($C_{building}$) is calculated using the steady-state solution of Johnson and Ettinger (1991) such that:

$$C_{building} = \alpha C_{source} . \qquad (10)$$

The steady-state attenuation coefficient (α) is calculated by:

$$\alpha = \frac{\left[\left(\frac{D_T^{eff} A_B}{Q_{building} L_T}\right) \times \exp\left(\frac{Q_{soil} L_{crack}}{D^{crack} A_{crack}}\right)\right]}{\left[\exp\left(\frac{Q_{soil} L_{crack}}{D^{crack} A_{crack}}\right) + \left(\frac{D_T^{eff} A_B}{Q_{building} L_T}\right) + \left(\frac{D_T^{eff} A_B}{Q_{soil} L_T}\right)\left[\exp\left(\frac{Q_{soil} L_{crack}}{D^{crack} A_{crack}}\right) - 1\right]\right]} \qquad (11)$$

where: α = Steady-state attenuation coefficient, unitless
D_T^{eff} = Total overall effective diffusion coefficient, cm^2/s
A_B = Area of the enclosed space below grade, cm^2
$Q_{building}$ = Building ventilation rate, cm^3/s
L_T = Source-building separation, cm
Q_{soil} = Volumetric flow rate of soil gas into the enclosed space, cm^3/s
L_{crack} = Enclosed space foundation or slab thickness, cm
A_{crack} = Area of total cracks, cm^2
D^{crack} = Effective diffusion coefficient through the cracks, cm^2/s.

The reader is referred to Section 2.5 of this Guidance for a more detailed discussion of the derivation of Equation 11 and procedures for determining values for model input parameters. Except for the calculation of the equilibrium vapor concentration at the source of emissions, NAPL-SCREEN is identical to the three-phase model SL-SCREEN and NAPL-ADV is identical to the three-phase model SL-ADV.

The NAPL-SCREEN and NAPL-ADV models explicitly solve for the time-averaged building concentration over the exposure duration using a forward finite-difference numerical approach. For each time-step δ*t*:

$$M_i(t + \delta t) = M_i(t) - \delta t\left(C_{building} \times Q_{building} / MW_i\right) \qquad (12)$$

where $M_i\,(t)$ is the number of moles of component i in soil at the previous time and $M_i(t+\delta t)$ is the number of moles at the new time. The time-step interval is variable as a function of the percent of mass lost over the time-step. The user may specify a minimum and maximum percent loss allowed; these values are applied to the single component of the residual phase mixture with the highest mass loss rate during each time-step interval. If the user-specified maximum percent loss is exceeded, the next time-step interval is reduced by half; likewise, if the user-specified minimum percent loss is not achieved, the next time-step interval is increased by a factor of two. The instantaneous building concentration at time = t is calculated using Equation 10 for each time-step. The time-averaged building concentration is estimated using a trapezoidal approximation of the integral.

Model Assumptions and Limitations

The NAPL-SCREEN and NAPL-ADV models operate under the assumption that sufficient time has elapsed since the time of initial soil contamination for steady-state conditions to have been achieved. This means that the subsurface vapor plume has reached the bottom of the enclosed space floor and that the vapor concentration has reached its maximum value. An estimate of the time required to reach near steady-state conditions (τ_{ss}) can be made using the following equations from API (1998):

$$\tau_{ss} \cong \frac{R_v \theta_a L_T{}^2}{D^{eff}} \qquad (13)$$

and,

$$R_v = 1 + \frac{\theta_w}{\theta_a H'_{TS}} + \frac{\rho_b K_d}{\theta_a H'_{TS}} \qquad (14)$$

and,

$$D^{eff} = D_a \frac{\theta_a{}^{10/3}}{n^2} + \left(\frac{D_w}{H'_{TS}} \right) \frac{\theta_w{}^{10/3}}{n^2} \qquad (15)$$

where R_v is the unitless vapor phase retardation factor, L_T is the source-building separation (cm), D^{eff} is the effective diffusion coefficient (cm^2/s), D_a is the diffusivity in air (cm^2/s), D_w is the diffusivity in water (cm^2/s), and n is the soil total porosity (cm^3/cm^3). The NAPL-SCREEN and NAPL-ADV models are applicable only when the elapsed time since initial soil contamination meets or exceeds the value of τ_{ss} (see **Using the Models**).

Emission source depletion is calculated by estimating the rate of vapor loss as a function of time such that the mass lost at each time-step is subtracted from a finite mass of contamination at the source. This requires the model user to estimate the dimensions of the emission source, e.g., the length, width, and thickness of the contaminated zone. The model should only be used, therefore, when the extent of soil contamination has been sufficiently determined. It should be noted that because the NAPL-SCREEN and NAPL-ADV models are one-dimensional, the areal extent of soil contamination (i.e., length × width) can be less than but not greater than the areal extent of the building floor in contact with the soil.

Each model treats the contaminated zone directly below the building as a box containing a finite mass of each specified compound. The initial contamination contained within the box is assumed to be homogeneously distributed. After each time-step, the remaining contamination is assumed to be instantaneously redistributed within the box to homogeneous conditions. The diffusion path length from the top of contamination to the bottom of the enclosed space floor therefore remains constant with time. Use of this simplifying assumption means that the degree of NAPL soil saturation is not required in the calculation of the total overall effective diffusion coefficient (D_T^{eff}).

As time proceeds, the concentration of the mixture of compounds within the soil column may reach the soil saturation limit. Below this point, a residual phase will cease to exist and the vapor concentration of each chemical will decrease proportional to its total volume soil concentration. Theoretically, the vapor concentration will decrease asymptotically, approaching but never reaching zero. Because of the nature of the numerical solution to equilibrium vapor concentration, however, compounds with high effective diffusion coefficients (e.g., vinyl chloride) may reach zero soil concentrations while other less volatile contaminants will not. If the initial soil concentrations are significantly higher than their respective values of the soil saturation concentration, a residual phase may persist up to the user-defined exposure duration.

Model assumptions and limitations concerning vapor transport and vapor intrusion into buildings are those specified for the three-phase models.

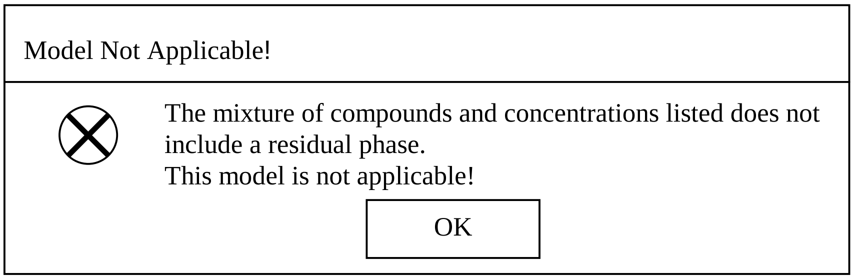
Using the Models

Each model is constructed as a Microsoft® Excel workbook containing five worksheets. The DATENTER worksheet is the data entry worksheet and also provides model results. The VLOOKUP worksheet contains the “Chemical Properties Lookup Table” with listed chemicals and associated chemical and toxicological properties. It should be noted that the toxicological properties for many of these chemicals were derived by route-to-route extrapolation. In addition, the VLOOKUP worksheet includes the “Soil Properties Lookup Table” containing values for model intermediate variables used in estimating the soil vapor permeability. The CHEMPROPS worksheet provides a summary of the chemical and toxicological properties of the soil contaminants selected by the user. In addition, the CHEMPROPS worksheet provides calculated values for the soil saturation concentration (C_{sat}) and the time to reach steady-state conditions (τ_{ss}) once all required data are entered into the DATENTER worksheet. The INTERCALCS worksheet contains calculated values of intermediate model variables. Finally, the COMPUTE worksheet contains the numerical solutions for equilibrium vapor concentration and building vapor concentration as a function of time.

Both models use the Microsoft® SOLVER add-in algorithms to simultaneously solve Equations 3 and 4 for each of up to 10 chemicals specified by the user. In order to run NAPL-SCREEN or NAPL-ADV, the SOLVER add-in <u>must</u> be loaded into EXCEL. The user is referred to the EXCEL instructions for loading the SOLVER add-in.

On the DATENTER worksheet, the user may specify up to 10 soil contaminants by CAS number along with associated soil concentrations in units of mg/kg. The CAS number entered must match exactly one of the 93 chemicals listed in the VLOOKUP worksheet or the error message "CAS No. not found" will appear in the "Chemical" box. If the list of chemicals and concentrations entered does not constitute a residual phase, the error message in Figure 1 will appear after starting the model.

Figure 1. Residual Phase Error Message



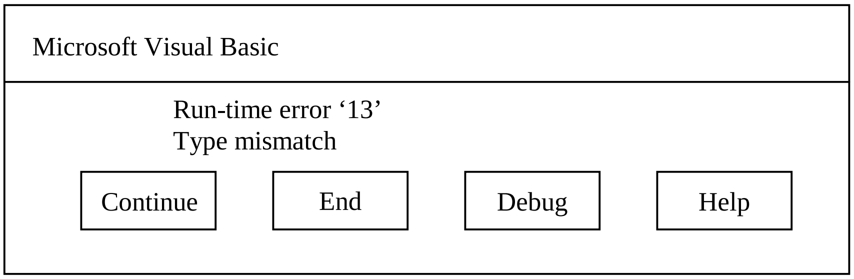
Model Not Applicable!

The mixture of compounds and concentrations listed does not include a residual phase.
This model is not applicable!

If this error message box appears, use either the SL-SCREEN or SL-ADV model to estimate subsurface vapor intrusion into the building.

After starting the model calculations, other error message boxes may appear if data entry values are missing on the DATENTER worksheet or if entered values do not conform to model assumptions. If such an error message box appears, fill-in missing data or re-enter data as appropriate. If entered data values are outside the expected range or if text values are entered where numeric values are expected, the model calculation macro will be suspended and the run-time error message in Figure 2 will appear.

Figure 2. Run-Time Error Message



Microsoft Visual Basic

Run-time error '13'
Type mismatch

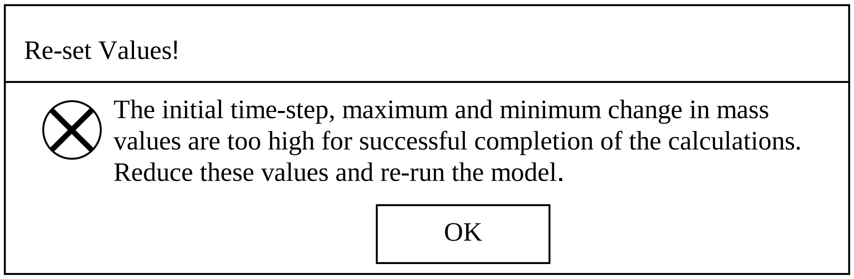
Should this error message appear, click on the "End" button to terminate the macro and return to the DATENTER worksheet. At this point, the user should review all of the entered values and make the appropriate corrections.

In addition to contaminant data, soil properties data, zone of contamination data, and exposure assumptions must also be specified in the DATENTER worksheet. Similar to the SL-SCREEN three-phase model, the NAPL-SCREEN model allows for only one soil stratum between the top of contamination and the bottom of the building floor in contact with the soil. In addition, the NAPL-SCREEN model uses built-in default values for all building variables (e.g., building dimensions, air exchange rate, total crack area, etc.). These default values are for single-family detached residences; therefore, the NAPL-SCREEN model should only be used for the residential exposure scenario.

The NAPL-ADV model, like the SL-ADV model, allows for up to three different soil strata between the top of contamination and the bottom of the building floor. In addition, the NAPL-ADV model allows the user to enter values for all model variables. This allows for the estimation of soil vapor intrusion into buildings other than single-family residences.

For each model, the user must also enter the duration of the first (initial) time-step interval. The maximum and minimum change in mass for each time-step must also be specified. The values of the initial time-step interval, and the maximum and minimum change in mass are important. If these values are too low, the model will calculate very small increments in the mass lost over time which will greatly extend the run-time of the model. In general, if the concentrations of the least volatile chemicals in the mixture are well above their respective values of the soil saturation concentration, a relatively large initial time-step interval, and maximum and minimum change in mass should be specified (e.g., 4 days, 10%, and 5%, respectively). For comparison, the value of the soil saturation concentration (C_{sat}) for each chemical specified by the user may be found in the CHEMPROPS worksheet after all data have been entered on the DATENTER worksheet. If, however, the soil concentrations of the most volatile constituents are very close to their respective saturation limits, large values of the initial time-step interval, and the maximum and minimum change in mass will result in the error message in Figure 3 after starting the model.

Figure 3. Time-Step and Change in Mass Error Message



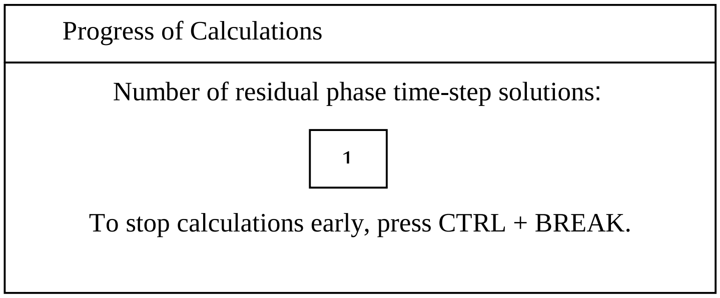
Re-set Values!

The initial time-step, maximum and minimum change in mass values are too high for successful completion of the calculations. Reduce these values and re-run the model.

Should this error message occur, reduce the value of the initial time-step interval and the values of the maximum and minimum change in mass to smaller values and re-run the model. The error message will be repeated until the values of these variables are sufficiently small.

After all required data are entered into the DATENTER worksheet, the model is run by clicking on the “Execute Model” button which will change from reading “Execute” to “Stand by...”. In addition, the message box in Figure 4 will appear keeping a running count of the number of residual phase time-step solutions achieved by the model.

Figure 4. Progress of Calculations Message Box



Progress of Calculations

Number of residual phase time-step solutions:

1

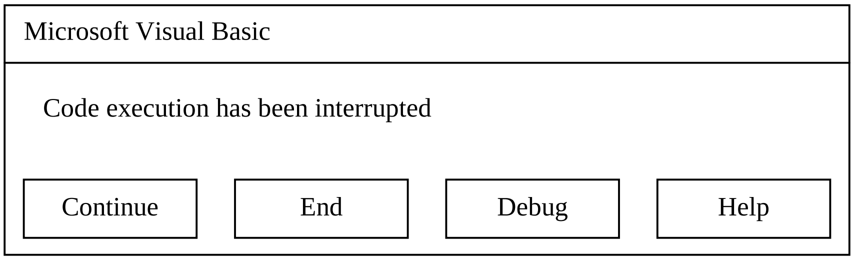
To stop calculations early, press CTRL + BREAK.

Each SOLVER trial solution can also be seen running in the status bar at the bottom of the screen. When the model is finished calculating, the “Execute Model” button will read “Done” and the Progress of Calculations message box in Figure 4 will disappear. The time-averaged building concentrations, incremental cancer risks, and/or hazard quotients will then be displayed under the “RESULTS” section of the DATENTER worksheet. In addition, an “X” will appear beside the calculated risk or hazard quotient of each contaminant for which a route-to-route extrapolation was employed. It should be noted that a route-to-route extrapolation was used for any chemical without a unit risk factor (URF) or a reference concentration (RfC). Therefore, the user should evaluate the resulting cancer risks and/or hazard quotients of such chemicals. Once a solution has been achieved and the user wishes to save the results, the file should be saved under a new file name. If the user wishes to delete all of the data previously entered on the DATENTER worksheet, this may be accomplished by clicking on the “Clear Data Entry Sheet” button.

Stopping Calculations Early

As mentioned previously, the user-defined values of the initial time-step interval, and the maximum and minimum change in mass should be chosen carefully. If the model run-time is excessive or if the user simply wishes to terminate the calculations, the model may be stopped by pressing CTRL + BREAK. If termination occurs in-between SOLVER solutions, the message box in Figure 5 will appear.

Figure 5. Code Interruption Message Box

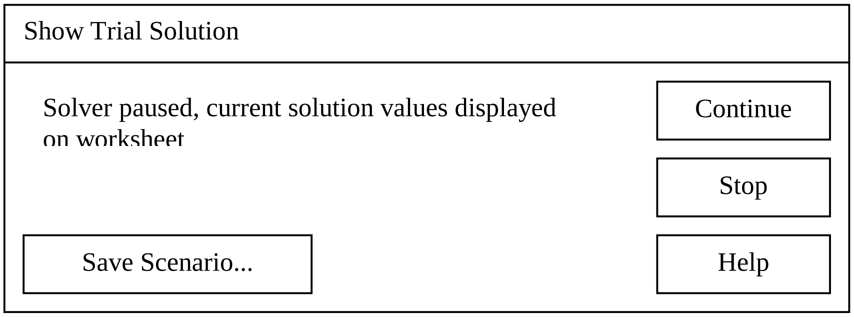


Code execution has been interrupted

If this message box appears, click on the “End” button to terminate the macro.

If the termination occurs during a SOLVER solution, the message box in Figure 6 will appear. If this message box appears, click on the “Stop” button. This will stop the SOLVER solution but not the program macro. Depending on where in the macro code the interruption occurs, the model may continue to operate after clicking on the “Stop” button in Figure 6. If this happens, press CTRL + BREAK again. At this point, the message box in Figure 5 will appear; click on the “End” button to terminate the macro.

Figure 6. Solver Interruption Message Box



Solver paused, current solution values displayed on worksheet

At this point, the user may examine the model results up to the point of termination on the COMPUTE worksheet. The values of the “Change in mass”, the “Time-step interval”, and the “Cumulative time” should be examined to determine if changes are necessary in the values of the initial time-step interval, and the maximum and minimum change in mass. After these or any other values are changed on the DATENTER worksheet, the model may be re-run by clicking on the “Execute Model” button.

Step-By-Step Procedures for Running the Models

The following gives the step-by-step procedures for running either the NAPL-SCREEN or the NAPL-ADV model.

1. On the DATENTER worksheet, enter the CAS number of each soil contaminant in the residual phase mixture (do not include dashes in the CAS numbers). After the CAS numbers have been entered, the respective chemical names will appear in the "Chemical" box.

2. On the DATENTER worksheet, enter the soil concentration of each contaminant in units of mg/kg as well as values for all remaining variables except the "Initial time-step", the "Maximum change in mass", and the "Minimum change in mass".

3. On the CHEMPROPS worksheet, note the calculated values of the "Time to steady state" (τ_{ss}) for each contaminant. Calculated values of the time-averaged building concentration and associated risks for contaminants with values of τ_{ss} greater than the actual elapsed time since initial soil contamination will be artificially high.

4. On the CHEMPROPS worksheet, note the calculated values of the "Soil saturation concentration" (C_{sat}) for each contaminant. Use these data to help determine appropriate user-defined values for the initial time-step, and the maximum and minimum change in mass. Typical values for these variables might be 2 days, 7%, and 4%, respectively, but may be considerably higher or lower depending on the number of chemicals in the analysis and the starting soil concentrations (see the discussion on page 8).

5. Click on the "Execute Model" button to begin the model calculations. If data are missing on the DATENTER worksheet, or entered values do not conform to model assumptions, an error message box will appear after the model is started informing the user of the type of error encountered. Enter the appropriate values on the DATENTER worksheet and re-run the model. Once the model has successfully started, note the number of residual phase time-step solutions achieved by the model in the Progress of Calculations message box (Figure 4). Use this information to help establish new values for the initial time-step interval and the maximum and minimum change in mass if the number of time-steps needs to be increased or decreased.

6. When the NAPL-SCREEN model has finished calculating, check column "O" on the COMPUTE worksheet to determine how many time-steps were calculated while a residual phase was present; one time-step is equal to one row (when using the NAPL-ADV model check column "P"). A residual phase is present when the value in column "O" or "P", as appropriate, is equal to 1.000. In general, a greater number of time-steps means a more accurate estimate of the time-averaged building concentration. If the starting soil concentrations of the most volatile contaminants are very close to their respective values of C_{sat}, a minimum of 5 to 10 time-steps should be calculated by the model. For all other cases, a reasonable number of time-steps is between 40 and 70. To increase the number of time-steps calculated by the model, decrease the values of the initial time-step interval and the maximum and minimum change in mass. The opposite is true when the number of time-steps is to be decreased.

7. If the message box in Figure 1 appears after starting the model, the mixture of compounds and concentrations specified does not include a residual phase. Use the SL-SCREEN or SL-ADV model to calculate indoor air concentrations and risks for each contaminant separately.

8. If the message box in Figure 3 appears after starting the model, reduce the input values of the initial time-step, and maximum and minimum change in mass and re-run the model.

9. If the run-time of the model is excessive, terminate the model macro by pressing CTRL + BREAK (see the discussion under **Stopping Calculations Early** on pages 9 and 10). Examine the calculated values of the "Change in mass", the "Time-step interval", and the "Cumulative time" on the COMPUTE worksheet. Re-enter new lower values for the initial time-step interval, and the maximum and minimum change in mass and re-run the model.

10. After successful completion of a model run, note the calculated values of the "Time-averaged building concentration", "Incremental cancer risk", and/or "Hazard quotient" in the "RESULTS" section of the DATENTER worksheet. Also note for which contaminants a route-to-route extrapolation was employed. If the model results are to be retained, save the file under a new file name.

Adding, Deleting or Revising Chemical Data

Additional chemicals can be listed in the "Chemical Properties Lookup Table" within the VLOOKUP worksheet. To add, delete or revise chemicals, the VLOOKUP worksheet must be unprotected using the password "ABC" in capital letters. Row number 171 is the last row that may be used to add new chemicals. If new chemicals are added or chemicals deleted, the user must sort all the data in the "Chemical Properties Lookup Table" (except the column headers) in ascending order by CAS number. After sorting is complete, the worksheet should again be protected.

APPENDIX B

CHEMICAL PROPERTIES LOOKUP TABLE AND REFERENCES

CAS No.	Chemical	Organic Carbon Partition Coefficient K_{oc} (cm^3/g)		Diffusivity in Air D_a (cm^2/s)		Diffusivity in Water D_w (cm^2/s)		Pure Component Water Solubility S (mg/L)		Henry's Law Constant H' (unitless)		Henry's Law Constant at Reference Temperature H (atm-m^3/mol)	Henry's Law Constant Reference Temperature T_R (^{o}C)	Normal Boiling Point T_B (^{o}K)		Critical Temperature T_C (^{o}K)		Enthalpy of Vaporization at the Normal Boiling Point deltaH$_{v,b}$ (cal/mol)		Unit Risk Factor URF (ug/m^3)$^{-1}$		Reference Concentration RfC (mg/m^3)		Density, r_i (g/cm^3)		Physical State at soil Temp (S,L,G)	Vapor Pressure VP (mm Hg)	Molecular Weight Mw (g/mole)		URF extrapolated (X)	Rfc extrapolated (X)
74873	Methyl chloride (chlorome	2.12E+00	2	1.26E-01	2	6.50E-06	2	5.33E+03	3	3.61E-01	3	8.80E-03	25	249.00	4	416.25	4	5.11E+03	4	1.00E-06	3	9.00E-02	3	0.9159	8	L	4.30E+03	5.05E+01	3		
74908	Hydrogen cyanide	3.80E+00	2	1.93E-01	2	2.10E-05	2	1.00E+06	3	5.44E-03	3	1.33E-04	25	299.00	4	456.70	4	6.68E+03	7	0.00E+00	3	3.00E-03	3	0.6876	4	L	7.42E+02	2.70E+01	3		
74953	Methylene bromide	1.26E+01	2	4.30E-02	2	8.44E-06	2	1.19E+04	3	3.52E-02	3	8.59E-04	25	370.00	4	583.00	6	7.87E+03	4	0.00E+00	3	3.50E-02	3	2.4969	4	L	4.44E+01	1.74E+02	3		X
75003	Chloroethane (ethyl chlori	4.40E+00	2	2.71E-01	2	1.15E-05	2	5.68E+03	3	3.61E-01	3	8.80E-03	25	285.30	4	460.40	4	5.88E+03	4	8.29E-07	3	1.00E+01	3	0.3242	8	L	1.01E+03	6.45E+01	3	X	
75014	Vinyl chloride (chloroethe	1.86E+01	1	1.06E-01	1	1.23E-05	1	8.80E+03	3	1.10E+00	3	2.69E-02	25	2.59E+02	1	4.32E+02	1	5.25E+03	1	8.80E-06	3	1.00E-01	3	9.11E-01	4	G	2.98E+03	6.25E+01	3		
75058	Acetonitrile	4.20E+00	2	1.28E-01	2	1.66E-05	2	1.00E+06	3	1.42E-03	3	3.45E-05	25	354.60	4	545.50	4	7.11E+03	4	0.00E+00	3	6.00E-02	3	0.7857	4	L	9.11E+01	4.11E+01	3		
75070	Acetaldehyde	1.06E+00	2	1.24E-01	2	1.41E-05	2	1.00E+06	3	3.23E-03	3	7.87E-05	25	293.10	4	466.00	4	6.16E+03	4	2.20E-06	3	9.00E-03	3	0.783	8	L	9.02E+02	4.41E+01	3		
75092	Methylene chloride	1.17E+01	1	1.01E-01	1	1.17E-05	1	1.30E+04	3	8.96E-02	3	2.18E-03	25	3.13E+02	1	5.10E+02	1	6.71E+03	1	4.70E-07	3	3.01E+00	3	1.33E+00	4	L	4.33E+02	8.49E+01	3		
75150	Carbon disulfide	4.57E+01	1	1.04E-01	1	1.00E-05	1	1.19E+03	3	1.24E+00	3	3.02E-02	25	3.19E+02	1	5.52E+02	1	6.39E+03	1	0.00E+00	3	7.00E-01	3	1.26E+00	4	L	3.59E+02	7.61E+01	3		
75218	Ethylene oxide	1.33E+00	2	1.04E-01	2	1.45E-05	2	3.04E+05	3	2.27E-02	3	5.54E-04	25	283.60	4	469.00	4	6.10E+03	4	1.00E-04	3	0.00E+00	3	0.3146	8	L	1.25E+03	4.41E+01	3		
75252	Bromoform	8.71E+01	1	1.49E-02	1	1.03E-05	1	3.10E+03	3	2.41E-02	3	5.88E-04	25	4.22E+02	1	6.96E+02	1	9.48E+03	1	1.10E-06	3	7.00E-02	3	2.90E+00	4	L	5.51E+00	2.53E+02	3		X
75274	Bromodichloromethane	5.50E+01	1	2.98E-02	1	1.06E-05	1	6.74E+03	3	6.54E-02	3	1.60E-03	25	3.63E+02	1	5.86E+02	1	7.80E+03	1	1.77E-05	3	7.00E-02	3	1.98E+00	4	L	5.00E+01	1.64E+02	3	X	X
75296	2-Chloropropane	9.14E+00	2	8.88E-02	2	1.01E-05	2	3.73E+03	3	5.93E-01	3	1.45E-02	25	308.70	4	485.00	6	6.29E+03	4	0.00E+00	3	1.02E-01	3	0.8617	4	L	5.23E+02	7.85E+01	3		
75343	1,1-Dichloroethane	3.16E+01	1	7.42E-02	1	1.05E-05	1	5.06E+03	3	2.30E-01	3	5.61E-03	25	3.31E+02	1	5.23E+02	1	6.90E+03	1	0.00E+00	3	5.00E-01	3	1.18E+00	4	L	2.27E+02	9.90E+01	3		
75354	1,1-Dichloroethylene	5.89E+01	1	9.00E-02	1	1.04E-05	1	2.25E+03	3	1.07E+00	3	2.60E-02	25	3.05E+02	1	5.76E+02	1	6.25E+03	1	0.00E+00	3	2.00E-01	3	1.21E+00	4	L	6.00E+02	9.69E+01	3		
75456	Chlorodifluoromethane	4.79E+01	2	1.01E-01	2	1.28E-05	2	2.00E+00	3	1.10E+00	3	2.70E-02	25	232.40	4	369.30	4	4.84E+03	6	0.00E+00	3	5.00E+01	3	1.209	8	L	7.48E+03	8.65E+01	3		
75694	Trichlorofluoromethane	4.97E+02	2	8.70E-02	2	9.70E-06	2	1.10E+03	3	3.97E+00	3	9.68E-02	25	296.70	4	471.00	6	6.00E+03	6*	0.00E+00	3	7.00E-01	3	1.4879	8	L	8.03E+02	1.37E+02	3		
75718	Dichlorodifluoromethane	4.57E+02	2	6.65E-02	2	9.92E-06	2	2.80E+02	3	1.40E+01	3	3.42E-01	25	243.20	4	384.95	4	9.42E+03	6	0.00E+00	3	2.00E-01	3	1.33	8	L	4.85E+03	1.21E+02	3		
76131	1,1,2-Trichloro-1,2,2-triflu	1.11E+04	2	7.80E-02	2	8.20E-06	2	1.70E+02	3	1.97E+01	3	4.80E-01	25	320.70	4	487.30	4	6.46E+03	4*	0.00E+00	3	3.01E+01	3	1.5635	8	L	3.32E+02	1.87E+02	3		
76448	Heptachlor	1.41E+06	1	1.12E-02	1	5.69E-06	1	1.80E-01	3	6.05E+01	3	1.48E+00	25	6.04E+02	1	8.46E+02	1	1.30E+04	1	1.30E-03	3	1.75E-03	3	NA	4	S	4.00E-04	3.73E+02	3		X
77474	Hexachlorocyclopentadie	2.00E+05	1	1.61E-02	1	7.21E-06	1	1.80E+00	3	1.10E+00	3	2.69E-02	25	5.12E+02	1	7.46E+02	1	1.09E+04	1	0.00E+00	3	2.00E-04	3	1.70E+00	4	L	6.00E-02	2.73E+02	3		
78831	Isobutanol	2.59E+00	2	8.60E-02	2	9.30E-06	2	8.50E+04	3	4.83E-04	3	1.18E-05	25	381.04	4	547.78	4	1.09E+04	6	0.00E+00	3	1.05E+00	3	0.8018	4	L	1.05E+01	7.41E+01	3		X
78875	1,2-Dichloropropane	4.37E+01	1	7.82E-02	1	8.73E-06	1	2.80E+03	3	1.15E-01	3	2.79E-03	25	3.70E+02	1	5.72E+02	1	7.59E+03	1	1.94E-05	3	4.00E-03	3	1.13E+00	4	L	5.20E+01	1.13E+02	3	X	
78933	Methylethylketone (2-buta	2.30E+00	2	8.08E-02	2	9.80E-06	2	2.23E+05	3	2.29E-03	3	5.58E-05	25	352.50	4	536.78	4	7.48E+03	4	0.00E+00	3	5.00E+00	3	0.8054	4	L	9.53E+01	7.21E+01	3		
79005	1,1,2-Trichloroethane	5.01E+01	1	7.80E-02	1	8.80E-06	1	4.42E+03	3	3.73E-02	3	9.11E-04	25	3.86E+02	1	6.02E+02	1	8.32E+03	1	1.60E-05	3	1.40E-02	3	1.44E+00	4	L	2.33E+01	1.33E+02	3		X
79016	Trichloroethylene	1.66E+02	1	7.90E-02	1	9.10E-06	1	1.47E+03	3	4.21E-01	3	1.03E-02	25	3.60E+02	1	5.44E+02	1	7.51E+03	1	1.10E-04	3	4.00E-02	3	1.46E+00	4	L	7.35E+01	1.31E+02	3	X	
79209	Methyl acetate	3.26E+00	2	1.04E-01	2	1.00E-05	2	2.00E+03	3	4.84E-03	3	1.18E-04	25	329.80	4	506.70	6	7.26E+03	6	0.00E+00	3	3.50E+00	3	0.9342	4	L	2.35E+02	7.41E+01	3		X
79345	1,1,2,2-Tetrachloroethane	9.33E+01	1	7.10E-02	1	7.90E-06	1	2.96E+03	3	1.41E-02	3	3.44E-04	25	4.20E+02	1	6.61E+02	1	9.00E+03	1	5.80E-05	3	2.10E-01	3	1.60E+00	4	L	4.62E+00	1.68E+02	3		X
79469	2-Nitropropane	1.17E+01	2	9.23E-02	2	1.01E-05	2	1.70E+04	3	5.03E-03	3	1.23E-04	25	393.20	4	594.00	8	8.38E+03	8	2.69E-03	3	2.00E-02	3	0.9876	8	L	1.80E+01	8.91E+01	3		
80626	Methylmethacrylate	6.98E+00	2	7.70E-02	2	8.60E-06	2	1.50E+04	3	1.38E-02	3	3.36E-04	25	373.50	4	567.00	6	8.97E+03	6	0.00E+00	3	7.00E-01	3	0.944	4	L	3.84E+01	1.00E+02	3		
83329	Acenaphthene	7.08E+03	1	4.21E-02	1	7.69E-06	1	3.57E+00	3	6.34E-03	3	1.55E-04	25	5.51E+02	1	8.03E+02	1	1.22E+04	1	0.00E+00	3	2.10E-01	3	NA	4	S	2.50E-03	1.54E+02	3		X
86737	Fluorene	1.38E+04	1	3.63E-02	1	7.88E-06	1	1.98E+00	3	2.60E-03	3	6.34E-05	25	5.70E+02	1	8.70E+02	1	1.27E+04	1	0.00E+00	3	1.40E-01	3	NA	4	S	6.33E-04	1.66E+02	3		X
87683	Hexachloro-1,3-butadiene	5.37E+04	1	5.61E-02	1	6.16E-06	1	3.20E+00	3	3.33E-01	3	8.13E-03	25	4.86E+02	1	7.38E+02	1	1.02E+04	1	2.20E-05	3	7.00E-04	3	1.56E+00	4	L	2.21E-01	2.61E+02	3		X
88722	o-Nitrotoluene	3.24E+02	2	5.87E-02	2	8.67E-06	2	6.50E+02	3	5.11E-04	3	1.25E-05	25	495.00	4	720.00	8	1.22E+04	6	0.00E+00	3	3.50E-02	3	1.163	8	L	4.50E-02	1.37E+02	3		X
91203	Naphthalene	2.00E+03	1	5.90E-02	1	7.50E-06	1	3.10E+01	3	1.98E-02	3	4.82E-04	25	4.91E+02	1	7.48E+02	1	1.04E+04	1	0.00E+00	3	3.00E-03	3	NA	4	S	8.50E-02	1.28E+02	3		
91576	2-Methylnaphthalene	2.81E+03	2	5.22E-02	2	7.75E-06	2	2.46E+01	3	2.12E-02	3	5.17E-04	25	514.26	4	761.00	4	1.26E+04	8	0.00E+00	3	7.00E-02	3	1.0058	4	S	5.50E-02	1.42E+02	3		X
92524	Biphenyl	4.38E+03	2	4.04E-02	2	8.15E-06	2	7.45E+00	3	1.23E-02	3	2.99E-04	25	529.10	4	789.00	4	1.09E+04	8	0.00E+00	3	1.75E-01	3	1.04	4	S	9.64E-03	1.54E+02	3		X
95476	o-Xylene	3.63E+02	1	8.70E-02	1	1.00E-05	1	1.78E+02	3	2.12E-01	3	5.18E-03	25	4.18E+02	1	6.30E+02	1	8.66E+03	1	0.00E+00	3	1.00E-01	3	8.80E-01	4	L	6.61E+00	1.06E+02	3		
95501	1,2-Dichlorobenzene	6.17E+02	1	6.90E-02	1	7.90E-06	1	1.56E+02	3	7.77E-02	3	1.90E-03	25	4.54E+02	1	7.05E+02	1	9.70E+03	1	0.00E+00	3	2.00E-01	3	1.31E+00	4	L	1.36E+00	1.47E+02	3		
95578	2-Chlorophenol	3.88E+02	1	5.01E-02	1	9.46E-06	1	2.20E+04	3	1.60E-02	3	3.90E-04	25	4.48E+02	1	6.75E+02	1	9.57E+03	1	0.00E+00	3	1.75E-02	3	1.26E+00	4	L	2.34E+00	1.29E+02	3		X
95636	1,2,4-Trimethylbenzene	1.35E+03	2	6.06E-02	2	7.92E-06	2	5.70E+01	3	2.52E-01	3	6.14E-03	25	442.30	4	649.17	4	9.37E+03	6	0.00E+00	3	5.95E-03	3	0.8758	4	L	2.10E+00	1.20E+02	3		
96184	1,2,3-Trichloropropane	2.20E+01	2	7.10E-02	2	7.90E-06	2	1.75E+03	3	1.67E-02	3	4.08E-04	25	430.00	4	652.00	6	9.17E+03	8	5.71E-04	3	4.90E-03	3	1.3889	4	L	3.69E+00	1.47E+02	3	X	
96333	Methyl acrylate	4.53E+00	2	9.76E-02	2	1.02E-05	2	6.00E+04	3	7.68E-03	3	1.87E-04	25	353.70	4	536.00	7	7.75E+03	7	0.00E+00	3	1.05E-01	3	0.9535	4	L	8.80E+01	8.61E+01	3		X
97632	Ethylmethacrylate	2.95E+01	2	6.53E-02	2	8.37E-06	2	3.67E+03	3	3.44E-02	3	8.40E-04	25	390.00	4	571.00	8	1.10E+04	6	0.00E+00	3	3.15E-01	3	0.9135	4	L	2.06E+01	1.14E+02	3		X
98066	tert-Butylbenzene	7.71E+02	2	5.65E-02	2	8.02E-06	2	2.95E+01	3	4.87E-01	3	1.19E-02	25	442.10	4	1220.00	9	8.98E+03	8	0.00E+00	3	1.40E-01	3	0.8665	4	L	2.20E+00	1.34E+02	3		X
98828	Cumene	4.89E+02	2	6.50E-02	2	7.10E-06	2	6.13E+01	3	4.74E+01	3	1.46E-02	25	425.56	4	631.10	4	1.03E+04	6	0.00E+00	3	4.00E-01	3	0.8618	4	L	4.50E+00	1.20E+02	3		
98862	Acetophenone	5.77E+01	2	6.00E-02	2	8.73E-06	2	6.13E+03	3	4.38E-04	3	1.07E-05	25	475.00	4	709.50	4	1.17E+04	6	0.00E+00	3	3.50E-01	3	1.0281	4	S,L	3.97E-01	1.20E+02	3		X
98953	Nitrobenzene	6.46E+01	1	7.60E-02	1	8.60E-06	1	2.09E+03	3	9.82E-04	3	2.39E-05	25	4.84E+02	1	7.19E+02	1	1.06E+04	1	0.00E+00	3	2.00E-03	3	1.20E+00	4	L	2.45E-01	1.23E+02	3		
100414	Ethylbenzene	3.63E+02	1	7.50E-02	1	7.80E-06	1	1.69E+02	3	3.22E-01	3	7.86E-03	25	4.09E+02	1	6.17E+02	1	8.50E+03	1	0.00E+00	3	1.00E+00	3	8.67E-01	4	L	9.60E+00	1.06E+02	3		
100425	Styrene	7.76E+02	1	7.10E-02	1	8.00E-06	1	3.10E+02	3	1.12E-01	3	2.74E-03	25	4.18E+02	1	6.36E+02	1	8.74E+03	1	0.00E+00	3	1.00E+00	3	9.06E-01	4	L	6.12E+00	1.04E+02	3		
100447	Benzylchloride	6.14E+01	2	7.50E-02	2	7.80E-06	2	5.25E+02	3	1.70E-02	3	4.14E-04	25	452.00	4	685.00	8	8.77E+03	6	4.86E-05	3	0.00E+00	3	1.1004	4	L	1.31E+00	1.27E+02	3	X	
100527	Benzaldehyde	4.59E+01	2	7.21E-02	2	9.07E-06	2	3.30E+03	3	9.73E-04	3	2.37E-05	25	452.00	4	695.00	4	1.17E+04	6	0.00E+00	3	3.50E-01	3	1.0415	4	L	9.00E-01	1.06E+02	3		X
103651	n-Propylbenzene	5.62E+02	2	6.01E-02	2	7.83E-06	2	6.00E+01	3	4.37E-01	3	1.07E-02	25	432.20	4	630.00	4	9.12E+03	8	0.00E+00	3	1.40E-01	3	0.862	4	L	2.50E+00	1.20E+02	3		X
104518	n-Butylbenzene	1.11E+03	2	5.70E-02	2	8.12E-06	2	2.00E+00	3	5.38E-01	3	1.31E-02	25	456.46	4	660.50	4	9.29E+03	4	0.00E+00	3	1.40E-01	3	0.8601	4	L	1.00E+00	1.34E+02	3		X
106423	p-Xylene	3.89E+02	1	7.69E-02	1	8.44E-06	1	1.85E+02	3	3.13E-01	3	7.64E-03	25	4.12E+02	1	6.16E+02	1	8.53E+03	1	0.00E+00	3	1.00E-01	3	8.61E-01	4	L	8.90E+00	1.06E+02	3		
106467	1,4-Dichlorobenzene	6.17E+02	1	6.90E-02	1	7.90E-06	1	7.90E+01	3	9.82E-02	3	2.39E-03	25	4.47E+02	1	6.85E+02	1	9.27E+03	1	0.00E+00	3	8.00E-01	3	NA	4	S	1.00E+00	1.47E+02	3		
106934	1,2-Dibromoethane (ethyl	2.50E+01	2	2.17E-02	2	1.19E-05	2	4.18E+03	3	3.04E-02	3	7.41E-04	25	404.60	4	583.00	4	8.31E+03	4	2.20E-04	3	2.00E-04	3	2.1791	4	L	1.33E+01	1.88E+02	3		
106990	1,3-Butadiene	1.91E+01	2	2.49E-01	2	1.08E-05	2	7.35E+02	3	3.01E+00	3	7.34E-02	25	268.60	4	425.00	4	5.37E+03	4	3.00E-02	3	2.00E-03	3	0.29315	8	L	2.11E+03	5.41E+01	3		
107028	Acrolein	2.76E+00	2	1.05E-01	2	1.22E-05	2	2.13E+05	3	4.99E-03	3	1.22E-04	25	325.60	4	506.00	8	6.73E+03	6	0.00E+00	3	2.00E-05	3	0.84	4	L	2.74E+02	5.61E+01	3		
107062	1,2-Dichloroethane	1.74E+01	1	1.04E-01	1	9.90E-06	1	8.52E+03	3	4.00E-02	3	9.77E-04	25	3.57E+02	1	5.61E+02	1	7.64E+03	1	2.60E-05	3	0.00E+00	3	1.24E+00	4	L	7.89E+01	9.90E+01	3		
107131	Acrylonitrile	5.90E+00	2	1.22E-01	2	1.34E-05	2	7.40E+04	3	4.21E-03	3	1.03E-04	25	350.30	4	519.00	6	7.79E+03	8	6.80E-05	3	2.00E-03	3	0.806	4	L	1.09E+02	5.31E+01	3		
108054	Vinyl acetate	5.25E+00	1	8.50E-02	1	9.20E-06	1	2.00E+04	3	2.09E-02	3	5.10E-04	25	3.46E+02	1	5.19E+02	1	7.80E+03	1	0.00E+00	3	2.00E-01	3	9.32E-01	4	L	9.02E+01	8.61E+01	3		
108101	Methylisobutylketone (4-m	9.06E+00	2	7.50E-02	2	7.80E-06	2	1.90E+04	3	5.64E-03	3	1.38E-04	25	389.50	4	571.00	4	8.24E+03	4	0.00E+00	3	3.00E+00	3	0.7978	4	L	1.99E+01	1.00E+02	3		
108383	m-Xylene	4.07E+02	1	7.00E-02	1	7.80E-06	1	1.61E+02	3	3.00E-01	3	7.32E-03	25	4.12E+02	1	6.17E+02	1	8.52E+03	1	0.00E+00	3	1.00E-01	3	8.64E-01	4	L	8.45E+00	1.06E+02	3		
108678	1,3,5-Trimethylbenzene	1.35E+03	2	6.02E-02	2	8.67E-06	2	2.00E+00	3	2.41E-01	3	5.87E-03	25	437.89	4	637.25	4	9.32E+03	6	0.00E+00	3	5.95E-03	3	0.8652	4	L	2.40E+00	1.20E+02	3		
108872	Methylcyclohexane	7.85E+01	2	7.35E-02	2	8.52E-06	2	1.40E+01	3	4.22E+00	3	1.03E-01	25	373.90	4	572.20	4	7.47E+03	4	0.00E+00	3	3.01E+00	3	0.7694	4	L	4.30E+01	9.82E+01	3		
108883	Toluene	1.82E+02	1	8.70E-02	1	8.60E-06	1	5.26E+02	3	2.72E-01	3	6.62E-03	25	3.84E+02	1	5.92E+02	1	7.93E+03	1	0.00E+00	3	4.00E-01	3	8.67E-01	4	L	2.84E+01	9.21E+01	3		
108907	Chlorobenzene	2.19E+02	1	7.30E-02	1	8.70E-06	1	4.72E+02	3	1.51E-01	3	3.69E-03	25	4.05E+02	1	6.32E+02	1	8.41E+03	1	0.00E+00	3	5.95E-02	3	1.11E+00	4	L	1.20E+01	1.13E+02	3		
109693	1-Chlorobutane	1.72E+01	2	8.26E-02	2	1.00E-05	2	1.10E+03	3	6.93E-01	3	1.69E-02	25	351.60	4	542.00	6	7.26E+03	4	0.00E+00	3	1.40E+00	3	0.8862	4	L	1.01E+02	9.26E+01	3		X
110009	Furan	1.86E+01	2	1.04E-01	2	1.22E-05	2	1.00E+04	3	2.21E-01	3	5.39E-03	25	304.60	4	490.20	4	6.48E+03	4	0.00E+00	3	3.50E-03	3	0.9514	4	L	6.00E+02	6.81E+01	3		X
110543	Hexane	4.34E+01	2	2.00E-01	2	7.77E-06	2	1.24E+01	3	6.82E+01	3	1.66E+00	25	341.70	4	508.00	4	6.90E+03	4	0.00E+00	3	2.00E-01	3	0.6548	4	L	1.51E+02	8.62E+01	3		
111444	Bis(2-chloroethyl)ether	1.55E+01	1	6.92E-02	1	7.53E-06	1	1.72E+04	3	7.36E-04	3	1.80E-05	25	4.51E+02	1	6.60E+02	1	1.08E+04	1	3.30E-04	3	0.00E+00	3	1.22E+00	4	L	1.55E+00	1.43E+02	3		
115297	Endosulfan	2.14E+03	1	1.15E-02	1	4.55E-06	1	5.10E-01	3	4.58E-04	3	1.12E-05	25	6.74E+02	1	9.43E+02	1	1.40E+04	1	0.00E+00	3	2.10E-02	3	NA	4	S	1.00E-05	4.07E+02	3		X
118741	Hexachlorobenzene	5.50E+04	1	5.42E-02	1	5.91E-06	1	5.00E-03	3	5.40E-02	3	1.32E-03	25	5.83E+02	1	8.25E+02	1	1.44E+04	1	4.60E-04	3	2.80E-03	3	NA	4	S	1.80E-05	2.85E+02	3		X
120821	1,2,4-Trichlorobenzene	1.78E+03	1	3.00E-02	1	8.23E-06	1	4.88E+01	3	5.81E-02	3	1.42E-03	25	4.86E+02	1	7.25E+02	1	1.05E+04	1	0.00E+00	3	4.00E-03	3	1.46E+00	4	L	4.31E-01	1.81E+02	3		
123739	Crotonaldehyde (2-butena	4.82E+00	2	9.56E-02	2	1.07E-05	2	3.69E+04	3	7.99E-04	3	1.95E-05	25	375.20	4	568.00	7	8.62E+00	5	5.43E-04	3	0.00E+00	3	0.8516	4	L	7.81E+00	7.01E+01	3	X	
124481	Chlorodibromomethane	6.31E+01	1	1.96E-02	1	1.05E-05	1	2.60E+03	3	3.20E-02	3	7.81E-04	25	4.16E+02	1	6.78E+02	1	5.90E+03	1	2.40E-05	3	7.00E-02	3	2.45E+00	4	L	4.90E+00	2.08E+02	3	X	X
126987	Methacrylonitrile	3.58E+01	2	1.12E-01	2	1.32E-05	2	2.54E+04	3	1.01E-02	3	2.46E-04	25	363.30	4	554.00	8	7.60E+03	6	0.00E+00	3	7.00E-04	3	0.8001	4	L	7.12E+01	6.71E+01	3		
126998	2-Chloro-1,3-butadiene (c	6.73E+01	2	8.58E-02	2	1.03E-05	2	2.12E+03	3	4.91E-01	3	1.20E-02	25	332.40	4	525.00	8	8.07E+03	7	0.00E+00	3	7.00E-03	3	0.956	4	L	2.18E+02	8.85E+01	3		
127184	Tetrachloroethylene	1.55E+02	1	7.20E-02	1	8.20E-06	1	2.00E+02	3	7.53E-01	3	1.84E-02	25	3.94E+02	1	6.20E+02	1	8.29E+03	1	5.90E-06	3	6.00E-01	3	1.62E+00	4	L	1.86E+01	1.66E+02	3		
129000	Pyrene	1.05E+05	1	2.72E-02	1	7.24E-06	1	1.35E+00	3	4.50E-04	3	1.10E-05	25	6.68E+02	1	9.36E+02	1	1.44E+04	1	0.00E+00	3	1.05E-01	3	NA	4	S	4.59E-06	2.02E+02	3		X
132649	Dibenzofuran	5.15E+03	2	2.38E-02	2	6.00E-06	2	3.10E+00	3	5.15E-04	3	1.26E-05	25	560.00	4	824.00	6	6.64E+04	6*	0.00E+00	3	1.40E-02	3	1.1679	8	S	1.80E-04	1.68E+02	3		X

CAS No.	Chemical	Organic Carbon Partition Coefficient K_{oc} (cm^3/g)		Diffusivity in Air D_a (cm^2/s)		Diffusivity in Water D_w (cm^2/s)		Pure Component Water Solubility S (mg/L)		Henry's Law Constant H' (unitless)		Henry's Law Constant at Reference Temperature H (atm-m^3/mol)	Henry's Law Constant Reference Temperature T_R (^oC)	Normal Boiling Point T_B (^oK)		Critical Temperature T_C (^oK)		Enthalpy of Vaporization at the Normal Boiling Point deltaH$_{v,b}$ (cal/mol)		Unit Risk Factor URF (ug/m^3)$^{-1}$		Reference Concentration RfC (mg/m^3)		Density, r_i (g/cm^3)		Physical State at soil Temp (S,L,G)	Vapor Pressure VP (mm Hg)	Molecular Weight Mw (g/mole)		URF extrapolated (X)	Rfc extrapolated (X)
135988	sec-Butylbenzene	9.66E+02	2	5.70E-02	2	8.12E-06	2	3.94E+00	3	5.68E-01	3	1.39E-02	25	446.50	4	679.00	9	8.87E+04	8	0.00E+00	3	1.40E-01	3	0.8621	8	L	3.10E-01	1.34E+02	3		X
141786	Ethylacetate	6.44E+00	2	7.32E-02	2	9.70E-06	2	8.03E+04	3	5.64E-03	3	1.38E-04	25	350.26	4	523.30	4	7.63E+03	4	0.00E+00	3	3.15E+00	3	0.9003	4	L	9.37E+01	8.81E+01	3		X
156592	cis-1,2-Dichloroethylene	3.55E+01	1	7.36E-02	1	1.13E-05	1	3.50E+03	3	1.67E-01	3	4.07E-03	25	3.34E+02	1	5.44E+02	1	7.19E+03	1	0.00E+00	3	3.50E-02	3	1.28E+00	4	L	2.03E+02	9.69E+01	3		X
156605	trans-1,2-Dichloroethylene	5.25E+01	1	7.07E-02	1	1.19E-05	1	6.30E+03	3	3.84E-01	3	9.36E-03	25	3.21E+02	1	5.17E+02	1	6.72E+03	1	0.00E+00	3	7.00E-02	3	1.26E+00	4	L	3.33E+02	9.69E+01	3		X
205992	Benzo(b)fluoranthene	1.23E+06	1	2.26E-02	1	5.56E-06	1	1.50E-03	3	4.54E-03	3	1.11E-04	25	7.16E+02	1	9.69E+02	1	1.70E+04	1	2.09E-04	3	0.00E+00	3	NA	4	S	5.00E-07	2.52E+02	3	X	
218019	Chrysene	3.98E+05	1	2.48E-02	1	6.21E-06	1	6.30E-03	3	3.87E-03	3	9.44E-05	25	7.14E+02	1	9.79E+02	1	1.65E+04	1	2.09E-06	3	0.00E+00	3	NA	4	S	6.23E-09	2.28E+02	3	X	
309002	Aldrin	2.45E+06	1	1.32E-02	1	4.86E-06	1	1.70E-02	3	6.95E-03	3	1.70E-04	25	6.03E+02	1	8.39E+02	1	1.50E+04	1	4.90E-03	3	1.05E-04	3	NA	4	S	6.00E-06	3.65E+02	3		X
319846	alpha-HCH (alpha-BHC)	1.23E+03	1	1.42E-02	1	7.34E-06	1	2.00E+00	3	4.34E-04	3	1.06E-05	25	5.97E+02	1	8.39E+02	1	1.50E+04	1	1.80E-03	3	0.00E+00	3	NA	4	S	4.50E-05	2.91E+02	3		
541731	1,3-Dichlorobenzene	1.98E+03	2	6.92E-02	2	7.86E-06	2	1.34E+02	3	1.27E-01	3	3.09E-03	25	446.00	4	684.00	8	9.23E+03	4	0.00E+00	3	1.05E-01	3	1.2884	4	L	2.15E+00	1.47E+02	3		X
542756	1,3-Dichloropropene	4.57E+01	1	6.26E-02	1	1.00E-05	1	2.80E+03	3	7.24E-01	3	1.77E-02	25	3.81E+02	1	5.87E+02	1	7.90E+03	1	4.00E-06	3	2.00E-02	3	1.22E+00	4	L	3.40E+01	1.11E+02	3		
630206	1,1,1,2-Tetrachloroethane	1.16E+02	2	7.10E-02	2	7.90E-06	2	1.10E+03	3	9.90E-02	3	2.41E-03	25	4.04E+02	4	6.24E+02	6	9.77E+03	6	7.40E-06	3	1.05E-01	3	1.54E+00	4	L	1.20E+01	1.68E+02	3		X
1634044	MTBE	7.26E+00	2	1.02E-01	2	1.05E-05	2	5.10E+04	3	2.56E-02	3	6.23E-04	25	328.30	4	497.10	4	6.68E+03	4	0.00E+00	3	3.00E+00	3	0.7405	4	L	2.50E+02	8.82E+01	3		
7439976	Mercury (elemental)	5.20E+01	1	3.07E-02	1	6.30E-06	1	2.00E+01	3	4.40E-01	3	1.07E-02	25	6.30E+02	1	1.75E+03	1	1.41E+04	1	0.00E+00	3	3.00E-04	3	1.35E+01	4	L	2.00E-03	2.01E+02	3		

<u>Sources:</u>

1 User's Guide for the Johnson and Ettinger (1991) Model for Subsurface Vapor Intrusion Into Buildings (Revised), December, 2000
2 Water9 Database
3 VI Draft Guidance, November 2002
4 CRC Handbook of Chemistry and Physics, 76th Edition
5 The Merck Index, 10th Edition
6 Hazardous Substances Data Bank, February 2003 http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB
7 Weiss, G., Hazardous Chemicals Data Book, Second Edition. Noyes Data Corporation. 1986.
8 DECHEMA Web Datbase, March 2003 http://I-systems.dechema.de/
9 Flexware Engineering Solutions for Industry, Properties of Various Gases www.flexwareinc.com/gasprop.htm

* For enthalpy of vaporization, highlighted values are enthalpy of vaporization at value other than normal boiling point.
For density, highlighted values are taken at temperature other than 20^{o}C.

APPENDIX C

EXAMPLE WORKSHEETS FOR THE ADVANCED SOIL CONTAMINATION MODEL

DATA ENTRY SHEET

SL-ADV
Version 3.1; 02/04

Reset to Defaults

CALCULATE RISK-BASED SOIL CONCENTRATION (enter "X" in "YES" box)

YES ☒ X

OR

CALCULATE INCREMENTAL RISKS FROM ACTUAL SOIL CONCENTRATION (enter "X" in "YES" box and initial soil conc. below)

YES ☐

ENTER Chemical CAS No. (numbers only, no dashes)	**ENTER** Initial soil conc., C_R (µg/kg)		Chemical
71432			Benzene

MORE ↓

ENTER Average soil temperature, T_S (^oC)	**ENTER** Depth below grade to bottom of enclosed space floor, L_F (cm)	**ENTER** Depth below grade to top of contamination, L_t (cm)	**ENTER** Depth below grade to bottom of contamination, (enter value of 0 if value is unknown) L_b (cm)	**ENTER** Totals must add up to value of L_t (cell G28) Thickness of soil stratum A, h_A (cm)	**ENTER** Thickness of soil stratum B, (Enter value or 0) h_B (cm)	**ENTER** Thickness of soil stratum C, (Enter value or 0) h_C (cm)	**ENTER** Soil stratum A SCS soil type (used to estimate soil vapor permeability)		**ENTER** User-defined stratum A soil vapor permeability, k_v (cm^2)
10	200	400	600	200	100	100	L	OR	

MORE ↓

ENTER Stratum A SCS soil type Lookup Soil Parameters	**ENTER** Stratum A soil dry bulk density, ρ_b^A (g/cm^3)	**ENTER** Stratum A soil total porosity, n^A (unitless)	**ENTER** Stratum A soil water-filled porosity, θ_w^A (cm^3/cm^3)	**ENTER** Stratum A soil organic carbon fraction, f_{oc}^A (unitless)	**ENTER** Stratum B SCS soil type Lookup Soil Parameters	**ENTER** Stratum B soil dry bulk density, ρ_b^B (g/cm^3)	**ENTER** Stratum B soil total porosity, n^B (unitless)	**ENTER** Stratum B soil water-filled porosity, θ_w^B (cm^3/cm^3)	**ENTER** Stratum B soil organic carbon fraction, f_{oc}^B (unitless)	**ENTER** Stratum C SCS soil type Lookup Soil Parameters	**ENTER** Stratum C soil dry bulk density, ρ_b^C (g/cm^3)	**ENTER** Stratum C soil total porosity, n^C (unitless)	**ENTER** Stratum C soil water-filled porosity, θ_w^C (cm^3/cm^3)	**ENTER** Stratum C soil organic carbon fraction, f_{oc}^C (unitless)
L	1.59	0.399	0.148	0.002	L	1.59	0.399	0.148	0.002	S	1.66	0.375	0.054	0.002

MORE ↓

ENTER Enclosed space floor thickness, L_{crack} (cm)	**ENTER** Soil-bldg. pressure differential, ΔP ($g/cm\text{-}s^2$)	**ENTER** Enclosed space floor length, L_B (cm)	**ENTER** Enclosed space floor width, W_B (cm)	**ENTER** Enclosed space height, H_B (cm)	**ENTER** Floor-wall seam crack width, w (cm)	**ENTER** Indoor air exchange rate, ER (1/h)	**ENTER** Average vapor flow rate into bldg. OR Leave blank to calculate Q_{soil} (L/m)
10	40	1000	1000	366	0.1	0.25	5

ENTER Averaging time for carcinogens, AT_C (yrs)	**ENTER** Averaging time for noncarcinogens, AT_{NC} (yrs)	**ENTER** Exposure duration, ED (yrs)	**ENTER** Exposure frequency, EF (days/yr)	**ENTER** Target risk for carcinogens, TR (unitless)	**ENTER** Target hazard quotient for noncarcinogens, THQ (unitless)
70	30	30	350	1.0E-06	1
				Used to calculate risk-based soil concentration.	

END

CHEMICAL PROPERTIES SHEET

Diffusivity in air, D_a (cm^2/s)	Diffusivity in water, D_w (cm^2/s)	Henry's law constant at reference temperature, H ($atm\text{-}m^3/mol$)	Henry's law constant reference temperature, T_R (^oC)	Enthalpy of vaporization at the normal boiling point, $\Delta H_{v,b}$ (cal/mol)	Normal boiling point, T_B (^oK)	Critical temperature, T_C (^oK)	Organic carbon partition coefficient, K_{oc} (cm^3/g)	Pure component water solubility, S (mg/L)	Unit risk factor, URF ($\mu g/m^3)^{-1}$	Reference conc., RfC (mg/m^3)	Physical state at soil temperature, (S,L,G)
8.80E-02	9.80E-06	5.54E-03	25	7,342	353.24	562.16	5.89E+01	1.79E+03	7.8E-06	3.0E-02	L

END

INTERMEDIATE CALCULATIONS SHEET

Exposure duration, τ (sec)	Source-building separation, L_T (cm)	Stratum A soil air-filled porosity, θ_a^A (cm^3/cm^3)	Stratum B soil air-filled porosity, θ_a^B (cm^3/cm^3)	Stratum C soil air-filled porosity, θ_a^C (cm^3/cm^3)	Stratum A effective total fluid saturation, S_{te} (cm^3/cm^3)	Stratum A soil intrinsic permeability, k_i (cm^2)	Stratum A soil relative air permeability, k_{rg} (cm^2)	Stratum A soil effective vapor permeability, k_v (cm^2)	Floor-wall seam perimeter, X_{crack} (cm)	Initial soil concentration used, C_R ($\mu g/kg$)	Bldg. ventilation rate, $Q_{building}$ (cm^3/s)
9.46E+08	200	0.251	0.251	0.321	0.257	1.85E-09	0.854	1.58E-09	4,000	1.00E+00	2.54E+04

Area of enclosed space below grade, A_B (cm^2)	Crack-to-total area ratio, η (unitless)	Crack depth below grade, Z_{crack} (cm)	Enthalpy of vaporization at ave. soil temperature, $\Delta H_{v,TS}$ (cal/mol)	Henry's law constant at ave. soil temperature, H_{TS} ($atm\text{-}m^3/mol$)	Henry's law constant at ave. soil temperature, H'_{TS} (unitless)	Vapor viscosity at ave. soil temperature, μ_{TS} (g/cm-s)	Stratum A effective diffusion coefficient, $D^{eff}{}_A$ (cm^2/s)	Stratum B effective diffusion coefficient, $D^{eff}{}_B$ (cm^2/s)	Stratum C effective diffusion coefficient, $D^{eff}{}_C$ (cm^2/s)	Total overall effective diffusion coefficient, $D^{eff}{}_T$ (cm^2/s)	Diffusion path length, L_d (cm)	Convection path length, L_p (cm)
1.80E+06	2.22E-04	200	8,122	2.68E-03	1.15E-01	1.75E-04	5.54E-03	5.54E-03	1.42E-02	7.97E-03	200	200

Soil-water partition coefficient, K_d (cm^3/g)	Source vapor conc., C_{source} ($\mu g/m^3$)	Crack radius, r_{crack} (cm)	Average vapor flow rate into bldg., Q_{soil} (cm^3/s)	Crack effective diffusion coefficient, D^{crack} (cm^2/s)	Area of crack, A_{crack} (cm^2)	Exponent of equivalent foundation Peclet number, $\exp(Pe^f)$ (unitless)	Infinite source indoor attenuation coefficient, α (unitless)	Infinite source bldg. conc., $C_{building}$ ($\mu g/m^3$)	Finite source β term (unitless)	Finite source ψ term $(sec)^{-1}$	Time for source depletion, τ_D (sec)	Exposure duration > time for source depletion (YES/NO)
1.18E-01	6.68E+02	0.10	8.33E+01	5.54E-03	4.00E+02	2.06E+163	NA	NA	1.86E+00	8.02E-08	2.94E+07	YES

Finite source indoor attenuation coefficient, $<\alpha>$ (unitless)	Mass limit bldg. conc., $C_{building}$ ($\mu g/m^3$)	Finite source bldg. conc., $C_{building}$ ($\mu g/m^3$)	Final finite source bldg. conc., $C_{building}$ ($\mu g/m^3$)	Unit risk factor, URF $(\mu g/m^3)^{-1}$	Reference conc., RfC (mg/m^3)
NA	2.49E-02	NA	2.49E-02	7.8E-06	3.0E-02

END

RESULTS SHEET

RISK-BASED SOIL CONCENTRATION CALCULATIONS:

Indoor exposure soil conc., carcinogen (µg/kg)	Indoor exposure soil conc., noncarcinogen (µg/kg)	Risk-based indoor exposure soil conc., (µg/kg)	Soil saturation conc., C_{sat} (µg/kg)	Final indoor exposure soil conc., (µg/kg)
1.26E+01	1.26E+03	1.26E+01	3.09E+05	1.26E+01

INCREMENTAL RISK CALCULATIONS:

Incremental risk from vapor intrusion to indoor air, carcinogen (unitless)	Hazard quotient from vapor intrusion to indoor air, noncarcinogen (unitless)
NA	NA

MESSAGE AND ERROR SUMMARY BELOW: (DO NOT USE RESULTS IF ERRORS ARE PRESENT)

MESSAGE: The values of Csource and Cbuilding on the INTERCALCS worksheet are based on unity and do not represent actual values.

SCROLL DOWN TO "END"

END

VLOOKUP TABLES

Soil Properties Lookup Table

SCS Soil Type	K_s (cm/h)	α_1 (1/cm)	N (unitless)	M (unitless)	n (cm^3/cm^3)	θ_r (cm^3/cm^3)	Mean Grain Diameter (cm)	Bulk Density (g/cm^3)	θ_w (cm^3/cm^3)	SCS Soil Name
C	0.61	0.01496	1.253	0.2019	0.459	0.098	0.0092	1.43	0.215	Clay
CL	0.34	0.01581	1.416	0.2938	0.442	0.079	0.016	1.48	0.168	Clay Loam
L	0.50	0.01112	1.472	0.3207	0.399	0.061	0.020	1.59	0.148	Loam
LS	4.38	0.03475	1.746	0.4273	0.390	0.049	0.040	1.62	0.076	Loamy Sand
S	26.78	0.03524	3.177	0.6852	0.375	0.053	0.044	1.66	0.054	Sand
SC	0.47	0.03342	1.208	0.1722	0.385	0.117	0.025	1.63	0.197	Sandy Clay
SCL	0.55	0.02109	1.330	0.2481	0.384	0.063	0.029	1.63	0.146	Sandy Clay Loam
SI	1.82	0.00658	1.679	0.4044	0.489	0.050	0.0046	1.35	0.167	Silt
SIC	0.40	0.01622	1.321	0.2430	0.481	0.111	0.0039	1.38	0.216	Silty Clay
SICL	0.46	0.00839	1.521	0.3425	0.482	0.090	0.0056	1.37	0.198	Silty Clay Loam
SIL	0.76	0.00506	1.663	0.3987	0.439	0.065	0.011	1.49	0.180	Silt Loam
SL	1.60	0.02667	1.449	0.3099	0.387	0.039	0.030	1.62	0.103	Sandy Loam

Chemical Properties Lookup Table

CAS No.	Chemical	Organic carbon partition coefficient, K_{oc} (cm^3/g)	Diffusivity in air, D_a (cm^2/s)	Diffusivity in water, D_w (cm^2/s)	Pure component water solubility, S (mg/L)	Henry's law constant H' (unitless)	Henry's law constant at reference temperature, H ($atm\text{-}m^3/mol$)	Henry's law constant reference temperature, T_R (^oC)	Normal boiling point, T_B (^oK)	Critical temperature, T_C (^oK)	Enthalpy of vaporization at the normal boiling point, $\Delta H_{v,b}$ (cal/mol)	Unit risk factor, URF ($\mu g/m^3)^{-1}$	Reference conc., RfC (mg/m^3)	Physical state at soil temperature, (S,L,G)	URF extrapolated (X)	RfC extrapolated (X)
56235	Carbon tetrachloride	1.74E+02	7.80E-02	8.80E-06	7.93E+02	1.24E+00	3.03E-02	25	349.90	556.60	7,127	1.5E-05	0.0E+00	L		
57749	Chlordane	1.20E+05	1.18E-02	4.37E-06	5.60E-02	1.99E-03	4.85E-05	25	624.24	885.73	14,000	1.0E-04	7.0E-04	S		
58899	gamma-HCH (Lindane)	1.07E+03	1.42E-02	7.34E-06	7.30E+00	5.73E-04	1.40E-05	25	596.55	839.36	15,000	3.7E-04	1.1E-03	S	X	X
60297	Ethyl ether	5.73E+00	7.82E-02	8.61E-06	5.68E+04	1.35E+00	3.29E-02	25	307.50	466.74	6,338	0.0E+00	7.0E-01	L		X
60571	Dieldrin	2.14E+04	1.25E-02	4.74E-06	1.95E-01	6.18E-04	1.51E-05	25	613.32	842.25	17,000	4.6E-03	1.8E-04	S		X
67641	Acetone	5.75E-01	1.24E-01	1.14E-05	1.00E+06	1.59E-03	3.87E-05	25	329.20	508.10	6,955	0.0E+00	3.5E-01	L		X
67663	Chloroform	3.98E+01	1.04E-01	1.00E-05	7.92E+03	1.50E-01	3.66E-03	25	334.32	536.40	6,988	2.3E-05	0.0E+00	L		
67721	Hexachloroethane	1.78E+03	2.50E-03	6.80E-06	5.00E+01	1.59E-01	3.88E-03	25	458.00	695.00	9,510	4.0E-06	3.5E-03	S		X
71432	Benzene	5.89E+01	8.80E-02	9.80E-06	1.79E+03	2.27E-01	5.54E-03	25	353.24	562.16	7,342	7.8E-06	3.0E-02	L		
71556	1,1,1-Trichloroethane	1.10E+02	7.80E-02	8.80E-06	1.33E+03	7.03E-01	1.72E-02	25	347.24	545.00	7,136	0.0E+00	2.2E+00	L		
72435	Methoxychlor	9.77E+04	1.56E-02	4.46E-06	1.00E-01	6.46E-04	1.58E-05	25	651.02	848.49	16,000	0.0E+00	1.8E-02	S		X
72559	DDE	4.47E+06	1.44E-02	5.87E-06	1.20E-01	8.59E-04	2.09E-05	25	636.44	860.38	15,000	9.7E-05	0.0E+00	S	X	
74839	Methyl bromide	1.05E+01	7.28E-02	1.21E-05	1.52E+04	2.55E-01	6.22E-03	25	276.71	467.00	5,714	0.0E+00	5.0E-03	G		
74873	Methyl chloride (chloromethane)	2.12E+00	1.26E-01	6.50E-06	5.33E+03	3.61E-01	8.80E-03	25	249.00	416.25	5,115	1.0E-06	9.0E-02	L		
74908	Hydrogen cyanide	3.80E+00	1.93E-01	2.10E-05	1.00E+06	5.44E-03	1.33E-04	25	299.00	456.70	6,676	0.0E+00	3.0E-03	L		
74953	Methylene bromide	1.26E+01	4.30E-02	8.44E-06	1.19E+04	3.52E-02	8.59E-04	25	370.00	583.00	7,868	0.0E+00	3.5E-02	L		X
75003	Chloroethane (ethyl chloride)	4.40E+00	2.71E-01	1.15E-05	5.68E+03	3.61E-01	8.80E-03	25	285.30	460.40	5,879	8.3E-07	1.0E+01	L	X	
75014	Vinyl chloride (chloroethene)	1.86E+01	1.06E-01	1.23E-05	8.80E+03	1.10E+00	2.69E-02	25	259.25	432.00	5,250	8.8E-06	1.0E-01	G		
75058	Acetonitrile	4.20E+00	1.28E-01	1.66E-05	1.00E+06	1.42E-03	3.45E-05	25	354.60	545.50	7,110	0.0E+00	6.0E-02	L		
75070	Acetaldehyde	1.06E+00	1.24E-01	1.41E-05	1.00E+06	3.23E-03	7.87E-05	25	293.10	466.00	6,157	2.2E-06	9.0E-03	L		
75092	Methylene chloride	1.17E+01	1.01E-01	1.17E-05	1.30E+04	8.96E-02	2.18E-03	25	313.00	510.00	6,706	4.7E-07	3.0E+00	L		
75150	Carbon disulfide	4.57E+01	1.04E-01	1.00E-05	1.19E+03	1.24E+00	3.02E-02	25	319.00	552.00	6,391	0.0E+00	7.0E-01	L		
75218	Ethylene oxide	1.33E+00	1.04E-01	1.45E-05	3.04E+05	2.27E-02	5.54E-04	25	283.60	469.00	6,104	1.0E-04	0.0E+00	L		
75252	Bromoform	8.71E+01	1.49E-02	1.03E-05	3.10E+03	2.41E-02	5.88E-04	25	422.35	696.00	9,479	1.1E-06	7.0E-02	L		X
75274	Bromodichloromethane	5.50E+01	2.98E-02	1.06E-05	6.74E+03	6.54E-02	1.60E-03	25	363.15	585.85	7,800	1.8E-05	7.0E-02	L	X	X
75296	2-Chloropropane	9.14E+00	8.88E-02	1.01E-05	3.73E+03	5.93E-01	1.45E-02	25	308.70	485.00	6,286	0.0E+00	1.0E-01	L		
75343	1,1-Dichloroethane	3.16E+01	7.42E-02	1.05E-05	5.06E+03	2.30E-01	5.61E-03	25	330.55	523.00	6,895	0.0E+00	5.0E-01	L		
75354	1,1-Dichloroethylene	5.89E+01	9.00E-02	1.04E-05	2.25E+03	1.07E+00	2.60E-02	25	304.75	576.05	6,247	0.0E+00	2.0E-01	L		
75456	Chlorodifluoromethane	4.79E+01	1.01E-01	1.28E-05	2.00E+00	1.10E+00	2.70E-02	25	232.40	369.30	4,836	0.0E+00	5.0E+01	L		
75694	Trichlorofluoromethane	4.97E+02	8.70E-02	9.70E-06	1.10E+03	3.97E+00	9.68E-02	25	296.70	471.00	5,999	0.0E+00	7.0E-01	L		
75718	Dichlorodifluoromethane	4.57E+02	6.65E-02	9.92E-06	2.80E+02	1.40E+01	3.42E-01	25	243.20	384.95	9,421	0.0E+00	2.0E-01	L		
76131	1,1,2-Trichloro-1,2,2-trifluoroetha	1.11E+04	7.80E-02	8.20E-06	1.70E+02	1.97E+01	4.80E-01	25	320.70	487.30	6,463	0.0E+00	3.0E+01	L		
76448	Heptachlor	1.41E+06	1.12E-02	5.69E-06	1.80E-01	6.05E+01	1.48E+00	25	603.69	846.31	13,000	1.3E-03	1.8E-03	S		X
77474	Hexachlorocyclopentadiene	2.00E+05	1.61E-02	7.21E-06	1.80E+00	1.10E+00	2.69E-02	25	512.15	746.00	10,931	0.0E+00	2.0E-04	L		
78831	Isobutanol	2.59E+00	8.60E-02	9.30E-06	8.50E+04	4.83E-04	1.18E-05	25	381.04	547.78	10,936	0.0E+00	1.1E+00	L		X
78875	1,2-Dichloropropane	4.37E+01	7.82E-02	8.73E-06	2.80E+03	1.15E-01	2.79E-03	25	369.52	572.00	7,590	1.9E-05	4.0E-03	L	X	
78933	Methylethylketone (2-butanone)	2.30E+00	8.08E-02	9.80E-06	2.23E+05	2.29E-03	5.58E-05	25	352.50	536.78	7,481	0.0E+00	5.0E+00	L		
79005	1,1,2-Trichloroethane	5.01E+01	7.80E-02	8.80E-06	4.42E+03	3.73E-02	9.11E-04	25	386.15	602.00	8,322	1.6E-05	1.4E-02	L		X
79016	Trichloroethylene	1.66E+02	7.90E-02	9.10E-06	1.47E+03	4.21E-01	1.03E-02	25	360.36	544.20	7,505	1.1E-04	4.0E-02	L	X	
79209	Methyl acetate	3.26E+00	1.04E-01	1.00E-05	2.00E+03	4.84E-03	1.18E-04	25	329.80	506.70	7,260	0.0E+00	3.5E+00	L		X
79345	1,1,2,2-Tetrachloroethane	9.33E+01	7.10E-02	7.90E-06	2.96E+03	1.41E-02	3.44E-04	25	419.60	661.15	8,996	5.8E-05	2.1E-01	L		X
79469	2-Nitropropane	1.17E+01	9.23E-02	1.01E-05	1.70E+04	5.03E-03	1.23E-04	25	393.20	594.00	8,383	2.7E-03	2.0E-02	L		
80626	Methylmethacrylate	6.98E+00	7.70E-02	8.60E-06	1.50E+04	1.38E-02	3.36E-04	25	373.50	567.00	8,975	0.0E+00	7.0E-01	L		
83329	Acenaphthene	7.08E+03	4.21E-02	7.69E-06	3.57E+00	6.34E-03	1.55E-04	25	550.54	803.15	12,155	0.0E+00	2.1E-01	S		X
86737	Fluorene	1.38E+04	3.63E-02	7.88E-06	1.98E+00	2.60E-03	6.34E-05	25	570.44	870.00	12,666	0.0E+00	1.4E-01	S		X
87683	Hexachloro-1,3-butadiene	5.37E+04	5.61E-02	6.16E-06	3.20E+00	3.33E-01	8.13E-03	25	486.15	738.00	10,206	2.2E-05	7.0E-04	L		X
88722	o-Nitrotoluene	3.24E+02	5.87E-02	8.67E-06	6.50E+02	5.11E-04	1.25E-05	25	495.00	720.00	12,239	0.0E+00	3.5E-02	L		X
91203	Naphthalene	2.00E+03	5.90E-02	7.50E-06	3.10E+01	1.98E-02	4.82E-04	25	491.14	748.40	10,373	0.0E+00	3.0E-03	S		
91576	2-Methylnaphthalene	2.81E+03	5.22E-02	7.75E-06	2.46E+01	2.12E-02	5.17E-04	25	514.26	761.00	12,600	0.0E+00	7.0E-02	S		X
92524	Biphenyl	4.38E+03	4.04E-02	8.15E-06	7.45E+00	1.23E-02	2.99E-04	25	529.10	789.00	10,890	0.0E+00	1.8E-01	S		X
95476	o-Xylene	3.63E+02	8.70E-02	1.00E-05	1.78E+02	2.12E-01	5.18E-03	25	417.60	630.30	8,661	0.0E+00	1.0E-01	L		X
95501	1,2-Dichlorobenzene	6.17E+02	6.90E-02	7.90E-06	1.56E+02	7.77E-02	1.90E-03	25	453.57	705.00	9,700	0.0E+00	2.0E-01	L		
95578	2-Chlorophenol	3.88E+02	5.01E-02	9.46E-06	2.20E+04	1.60E-02	3.90E-04	25	447.53	675.00	9,572	0.0E+00	1.8E-02	L		X
95636	1,2,4-Trimethylbenzene	1.35E+03	6.06E-02	7.92E-06	5.70E+01	2.52E-01	6.14E-03	25	442.30	649.17	9,369	0.0E+00	6.0E-03	L		

96184	1,2,3-Trichloropropane	2.20E+01	7.10E-02	7.90E-06	1.75E+03	1.67E-02	4.08E-04	25	430.00	652.00	9,171	5.7E-04	4.9E-03	L	X	
96333	Methyl acrylate	4.53E+00	9.76E-02	1.02E-05	6.00E+04	7.68E-03	1.87E-04	25	353.70	536.00	7,749	0.0E+00	1.1E-01	L		X
97632	Ethylmethacrylate	2.95E+01	6.53E-02	8.37E-06	3.67E+03	3.44E-02	8.40E-04	25	390.00	571.00	10,957	0.0E+00	3.2E-01	L		X
98066	tert-Butylbenzene	7.71E+02	5.65E-02	8.02E-06	2.95E+01	4.87E-01	1.19E-02	25	442.10	1220.00	8,980	0.0E+00	1.4E-01	L		X
98828	Cumene	4.89E+02	6.50E-02	7.10E-06	6.13E+01	4.74E+01	1.46E-02	25	425.56	631.10	10,335	0.0E+00	4.0E-01	L		
98862	Acetophenone	5.77E+01	6.00E-02	8.73E-06	6.13E+03	4.38E-04	1.07E-05	25	475.00	709.50	11,732	0.0E+00	3.5E-01	S,L		X
98953	Nitrobenzene	6.46E+01	7.60E-02	8.60E-06	2.09E+03	9.82E-04	2.39E-05	25	483.95	719.00	10,566	0.0E+00	2.0E-03	L		
100414	Ethylbenzene	3.63E+02	7.50E-02	7.80E-06	1.69E+02	3.22E-01	7.86E-03	25	409.34	617.20	8,501	0.0E+00	1.0E+00	L		
100425	Styrene	7.76E+02	7.10E-02	8.00E-06	3.10E+02	1.12E-01	2.74E-03	25	418.31	636.00	8,737	0.0E+00	1.0E+00	L		
100447	Benzylchloride	6.14E+01	7.50E-02	7.80E-06	5.25E+02	1.70E-02	4.14E-04	25	452.00	685.00	8,773	4.9E-05	0.0E+00	L	X	
100527	Benzaldehyde	4.59E+01	7.21E-02	9.07E-06	3.30E+03	9.73E-04	2.37E-05	25	452.00	695.00	11,658	0.0E+00	3.5E-01	L		X
103651	n-Propylbenzene	5.62E+02	6.01E-02	7.83E-06	6.00E+01	4.37E-01	1.07E-02	25	432.20	630.00	9,123	0.0E+00	1.4E-01	L		X
104518	n-Butylbenzene	1.11E+03	5.70E-02	8.12E-06	2.00E+00	5.38E-01	1.31E-02	25	456.46	660.50	9,290	0.0E+00	1.4E-01	L		X
106423	p-Xylene	3.89E+02	7.69E-02	8.44E-06	1.85E+02	3.13E-01	7.64E-03	25	411.52	616.20	8,525	0.0E+00	1.0E-01	L		X
106467	1,4-Dichlorobenzene	6.17E+02	6.90E-02	7.90E-06	7.90E+01	9.82E-02	2.39E-03	25	447.21	684.75	9,271	0.0E+00	8.0E-01	S		
106934	1,2-Dibromoethane (ethylene dibr	2.50E+01	2.17E-02	1.19E-05	4.18E+03	3.04E-02	7.41E-04	25	404.60	583.00	8,310	2.2E-04	2.0E-04	L		
106990	1,3-Butadiene	1.91E+01	2.49E-01	1.08E-05	7.35E+02	3.01E+00	7.34E-02	25	268.60	425.00	5,370	3.0E-02	2.0E-03	L		
107028	Acrolein	2.76E+00	1.05E-01	1.22E-05	2.13E+05	4.99E-03	1.22E-04	25	325.60	506.00	6,731	0.0E+00	2.0E-05	L		
107062	1,2-Dichloroethane	1.74E+01	1.04E-01	9.90E-06	8.52E+03	4.00E-02	9.77E-04	25	356.65	561.00	7,643	2.6E-05	0.0E+00	L		
107131	Acrylonitrile	5.90E+00	1.22E-01	1.34E-05	7.40E+04	4.21E-03	1.03E-04	25	350.30	519.00	7,786	6.8E-05	2.0E-03	L		
108054	Vinyl acetate	5.25E+00	8.50E-02	9.20E-06	2.00E+04	2.09E-02	5.10E-04	25	345.65	519.13	7,800	0.0E+00	2.0E-01	L		
108101	Methylisobutylketone (4-methyl-2-	9.06E+00	7.50E-02	7.80E-06	1.90E+04	5.64E-03	1.38E-04	25	389.50	571.00	8,243	0.0E+00	3.0E+00	L		
108383	m-Xylene	4.07E+02	7.00E-02	7.80E-06	1.61E+02	3.00E-01	7.32E-03	25	412.27	617.05	8,523	0.0E+00	1.0E-01	L		X
108678	1,3,5-Trimethylbenzene	1.35E+03	6.02E-02	8.67E-06	2.00E+00	2.41E-01	5.87E-03	25	437.89	637.25	9,321	0.0E+00	6.0E-03	L		
108872	Methylcyclohexane	7.85E+01	7.35E-02	8.52E-06	1.40E+01	4.22E+00	1.03E-01	25	373.90	572.20	7,474	0.0E+00	3.0E+00	L		
108883	Toluene	1.82E+02	8.70E-02	8.60E-06	5.26E+02	2.72E-01	6.62E-03	25	383.78	591.79	7,930	0.0E+00	4.0E-01	L		
108907	Chlorobenzene	2.19E+02	7.30E-02	8.70E-06	4.72E+02	1.51E-01	3.69E-03	25	404.87	632.40	8,410	0.0E+00	6.0E-02	L		
109693	1-Chlorobutane	1.72E+01	8.26E-02	1.00E-05	1.10E+03	6.93E-01	1.69E-02	25	351.60	542.00	7,263	0.0E+00	1.4E+00	L		X
110009	Furan	1.86E+01	1.04E-01	1.22E-05	1.00E+04	2.21E-01	5.39E-03	25	304.60	490.20	6,477	0.0E+00	3.5E-03	L		X
110543	Hexane	4.34E+01	2.00E-01	7.77E-06	1.24E+01	6.82E+01	1.66E+00	25	341.70	508.00	6,895	0.0E+00	2.0E-01	L		
111444	Bis(2-chloroethyl)ether	1.55E+01	6.92E-02	7.53E-06	1.72E+04	7.36E-04	1.80E-05	25	451.15	659.79	10,803	3.3E-04	0.0E+00	L		
115297	Endosulfan	2.14E+03	1.15E-02	4.55E-06	5.10E-01	4.58E-04	1.12E-05	25	674.43	942.94	14,000	0.0E+00	2.1E-02	S		X
118741	Hexachlorobenzene	5.50E+04	5.42E-02	5.91E-06	5.00E-03	5.40E-02	1.32E-03	25	582.55	825.00	14,447	4.6E-04	2.8E-03	S		X
120821	1,2,4-Trichlorobenzene	1.78E+03	3.00E-02	8.23E-06	4.88E+01	5.81E-02	1.42E-03	25	486.15	725.00	10,471	0.0E+00	4.0E-03	L		
123739	Crotonaldehyde (2-butenal)	4.82E+00	9.56E-02	1.07E-05	3.69E+04	7.99E-04	1.95E-05	25	375.20	568.00	9	5.4E-04	0.0E+00	L	X	
124481	Chlorodibromomethane	6.31E+01	1.96E-02	1.05E-05	2.60E+03	3.20E-02	7.81E-04	25	416.14	678.20	5,900	2.4E-05	7.0E-02	L	X	X
126987	Methacrylonitrile	3.58E+01	1.12E-01	1.32E-05	2.54E+04	1.01E-02	2.46E-04	25	363.30	554.00	7,600	0.0E+00	7.0E-04	L		
126998	2-Chloro-1,3-butadiene (chloropre	6.73E+01	8.58E-02	1.03E-05	2.12E+03	4.91E-01	1.20E-02	25	332.40	525.00	8,075	0.0E+00	7.0E-03	L		
127184	Tetrachloroethylene	1.55E+02	7.20E-02	8.20E-06	2.00E+02	7.53E-01	1.84E-02	25	394.40	620.20	8,288	5.9E-06	6.0E-01	L		
129000	Pyrene	1.05E+05	2.72E-02	7.24E-06	1.35E+00	4.50E-04	1.10E-05	25	667.95	936	14370	0.0E+00	1.1E-01	S		X
132649	Dibenzofuran	5.15E+03	2.38E-02	6.00E-06	3.10E+00	5.15E-04	1.26E-05	25	560	824	66400	0.0E+00	1.4E-02	S		X
135988	sec-Butylbenzene	9.66E+02	5.70E-02	8.12E-06	3.94E+00	5.68E-01	1.39E-02	25	446.5	679	88730	0.0E+00	1.4E-01	L		X
141786	Ethylacetate	6.44E+00	7.32E-02	9.70E-06	8.03E+04	5.64E-03	1.38E-04	25	350.26	523.3	7633.66	0.0E+00	3.2E+00	L		X
156592	cis-1,2-Dichloroethylene	3.55E+01	7.36E-02	1.13E-05	3.50E+03	1.67E-01	4.07E-03	25	333.65	544	7192	0.0E+00	3.5E-02	L		X
156605	trans-1,2-Dichloroethylene	5.25E+01	7.07E-02	1.19E-05	6.30E+03	3.84E-01	9.36E-03	25	320.85	516.5	6717	0.0E+00	7.0E-02	L		X
205992	Benzo(b)fluoranthene	1.23E+06	2.26E-02	5.56E-06	1.50E-03	4.54E-03	1.11E-04	25	715.9	969.27	17000	2.1E-04	0.0E+00	S	X	
218019	Chrysene	3.98E+05	2.48E-02	6.21E-06	6.30E-03	3.87E-03	9.44E-05	25	714.15	979	16455	2.1E-06	0.0E+00	S	X	
309002	Aldrin	2.45E+06	1.32E-02	4.86E-06	1.70E-02	6.95E-03	1.70E-04	25	603.01	839.37	15000	4.9E-03	1.1E-04	S		X
319846	alpha-HCH (alpha-BHC)	1.23E+03	1.42E-02	7.34E-06	2.00E+00	4.34E-04	1.06E-05	25	596.55	839.36	15000	1.8E-03	0.0E+00	S		
541731	1,3-Dichlorobenzene	1.98E+03	6.92E-02	7.86E-06	1.34E+02	1.27E-01	3.09E-03	25	446	684	9230.18	0.0E+00	1.1E-01	L		X
542756	1,3-Dichloropropene	4.57E+01	6.26E-02	1.00E-05	2.80E+03	7.24E-01	1.77E-02	25	381.15	587.38	7900	4.0E-06	2.0E-02	L		
630206	1,1,1,2-Tetrachloroethane	1.16E+02	7.10E-02	7.90E-06	1.10E+03	9.90E-02	2.41E-03	25	403.5	624	9768.282525	7.4E-06	1.1E-01	L		X
1634044	MTBE	7.26E+00	1.02E-01	1.05E-05	5.10E+04	2.56E-02	6.23E-04	25	328.3	497.1	6677.66	0.0E+00	3.0E+00	L		
7439976	Mercury (elemental)	5.20E+01	3.07E-02	6.30E-06	2.00E+01	4.40E-01	1.07E-02	25	629.88	1750	14127	0.0E+00	3.0E-04	L		

APPENDIX D

SAMPLE DATA ENTRY SHEETS FOR EACH MODEL

DATA ENTRY SHEET

SL-SCREEN
Version 3.1; 02/04

Reset to Defaults

CALCULATE RISK-BASED SOIL CONCENTRATION (enter "X" in "YES" box)

YES ☒

OR

CALCULATE INCREMENTAL RISKS FROM ACTUAL SOIL CONCENTRATION (enter "X" in "YES" box and initial soil conc. below)

YES ☐

ENTER Chemical CAS No. (numbers only, no dashes)	**ENTER** Initial soil conc., C_R (µg/kg)	Chemical
71432		Benzene

MORE ↓

ENTER Depth below grade to bottom of enclosed space floor, L_F (15 or 200 cm)	**ENTER** Depth below grade to top of contamination, L_t (cm)	**ENTER** Average soil temperature, T_S (^oC)	**ENTER** Vadose zone SCS soil type (used to estimate soil vapor permeability)		**ENTER** User-defined vadose zone soil vapor permeability, k_v (cm^2)
200	400	10	SCL	OR	

MORE ↓

ENTER Vandose zone SCS soil type Lookup Soil Parameters	**ENTER** Vadose zone soil dry bulk density, ρ_b^A (g/cm^3)	**ENTER** Vadose zone soil total porosity, n^V (unitless)	**ENTER** Vadose zone soil water-filled porosity, θ_w^V (cm^3/cm^3)	**ENTER** Vadose zone soil organic carbon fraction, f_{oc}^V (unitless)	**ENTER** Average vapor flow rate into bldg. (Leave blank to calculate) Q_{soil} (L/m)
SCL	1.63	0.384	0.146	0.002	5

MORE ↓

ENTER Averaging time for carcinogens, AT_C (yrs)	**ENTER** Averaging time for noncarcinogens, AT_{NC} (yrs)	**ENTER** Exposure duration, ED (yrs)	**ENTER** Exposure frequency, EF (days/yr)	**ENTER** Target risk for carcinogens, TR (unitless)	**ENTER** Target hazard quotient for noncarcinogens, THQ (unitless)
70	30	30	350	1.0E-06	1

Used to calculate risk-based soil concentration.

END

DATA ENTRY SHEET

SL-ADV
Version 3.1; 02/04

Reset to Defaults

CALCULATE RISK-BASED SOIL CONCENTRATION (enter "X" in "YES" box)

YES ☒ X

OR

CALCULATE INCREMENTAL RISKS FROM ACTUAL SOIL CONCENTRATION (enter "X" in "YES" box and initial soil conc. below)

YES ☐

ENTER Chemical CAS No. (numbers only, no dashes)	**ENTER** Initial soil conc., C_R (µg/kg)	Chemical
71432		Benzene

MORE ↓

ENTER Average soil temperature, T_S (^{o}C)	**ENTER** Depth below grade to bottom of enclosed space floor, L_F (cm)	**ENTER** Depth below grade to top of contamination, L_t (cm)	**ENTER** Depth below grade to bottom of contamination, (enter value of 0 if value is unknown) L_b (cm)	**ENTER** Totals must add up to value of L_t (cell G28) Thickness of soil stratum A, h_A (cm)	**ENTER** Thickness of soil stratum B, (Enter value or 0) h_B (cm)	**ENTER** Thickness of soil stratum C, (Enter value or 0) h_C (cm)	**ENTER** Soil stratum A SCS soil type (used to estimate soil vapor permeability)	OR	**ENTER** User-defined stratum A soil vapor permeability, k_v (cm^2)
10	200	400	600	200	100	100	L		

MORE ↓

ENTER Stratum A SCS soil type Lookup Soil Parameters	**ENTER** Stratum A soil dry bulk density, ρ_b^A (g/cm^3)	**ENTER** Stratum A soil total porosity, n^A (unitless)	**ENTER** Stratum A soil water-filled porosity, θ_w^A (cm^3/cm^3)	**ENTER** Stratum A soil organic carbon fraction, f_{oc}^A (unitless)	**ENTER** Stratum B SCS soil type Lookup Soil Parameters	**ENTER** Stratum B soil dry bulk density, ρ_b^B (g/cm^3)	**ENTER** Stratum B soil total porosity, n^B (unitless)	**ENTER** Stratum B soil water-filled porosity, θ_w^B (cm^3/cm^3)	**ENTER** Stratum B soil organic carbon fraction, f_{oc}^B (unitless)	**ENTER** Stratum C SCS soil type Lookup Soil Parameters	**ENTER** Stratum C soil dry bulk density, ρ_b^C (g/cm^3)	**ENTER** Stratum C soil total porosity, n^C (unitless)	**ENTER** Stratum C soil water-filled porosity, θ_w^C (cm^3/cm^3)	**ENTER** Stratum C soil organic carbon fraction, f_{oc}^C (unitless)
L	1.59	0.399	0.148	0.002	L	1.59	0.399	0.148	0.002	S	1.66	0.375	0.054	0.002

MORE ↓

ENTER Enclosed space floor thickness, L_{crack} (cm)	**ENTER** Soil-bldg. pressure differential, ΔP (g/cm-s^2)	**ENTER** Enclosed space floor length, L_B (cm)	**ENTER** Enclosed space floor width, W_B (cm)	**ENTER** Enclosed space height, H_B (cm)	**ENTER** Floor-wall seam crack width, w (cm)	**ENTER** Indoor air exchange rate, ER (1/h)	**ENTER** Average vapor flow rate into bldg. OR Leave blank to calculate Q_{soil} (L/m)
10	40	1000	1000	366	0.1	0.25	5

ENTER Averaging time for carcinogens, AT_C (yrs)	**ENTER** Averaging time for noncarcinogens, AT_{NC} (yrs)	**ENTER** Exposure duration, ED (yrs)	**ENTER** Exposure frequency, EF (days/yr)	**ENTER** Target risk for carcinogens, TR (unitless)	**ENTER** Target hazard quotient for noncarcinogens, THQ (unitless)
70	30	30	350	1.0E-06	1

Used to calculate risk-based soil concentration.

END

DATA ENTRY SHEET

SG-SCREEN
Version 3.1; 02/04

Reset to Defaults

Soil Gas Concentration Data

ENTER Chemical CAS No. (numbers only, no dashes)	ENTER Soil gas conc., C_g ($\mu g/m^3$)	OR	ENTER Soil gas conc., C_g (ppmv)	Chemical
71432			2.00E+01	Benzene

MORE ↓

ENTER Depth below grade to bottom of enclosed space floor, L_F (15 or 200 cm)	ENTER Soil gas sampling depth below grade, L_s (cm)	ENTER Average soil temperature, T_S (^oC)	ENTER Vadose zone SCS soil type (used to estimate soil vapor permeability)	OR	ENTER User-defined vadose zone soil vapor permeability, k_v (cm^2)
200	400	10	L		

MORE ↓

ENTER Vandose zone SCS soil type Lookup Soil Parameters	ENTER Vadose zone soil dry bulk density, ρ_b^A (g/cm^3)	ENTER Vadose zone soil total porosity, n^V (unitless)	ENTER Vadose zone soil water-filled porosity, θ_w^V (cm^3/cm^3)	ENTER Average vapor flow rate into bldg. (Leave blank to calculate) Q_{soil} (L/m)
L	1.59	0.399	0.148	5

MORE ↓

ENTER Averaging time for carcinogens, AT_C (yrs)	ENTER Averaging time for noncarcinogens, AT_{NC} (yrs)	ENTER Exposure duration, ED (yrs)	ENTER Exposure frequency, EF (days/yr)
70	30	30	350

END

DATA ENTRY SHEET

SG-ADV
Version 3.1; 02/04

Reset to Defaults

	Soil Gas Concentration Data			
ENTER Chemical CAS No. (numbers only, no dashes)	ENTER Soil gas conc., C_g ($\mu g/m^3$)	OR	ENTER Soil gas conc., C_g (ppmv)	Chemical
71432				Benzene

Enter soil gas concentration above.

MORE ↓

			Totals must add up to value of Ls (cell F24)					
ENTER Depth below grade to bottom of enclosed space floor, L_F (cm)	ENTER Soil gas sampling depth below grade, L_s (cm)	ENTER Average soil temperature, T_S (^oC)	ENTER Thickness of soil stratum A, h_A (cm)	ENTER Thickness of soil stratum B, (Enter value or 0) h_B (cm)	ENTER Thickness of soil stratum C, (Enter value or 0) h_C (cm)	ENTER Soil stratum A SCS soil type (used to estimate soil vapor permeability)	OR	ENTER User-defined stratum A soil vapor permeability, k_v (cm^2)
200	400	10	200	100	100	L		

MORE ↓

ENTER Stratum A SCS soil type	ENTER Stratum A soil dry bulk density, ρ_b^A (g/cm^3)	ENTER Stratum A soil total porosity, n^A (unitless)	ENTER Stratum A soil water-filled porosity, θ_w^A (cm^3/cm^3)	ENTER Stratum B SCS soil type	ENTER Stratum B soil dry bulk density, ρ_b^B (g/cm^3)	ENTER Stratum B soil total porosity, n^B (unitless)	ENTER Stratum B soil water-filled porosity, θ_w^B (cm^3/cm^3)	ENTER Stratum C SCS soil type	ENTER Stratum C soil dry bulk density, ρ_b^C (g/cm^3)	ENTER Stratum C soil total porosity, n^C (unitless)	ENTER Stratum C soil water-filled porosity, θ_w^C (cm^3/cm^3)
Lookup Soil Parameters				Lookup Soil Parameters				Lookup Soil Parameters			
L	1.59	0.399	0.148	L	1.59	0.399	0.148	S	1.66	0.375	0.054

MORE ↓

ENTER Enclosed space floor thickness, L_{crack} (cm)	ENTER Soil-bldg. pressure differential, ΔP ($g/cm\text{-}s^2$)	ENTER Enclosed space floor length, L_B (cm)	ENTER Enclosed space floor width, W_B (cm)	ENTER Enclosed space height, H_B (cm)	ENTER Floor-wall seam crack width, w (cm)	ENTER Indoor air exchange rate, ER (1/h)		ENTER Average vapor flow rate into bldg. OR Leave blank to calculate Q_{soil} (L/m)
10	40	1000	1000	366	0.1	0.25		5

ENTER Averaging time for carcinogens, AT_C (yrs)	ENTER Averaging time for noncarcinogens, AT_{NC} (yrs)	ENTER Exposure duration, ED (yrs)	ENTER Exposure frequency, EF (days/yr)
70	30	30	350

END

DATA ENTRY SHEET

GW-SCREEN
Version 3.1; 02/04

Reset to Defaults

CALCULATE RISK-BASED GROUNDWATER CONCENTRATION (enter "X" in "YES" box)

YES ☒

OR

CALCULATE INCREMENTAL RISKS FROM ACTUAL GROUNDWATER CONCENTRATION
(enter "X" in "YES" box and initial groundwater conc. below)

YES ☐

ENTER Chemical CAS No. (numbers only, no dashes)	**ENTER** Initial groundwater conc., C_W (μg/L)	Chemical
71432		Benzene

MORE ↓

ENTER Depth below grade to bottom of enclosed space floor, L_F (cm)	**ENTER** Depth below grade to water table, L_{WT} (cm)	**ENTER** SCS soil type directly above water table	**ENTER** Average soil/ groundwater temperature, T_S (^{o}C)	**ENTER** Average vapor flow rate into bldg. (Leave blank to calculate) Q_{soil} (L/m)
200	400	SC	10	5

MORE ↓

ENTER Vadose zone SCS soil type (used to estimate soil vapor permeability)	OR	**ENTER** User-defined vandose zone soil vapor permeability, k_v (cm^2)	**ENTER** Vadose zone SCS soil type Lookup Soil Parameters	**ENTER** Vadose zone soil dry bulk density, ρ_b^V (g/cm^3)	**ENTER** Vadose zone soil total porosity, n^V (unitless)	**ENTER** Vadose zone soil water-filled porosity, θ_w^V (cm^3/cm^3)
SCL			SCL	1.63	0.384	0.146

MORE ↓

ENTER Target risk for carcinogens, TR (unitless)	**ENTER** Target hazard quotient for noncarcinogens, THQ (unitless)	**ENTER** Averaging time for carcinogens, AT_C (yrs)	**ENTER** Averaging time for noncarcinogens, AT_{NC} (yrs)	**ENTER** Exposure duration, ED (yrs)	**ENTER** Exposure frequency, EF (days/yr)
1.0E-06	1	70	30	30	350

Used to calculate risk-based groundwater concentration.

DATA ENTRY SHEET

GW-ADV
Version 3.1; 02/04

Reset to Defaults

CALCULATE RISK-BASED GROUNDWATER CONCENTRATION (enter "X" in "YES" box)

YES X

OR

CALCULATE INCREMENTAL RISKS FROM ACTUAL GROUNDWATER CONCENTRATION (enter "X" in "YES" box and initial groundwater conc. below)

YES ☐

ENTER Chemical CAS No. (numbers only, no dashes)	ENTER Initial groundwater conc., C_W (µg/L)	Chemical
71432		Benzene

MORE ↓

Totals must add up to value of L_{WT} (cell G28)

ENTER Average soil/ groundwater temperature, T_S (^oC)	ENTER Depth below grade to bottom of enclosed space floor, L_F (cm)	ENTER Depth below grade to water table, L_{WT} (cm)	ENTER Thickness of soil stratum A, h_A (cm)	ENTER Thickness of soil stratum B, (Enter value or 0) h_B (cm)	ENTER Thickness of soil stratum C, (Enter value or 0) h_C (cm)	ENTER Soil stratum directly above water table, (Enter A, B, or C)	ENTER SCS soil type directly above water table	ENTER Soil stratum A SCS soil type (used to estimate soil vapor permeability)	OR	ENTER User-defined stratum A soil vapor permeability, k_v (cm^2)
10	200	400	300	50	50	C	SC	L		

MORE ↓

ENTER Stratum A SCS soil type Lookup Soil Parameters	ENTER Stratum A soil dry bulk density, ρ_b^A (g/cm^3)	ENTER Stratum A soil total porosity, n^A (unitless)	ENTER Stratum A soil water-filled porosity, θ_w^A (cm^3/cm^3)	ENTER Stratum B SCS soil type Lookup Soil Parameters	ENTER Stratum B soil dry bulk density, ρ_b^B (g/cm^3)	ENTER Stratum B soil total porosity, n^B (unitless)	ENTER Stratum B soil water-filled porosity, θ_w^B (cm^3/cm^3)	ENTER Stratum C SCS soil type Lookup Soil Parameters	ENTER Stratum C soil dry bulk density, ρ_b^C (g/cm^3)	ENTER Stratum C soil total porosity, n^C (unitless)	ENTER Stratum C soil water-filled porosity, θ_w^C (cm^3/cm^3)
L	1.59	0.399	0.148	L	1.59	0.399	0.148	SC	1.63	0.385	0.197

MORE ↓

ENTER Enclosed space floor thickness, L_{crack} (cm)	ENTER Soil-bldg. pressure differential, ΔP (g/cm-s^2)	ENTER Enclosed space floor length, L_B (cm)	ENTER Enclosed space floor width, W_B (cm)	ENTER Enclosed space height, H_B (cm)	ENTER Floor-wall seam crack width, w (cm)	ENTER Indoor air exchange rate, ER (1/h)	ENTER Average vapor flow rate into bldg. OR Leave blank to calculate Q_{soil} (L/m)
10	40	1000	1000	366	0.1	0.25	5

MORE ↓

ENTER Averaging time for carcinogens, AT_C (yrs)	ENTER Averaging time for noncarcinogens, AT_{NC} (yrs)	ENTER Exposure duration, ED (yrs)	ENTER Exposure frequency, EF (days/yr)	ENTER Target risk for carcinogens, TR (unitless)	ENTER Target hazard quotient for noncarcinogens, THQ (unitless)
70	30	30	350	1.0E-06	1

Used to calculate risk-based groundwater concentration.

END

APPENDIX E

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