# USER'S GUIDE FOR THE JOHNSON AND ETTINGER (1991) MODEL FOR SUBSURFACE VAPOR INTRUSION INTO BUILDINGS

Prepared By

Environmental Quality Management, Inc.
Cedar Terrace Office Park, Suite 250
3325 Durham-Chapel Hill Boulevard
Durham, North Carolina  27707-2646

Prepared For

E.H. Pechan & Associates, Inc.
5537-C Hempstead way
Springfield, Virginia  22151

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Janine Dinan, Work Assignment Manager

U.S. ENVIRONMENTAL PROTECTION AGENCY
OFFICE OF EMERGENCY AND REMEDIAL RESPONSE
TOXICS INTEGRATION BRANCH (5202G)
401 M STREET, S.W.
WASHINGTON, D.C.  20450

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# DISCLAIMER

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# SECTION 1

# INTRODUCTION

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 (1991) introduced a screening-level model which 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 or in close proximity to the source of contamination. In their article, Johnson and Ettinger 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 (Loureiro, et al., 1990).

The Johnson and Ettinger 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 nondiminishing 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 Johnson and Ettinger model as provided in the accompanying spreadsheets. The infinite source model and the finite source model are provided in both MICROSOFT EXCEL and LOTUS 1-2-3 formats for soil contamination and the infinite source model for contamination occurring below the water table. Model results (both screening and tier-2) 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.

Second-tier 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 second-tier 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.

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 of input parameters and to explore and quantity 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 6).

# SECTION 2

# MODEL THEORY

Chemical fate and transport within soils and between the soil column and enclosed spaces is determined by a number of physical and chemical processes. This section presents the theoretical framework on which the Johnson and Ettinger 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 Johnson and Ettinger (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 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 towards 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.

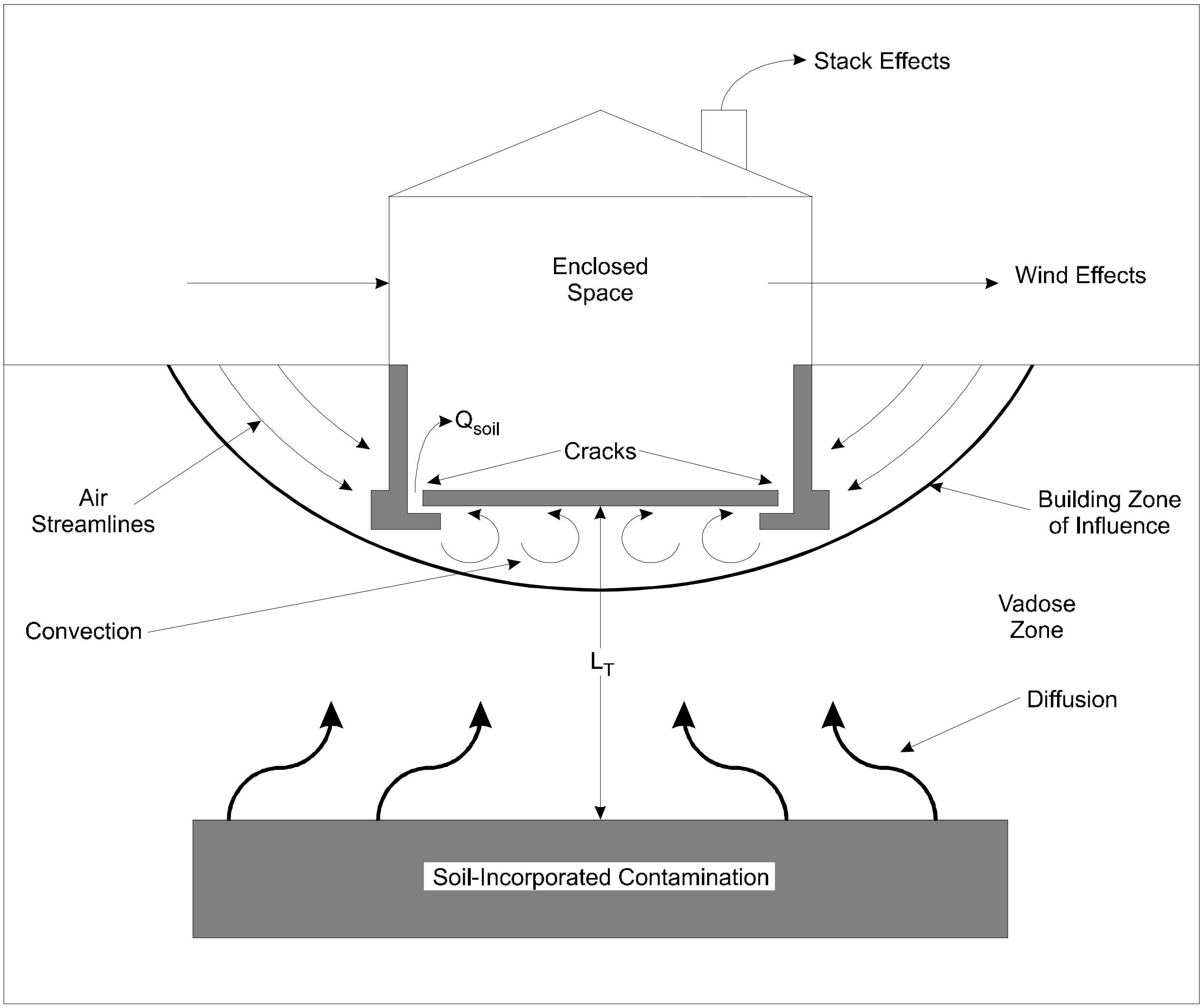


Figure 1.  Conceptual Diagram of Soil Contamination

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 rate of soil gas entry ($Q_{soil}$) 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 CONTAMINATION

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

$C_R$ = Initial soil concentration, g/g

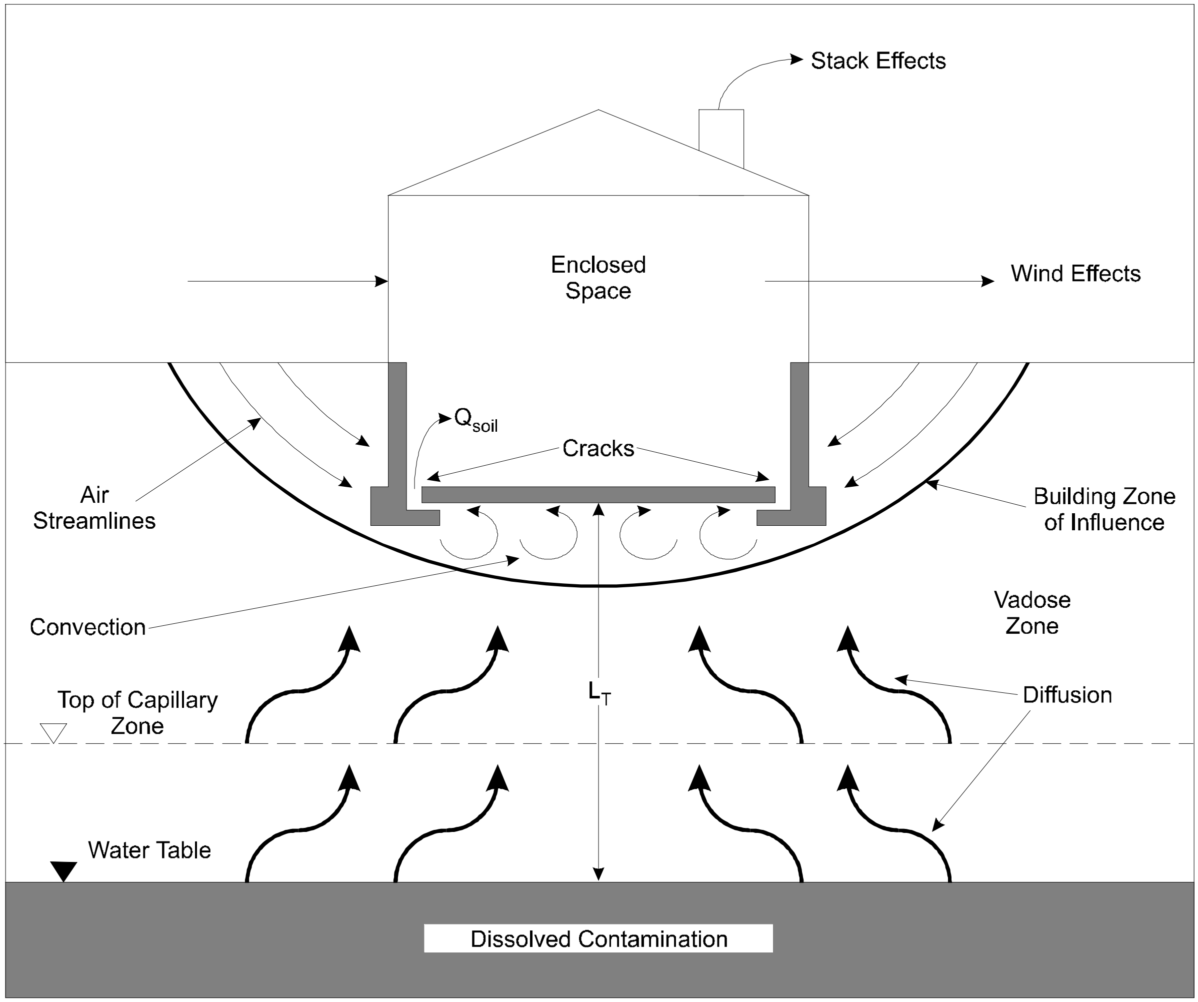


Figure 2. Conceptual Diagram of Groundwater Contamination

$\rho_b$ = Soil dry bulk density, g/cm$^3$

$\theta_w$ = Soil water-filled porosity, cm$^3$/cm$^3$

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

$\theta_a$ = 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.

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

$$C_{source} = H'_{TS} C_w \tag{2}$$

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:

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

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, °K

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

$R_C$ = Gas constant (= 1.9872 cal/mol - °K)

R = Gas constant (= 8.206 E-05 atm-m$^3$/mol-°K).

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

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

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, °K

$T_C$ = Critical temperature, °K

$T_B$ = Normal boiling point, °K

n = Constant, unitless.

Table 1 gives the value of n as a function of the ratio $T_B/T_C$.

TABLE 1. 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 |

Chemical properties are included in the accompanying spreadsheets for the 93 volatile chemicals listed in the U.S. Environmental Protection Agency (EPA) Soil Screening Guidance (EPA 1996a and b) and for four PCB aroclors. See Appendix C for the complete list of references by chemical.

## 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 implying 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 which corresponded to the air-entry pressure head. The air-entry pressure head corresponds with the top of the saturated capillary zone. Therefore, to account for the variation in the air content of the capillary zone, and 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:

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

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

$\theta_r$ = Residual soil water content, $cm^3/cm^3$

$\theta_s$ = Saturated soil water content, $cm^3/cm^3$

$\alpha$ = Point of inflection in the water retention curve where d $\theta_w$/dh is maximal, $cm^{-1}$

h = Air-entry pressure head, cm (= 1/$\alpha$ 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 $\theta_{w,cz}$.

Carsel and Parrish (1988) computed mean values of the van Genuchten soil water retention curve parameters for the 12 Soil Conservation Service (SCS) soil textural classifications. The data base used to develop the mean values presented in Table 2 was developed from sampling data representing 42 States and ranged from sample population sizes of 46 to 1,183. With these data, a general estimate can be made of the values of $\theta_{w,cz}$ and $\theta_{a,cz}$ for each soil 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:

## TABLE 2. MEAN VALUES OF THE VAN GENUCHTEN SOIL WATER RETENTION PARAMETERS FOR THE 12 SCS SOIL TYPES

| Soil texture (USDA) | Saturated water content, $\theta_s$ | Residual water Content, $\theta_r$ | Van Genuchten parameters | | | Number of samples[a] |
|---|---|---|---|---|---|---|
| | | | $\alpha$ (1/cm) | N | M | |
| Clayey soil[b] | 0.38 | 0.068 | 0.008 | 1.09 | 0.083 | 400 |
| Clay loam | 0.41 | 0.095 | 0.019 | 1.31 | 0.237 | 364 |
| Loam | 0.43 | 0.078 | 0.036 | 1.56 | 0.359 | 735 |
| Loamy sand | 0.41 | 0.057 | 0.124 | 2.28 | 0.561 | 315 |
| Silt | 0.46 | 0.034 | 0.016 | 1.37 | 0.270 | 82 |
| Silt loam | 0.45 | 0.067 | 0.020 | 1.41 | 0.291 | 1093 |
| Silty clay | 0.26 | 0.070 | 0.005 | 1.09 | 0.083 | 374 |
| Silty clay loam | 0.43 | 0.089 | 0.010 | 1.23 | 0.187 | 641 |
| Sand | 0.43 | 0.045 | 0.145 | 2.68 | 0.627 | 246 |
| Sandy clay | 0.38 | 0.100 | 0.027 | 1.23 | 0.187 | 46 |
| Sandy clay loam | 0.39 | 0.100 | 0.059 | 1.48 | 0.324 | 214 |
| Sandy loam | 0.41 | 0.065 | 0.075 | 1.89 | 0.471 | 1183 |

[a] Number of samples as indicated with minor exceptions; see Carsel and Parrish (1988).
[b] Clay soil refers to agricultural soil with < 60 percent clay.

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

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.

The value of $C_{source}$ is calculated using Equation 2; the value of A is assumed to be one $cm^2$; 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 capillarity 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:

$$L_{cz} = \frac{2 \;\; \alpha \;\; COS \;\; \lambda}{\rho_w \;\; g \;\; R} \tag{8}$$

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

$\sigma$ = Surface tension of water, g/s (= 73)

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

$\rho_w$ = Density of water, g/cm$^3$ (= 0.999)

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

R = Mean interparticle pore radius, cm

and,

$$R = 0.2D \tag{9}$$

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 10° and 20°C, Equation 8 reduces to:

$$L_{cz} = \frac{0.15}{R} \quad . \tag{10}$$

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 3 shows the centroid compositions and mean particle sizes of the 12 SCS soil textural classes.

Given the mean particle diameter data in Table 3, 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:

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

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.

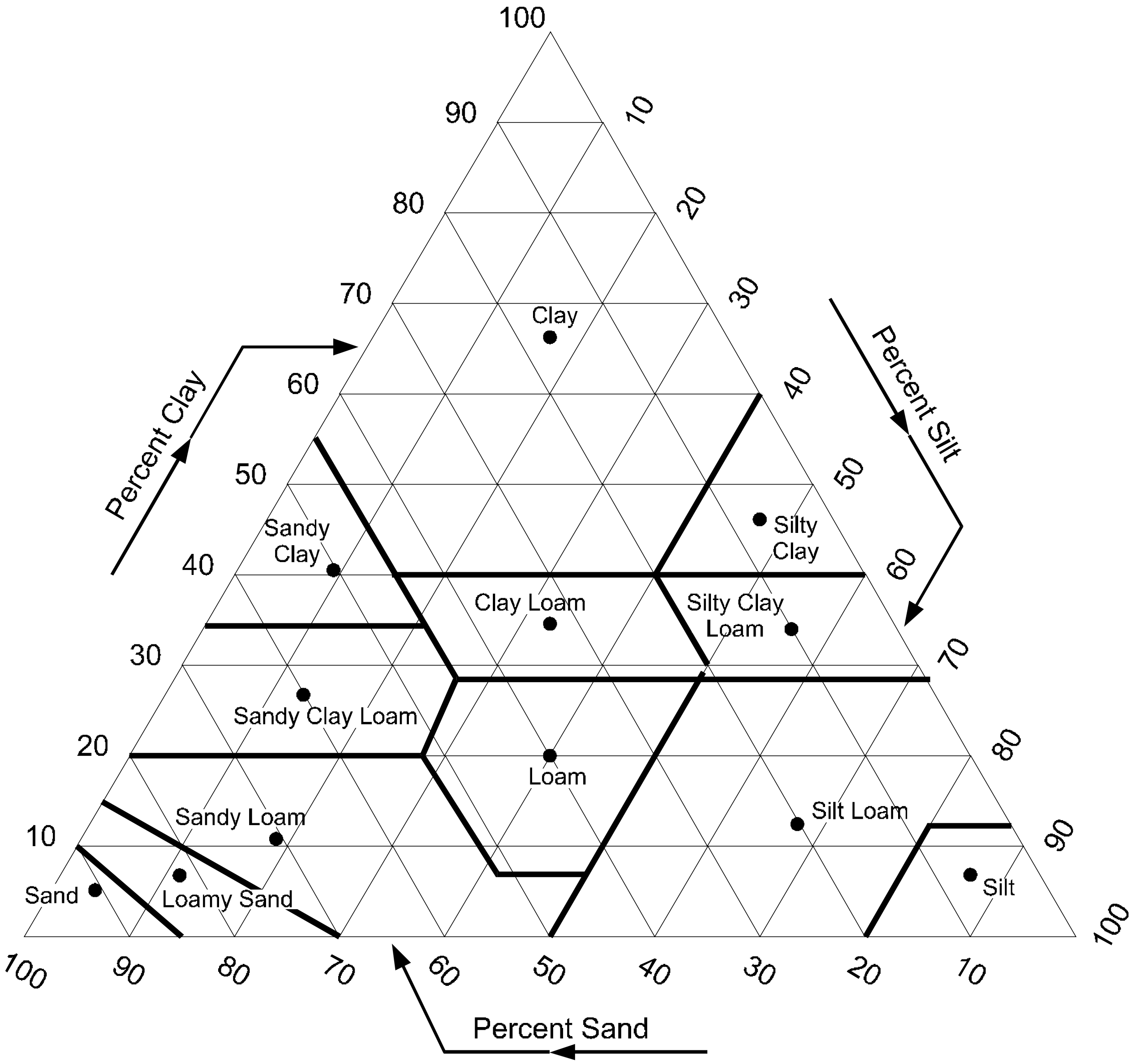


Figure 3. U.S. Soil Conservation Service Classification Chart Showing Centroid Compostions (Solid Circles)

TABLE 3. CENTROID COMPOSITIONS AND MEAN PARTICLE DIAMETERS OF THE 12 SCS SOIL CLASSIFICATIONS

| Textural class | % clay | % silt | % sand | Arithmetic mean particle diameter, cm |
|---|---|---|---|---|
| Sand | 3.33 | 5.00 | 91.67 | 0.044 |
| Loamy sand | 6.25 | 11.25 | 82.50 | 0.040 |
| Sandy loam | 10.81 | 27.22 | 61.97 | 0.030 |
| Sandy clay loam | 26.73 | 12.56 | 60.71 | 0.029 |
| Sandy clay | 41.67 | 6.67 | 51.66 | 0.025 |
| Loam | 18.83 | 41.01 | 40.16 | 0.020 |
| Clay loam | 33.50 | 34.00 | 32.50 | 0.016 |
| Silt loam | 12.57 | 65.69 | 21.74 | 0.011 |
| Clay | 64.83 | 16.55 | 18.62 | 0.0092 |
| Silty clay loam | 33.50 | 56.50 | 10.00 | 0.0056 |
| Silt | 6.00 | 87.00 | 7.00 | 0.0046 |
| Silty clay | 46.67 | 46.67 | 6.66 | 0.0039 |

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 (infinite source), Johnson and Ettinger (1991) give the solution for the attenuation coefficient (α) as:

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

where α = Infinite source 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:

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

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, $cm^3/s$

$\pi$ = 3.14159

$\Delta P$ = Pressure differential between the soil surface and the enclosed space, g/cm-s$^2$

$k_v$ = Soil vapor permeability, cm$^2$

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

$\mu$ = 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 Johnson and Ettinger (1991) as:

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

where $r_{crack}$ = Equivalent crack radius, cm

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

$A_B$ = 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 ($\eta$) 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 ($\eta$) remains constant, the value of $r_{crack}$ must also vary. The total area of cracks ($A_{crack}$) is the product of $\eta$ 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 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 $\alpha$ 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 $\alpha$ is set equal to Equation 18.

With a calculated value of $\alpha$, 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 Johnson and Ettinger (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 $\langle\alpha\rangle$ = Time-averaged finite source attenuation coefficient, unitless

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

$C_R$ = Initial soil concentration, g/g

$\Delta H_c$ = 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

$\tau$ = 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" ($\delta$) which grows with time; conversely, the "wet zone" of contamination retreats proportionally. When the thickness of the depletion zone ($\delta$) is equal to the initial thickness of contamination ($\Delta H_c$), 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 $\tau$. 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 ($\tau_D$) 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 ($\tau$) is greater than the time for source depletion ($\tau_D$), 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

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

$C_R$ = Initial soil concentration, g/g

$\Delta H_c$ = Initial thickness of contamination, cm

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

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

$\tau$ = Exposure interval, s.

## 2.7 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 hydraulic conductivity:

$$k_i = \frac{K_s \, \mu_w}{\rho_w \; g} \tag{26}$$

where $k_i$ = Soil intrinsic permeability, cm$^2$

$K_s$ = Soil saturated hydraulic conductivity, cm/s

$\mu_w$ = Dynamic viscosity of water, g/cm-s (= 0.01307 at 10°C)

$\rho_w$ = Density of water, g/cm$^3$ (= 0.999)

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

Carsel and Parrish (1988) estimated the mean saturated hydraulic conductivity ($K_s$) of the 12 SCS soil textural classifications (Table 4). With these values, a general estimate of the value of $k_i$ can be made by soil type.

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.

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.

## TABLE 4. MEAN VALUES OF SATURATED HYDRAULIC CONDUCTIVITY FOR THE 12 SCS SOIL TEXTURAL CLASSIFICATIONS

| Soil texture , USDA | Saturated hydraulic conductivity, cm/h |
|---|---|
| Sand | 29.70 |
| Loamy sand | 14.59 |
| Sandy loam | 4.42 |
| Sandy clay loam | 1.31 |
| Sandy clay | 0.12 |
| Loam | 1.04 |
| Clay loam | 0.26 |
| Silt loam | 0.45 |
| Clay | 0.20 |
| Silty clay loam | 0.07 |
| Silt | 0.25 |
| Silty clay | 0.02 |

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

$\theta_w$ = Soil water-filled porosity, $cm^3/cm^3$

$\theta_r$ = Residual soil water content, $cm^3/cm^3$

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

Mean values for the parameters $\theta_r$ and M by SCS soil type may be obtained from Table 2.

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 fixed soil water-filled porosity $\theta_w$.

## 2.8 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:

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

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 accompanying 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.

## 2.9 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:

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

## 2.10 MAJOR MODEL ASSUMPTIONS/LIMITATIONS

The following represent the major assumptions/limitations of the Johnson and Ettinger model. Additional assumptions specific to the application of the model as applied in the accompanying spreadsheets are contained in Section 5.

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.

# SECTION 3

# MODEL APPLICATION

This section provides step-by-step instructions on how to implement the Johnson and Ettinger model using the accompanying spreadsheets. 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, out of range, or outside of permitted limits.

## 3.1 RUNNING THE MODELS

Four different models are provided as both MICROSOFT EXCEL and LOTUS 1-2-3 spreadsheets.

1. Screening-Level Models for Soil Contamination:
    - SLSCREEN.XLS (EXCEL)
    - SLSCREEN.WK4 (1-2-3)
2. Screening-Level Models for Groundwater Contamination:
    - GWSCREEN.XLS (EXCEL)
    - GWSCREEN.WK4 (1-2-3)
3. Tier-2 Models for Soil Contamination:
    - SLTIER2.XLS (EXCEL)
    - SLTIER2.WK4 (1-2-3)

4. Tier-2 Models for Groundwater Contamination:

   - GWTIER2.XLS (EXCEL)
   - GWTIER2.WK4 (1-2-3).

Both the screening-level models and the tier-2 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 tier-2 models provide the user with the ability to enter data for all of the model parameters and also incorporates 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 either MICROSOFT EXCEL or LOTUS 1-2-3. 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, data entry conventions, how to interpret model results, and how to add/revise the chemical properties data found in the VLOOKUP Tables. As an example, Appendix A contains all the worksheets for the tier-2 soil contamination model SLTIER2.

Note: Because of the limitations of LOTUS 1-2-3, variable names (e.g., $\Delta H_C$) appear in alphanumeric characters. Subscripts are preceded by the symbol "~" and superscripts are preceded by the symbol "∧." Upper case greek characters are spelled with an initial capital letter and lower case greek characters are spelled in lower case. For example, the variable $\Delta H_C$ would appear as "Delta H~c" while the variable $D_T^{eff}$ would appear as "D~T∧eff."

## 3.2 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 (GWSCREEN). Figure 5 is an example of a tier-2 model data entry sheet (GWTIER2). Note that the screening-level model sheet requires entry of considerably less data than does the tier-2 sheet. To enter data, simply position the cursor within the appropriate box and type the value; all other cells are protected.

### 3.2.1 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 tier-2 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.

Figure 6 is an example of an error message appearing on the data entry sheet. Figure 7 illustrates error messages appearing within the error summary section on the results sheet (tier-2 models only).

### 3.2.2 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 tier-2 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

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**<br>Chemical CAS No. (numbers only, no dashes) | **ENTER**<br>Initial groundwater conc., $C_W$ ($\mu$g/L) | Chemical |
|---|---|---|
| 56235 | | Carbon tetrachloride |

| **ENTER**<br>Depth below grade to bottom of enclosed space floor, $L_F$ (cm) | **ENTER**<br>Depth below grade to water table, $L_{WT}$ (cm) | **ENTER**<br>SCS soil type directly above water table | **ENTER**<br>Average soil/ groundwater temperature, $T_S$ ($^{o}$C) |
|---|---|---|---|
| 200 | 400 | SC | 10 |

| **ENTER**<br>Vadose zone SCS soil type (used to estimate soil vapor permeability) | OR | **ENTER**<br>User-defined vadose zone soil vapor permeability, $k_v$ (cm$^2$) | **ENTER**<br>Vadose zone soil dry bulk density, $\rho_b^V$ (g/cm$^3$) | **ENTER**<br>Vadose zone soil total porosity, $n^V$ (unitless) | **ENTER**<br>Vadose zone soil water-filled porosity, $\theta_w^V$ (cm$^3$/cm$^3$) |
|---|---|---|---|---|---|
| SC | | | 1.5 | 0.43 | 0.3 |

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

Figure 4. GWSCREEN 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. below)

YES ☐

| **ENTER**<br>Chemical CAS No. (numbers only, no dashes) | **ENTER**<br>Initial groundwater conc., $C_W$ ($\mu$g/L) | Chemical |
|---|---|---|
| 56235 | | Carbon tetrachloride |

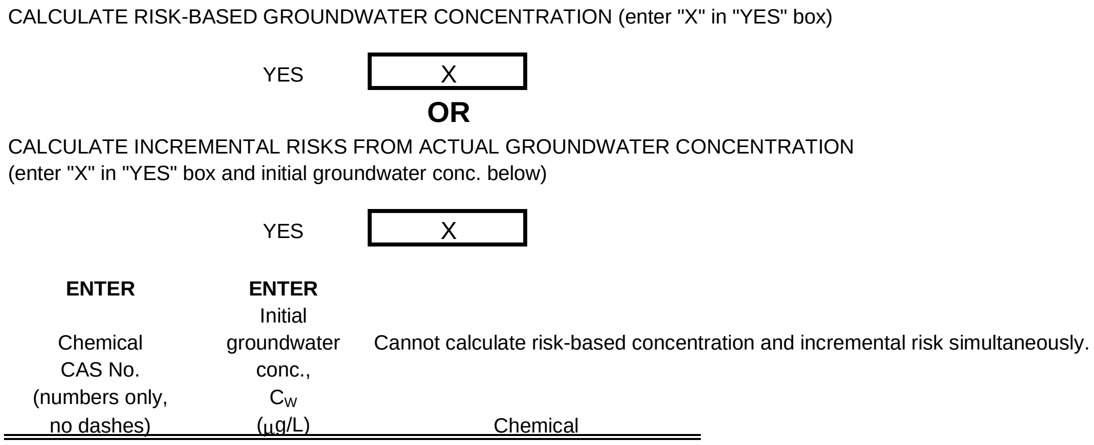
| **ENTER**<br>Average soil/ groundwater temperature, $T_S$ (°C) | **ENTER**<br>Depth below grade to bottom of enclosed space floor, $L_F$ (cm) | **ENTER**<br>Depth below grade to water table, $L_{WT}$ (cm) | **ENTER**<br>Totals must add up to value of $L_{WT}$ (cell D28)<br>Thickness of soil stratum A, $h_A$ (cm) | **ENTER**<br>Thickness of soil stratum B, (Enter value or 0) $h_B$ (cm) | **ENTER**<br>Thickness of soil stratum C, (Enter value or 0) $h_C$ (cm) | **ENTER**<br>Soil stratum directly above water table, (Enter A, B, or C) | **ENTER**<br>SCS soil type directly above water table | **ENTER**<br>Soil stratum A SCS soil type (used to estimate soil vapor permeability) | OR | **ENTER**<br>User-defined stratum A soil vapor permeability, $k_v$ (cm$^2$) |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | 200 | 400 | 300 | 50 | 50 | C | SC | C | | |

| **ENTER**<br>Stratum A soil dry bulk density, $\rho_b^A$ (g/cm$^3$) | **ENTER**<br>Stratum A soil total porosity, $n^A$ (unitless) | **ENTER**<br>Stratum A soil water-filled porosity, $\theta_w^A$ (cm$^3$/cm$^3$) | **ENTER**<br>Stratum B soil dry bulk density, $\rho_b^B$ (g/cm$^3$) | **ENTER**<br>Stratum B soil total porosity, $n^B$ (unitless) | **ENTER**<br>Stratum B soil water-filled porosity, $\theta_w^B$ (cm$^3$/cm$^3$) | **ENTER**<br>Stratum C soil dry bulk density, $\rho_b^C$ (g/cm$^3$) | **ENTER**<br>Stratum C soil total porosity, $n^C$ (unitless) | **ENTER**<br>Stratum C soil water-filled porosity, $\theta_w^C$ (cm$^3$/cm$^3$) |
|---|---|---|---|---|---|---|---|---|
| 1.5 | 0.43 | 0.2 | 1.7 | 0.42 | 0.27 | 1.7 | 0.43 | 0.3 |

| **ENTER**<br>Enclosed space floor thickness, $L_{crack}$ (cm) | **ENTER**<br>Soil-bldg. pressure differential, $\Delta P$ (g/cm-s$^2$) | **ENTER**<br>Enclosed space floor length, $L_B$ (cm) | **ENTER**<br>Enclosed space floor width, $W_B$ (cm) | **ENTER**<br>Enclosed space height, $H_B$ (cm) | **ENTER**<br>Floor-wall seam crack width, w (cm) | **ENTER**<br>Indoor air exchange rate, ER (1/h) |
|---|---|---|---|---|---|---|
| 15 | 40 | 961 | 961 | 488 | 0.1 | 0.45 |

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

Figure 5. GWTIER2 Data Entry Sheet



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

YES ☒

**OR**

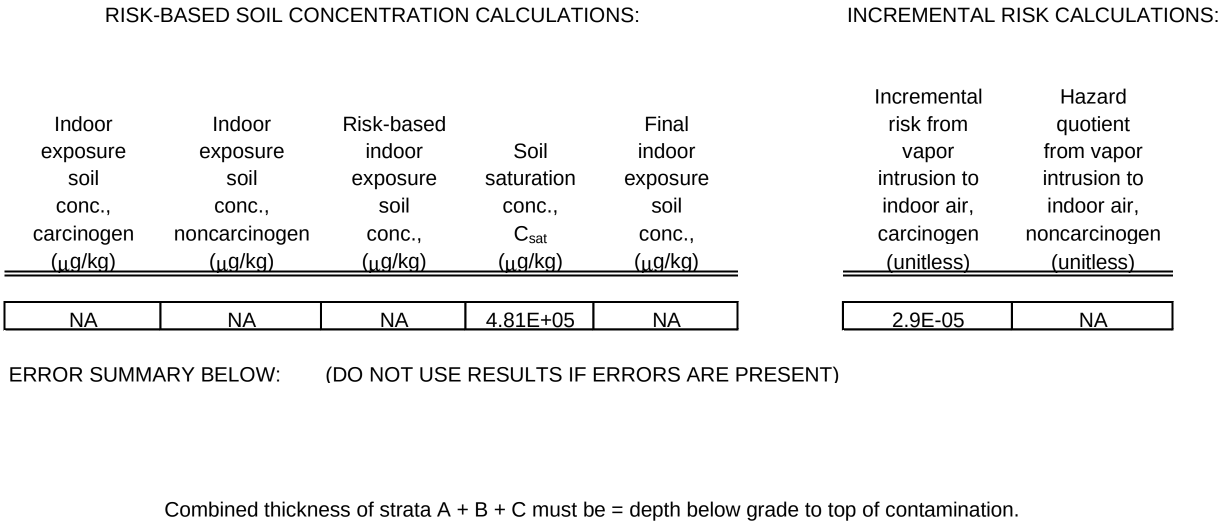
CALCULATE INCREMENTAL RISKS FROM ACTUAL GROUNDWATER CONCENTRATION
(enter "X" in "YES" box and initial groundwater conc. below)

YES ☒

| **ENTER**<br>Chemical CAS No. (numbers only, no dashes) | **ENTER**<br>Initial groundwater conc., $C_W$ ($\mu$g/L) | Chemical |
|---|---|---|

Cannot calculate risk-based concentration and incremental risk simultaneously.

Figure 6.  Example Error Message on Data Entry Sheet



RISK-BASED SOIL CONCENTRATION CALCULATIONS:

| Indoor exposure soil conc., carcinogen ($\mu$g/kg) | Indoor exposure soil conc., noncarcinogen ($\mu$g/kg) | Risk-based indoor exposure soil conc., ($\mu$g/kg) | Soil saturation conc., $C_{sat}$ ($\mu$g/kg) | Final indoor exposure soil conc., ($\mu$g/kg) |
|---|---|---|---|---|
| NA | NA | NA | 4.81E+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) |
|---|---|
| 2.9E-05 | NA |

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

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

Figure 7.  Example Error Message on Results Sheet

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 B.

1. *Calculate Risk-Based Concentration* OR *Calculate Incremental Risks from Actual Concentration* (All 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 97 chemicals and their associated properties are included with each model; see Section 4.4 for instructions on adding/revising chemicals.

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

   Enter a value only if incremental risks are to be calculated.  Be sure to enter the concentration in units of μg/kg (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)

   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.  Another source of information may be your State groundwater protection regulatory agency.

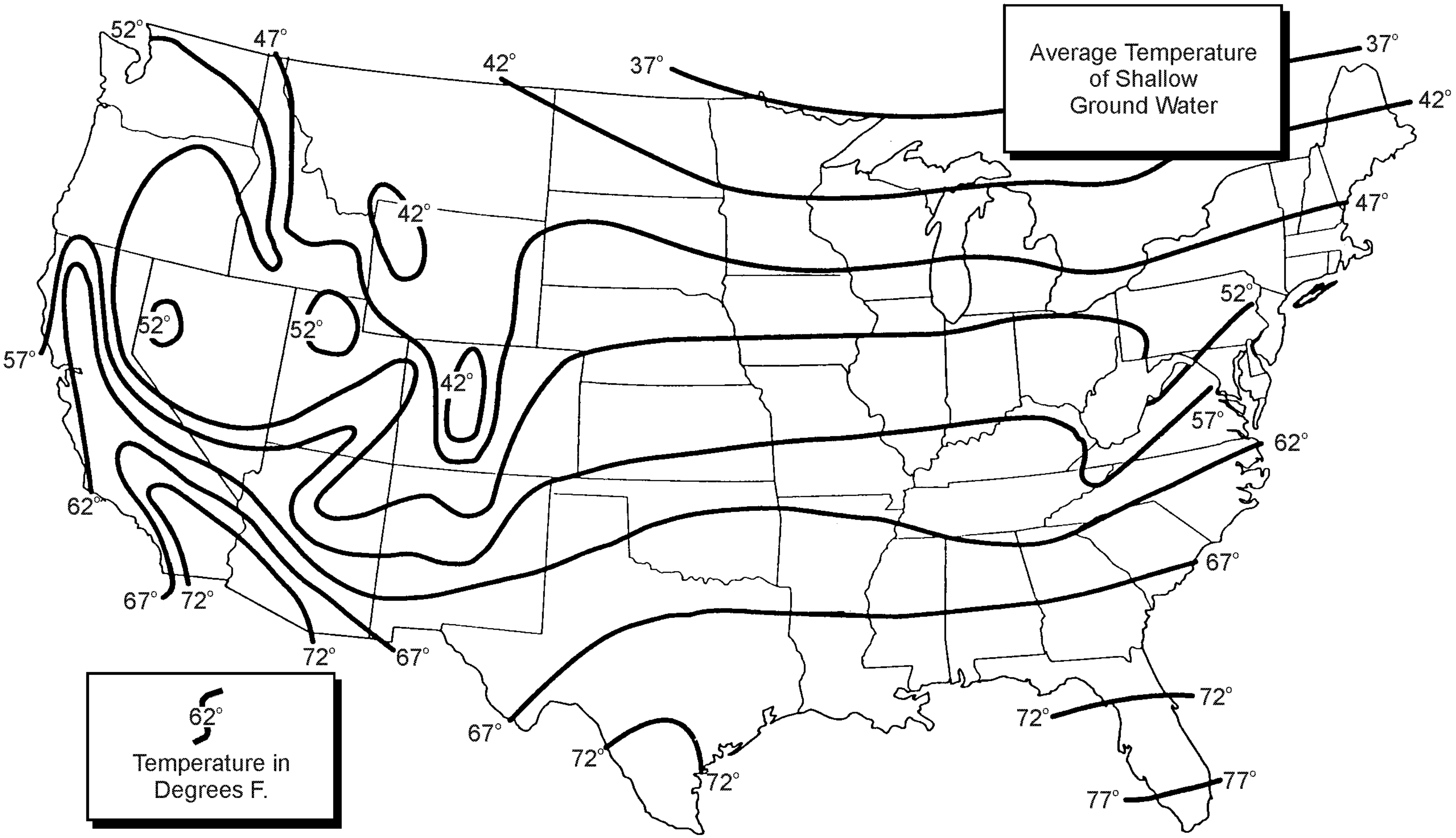


Figure 8.  Average Shallow Groundwater Temperature in the United States

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

   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)

   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.

7. *Depth Below Grade to Water Table* (Groundwater Models Only)

   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 type 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* (Soil Tier-2 Model Only)

   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"* (Tier-2 Models Only)

In the tier-2 models, the user can define up to three soil strata between the soil surface and the top of contamination. 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 top of the water table, 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* (Tier-2 Models Only)

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 | Silt loam |
| SL | Sandy loam |

To determine the correct soil type, see the SCS soil textural classification triangle in Figure 3.

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* (Tier-2 Models Only)

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 | $1.0 \times 10^{-7}$ to $1.0 \times 10^{-6}$ |
| Fine sand | $1.0 \times 10^{-8}$ to $1.0 \times 10^{-7}$ |
| Silty sand | $1.0 \times 10^{-9}$ to $1.0 \times 10^{-8}$ |
| Clayey silts | $1.0 \times 10^{-10}$ to $1.0 \times 10^{-9}$ |

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

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

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

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* (Groundwater Tier-2 Models Only)

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

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

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* (Tier-2 Models Only)

Enter the average soil dry bulk density for the appropriate soil stratum. 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* (Tier-2 Models Only)

Total soil porosity (n) is determined as:

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

where $\rho_b$ is the soil dry bulk density (g/cm$^3$) and $\rho_s$ is the soil particle density (usually 2.65 g/cm$^3$).

18. *Stratum "X" Soil Water-Filled Porosity* (Tier-2 Models Only)

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 as they may not be representative of long-term conditions.

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 rainfall 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 2 and 4 (i.e., $\theta_s$, $\theta_r$, N, $\alpha$, and $K_s$). The HYDRUS model is available from the U.S. Department of Agriculture - Agricultural Research Service in Riverside, California via their internet website at http://www.ussl.ars.usda.gov/MODELS/HYDRUS.HTM.

Schapp et al. (1997) recently developed a hierarchical neural network approach to predict van Genuchten (1980) soil hydraulic properties from basic soil properties. They concluded that of all the published models with which they compared their results, only the models of Vereecken et al. (1989) compared favorably. Vereecken et al. (1989) and Vereecken et al. (1990) developed a series of nonlinear regression equations to predict the soil hydraulic parameters of van Genuchten (1980) using simple soil properties such as particle size distribution, dry bulk density, and carbon content. With estimates of these values, the HYDRUS model may be employed to calculate long-term average soil moisture contents by soil stratum.

19. *Stratum "X" Soil Organic Carbon Fraction* (Soil Tier-2 Models Only)

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 (Nelson and Sommers, 1982). 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)

Because the screening-level models accommodate only one soil stratum above the top of contamination, enter the depth-averaged soil dry bulk density. The 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)

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)

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)

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* (Tier-2 Models Only)

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 15 cm which is consistent with Johnson and Ettinger (1991).

25. *Soil-Building Pressure Differential* (Tier-2 Models Only)

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 ($\Delta P$) 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 $\Delta P$ is 0-20 Pascals (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 $\Delta P$ was therefore chosen to be 4 Pa (40 $g/cm\text{-}s^2$).

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

26. *Enclosed Space Floor Length* (Tier-2 Models Only)

The default value is 961 cm (see Variable No. 28).

27. *Enclosed Space Floor Width* (Tier-2 Models Only)

The default value is 961 cm (see Variable No. 28).

28. *Enclosed Space Height* (Tier-2 Models Only)

The default values of the enclosed space length, width, and height were derived from the average estimated volume of both owner-occupied and rental single-family detached residences in the U.S. (U.S. DOE, 1995). These dimensions assume a living space volume of 451 $m^3$ divided into two stories of equal volume with ceiling heights of 8 ft (2.44 m). Each floor is assumed to be a square with a total floor area of 92.42 $m^2$ and equal lengths and widths of 9.61 m. The total height of the living space is 2 x 2.44 m or 4.88 m.

29. *Floor-Wall Seam Crack Width* (Tier-2 Models Only)

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-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 joints between wall and floor slabs of residential structures in Canada of approximately 300 $cm^2$. Therefore, given the default floor length and width of 961 cm, a gap width (w) of 0.1 cm equates to a total gap area of 384 $cm^2$, 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* (Tier-2 Models Only)

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 0.45/h. This value is consistent with both the geometric mean and the 50th percentile of houses in all regions of the U.S. as reported in Koontz and Rector (1995). This value is also consistent with the average 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.

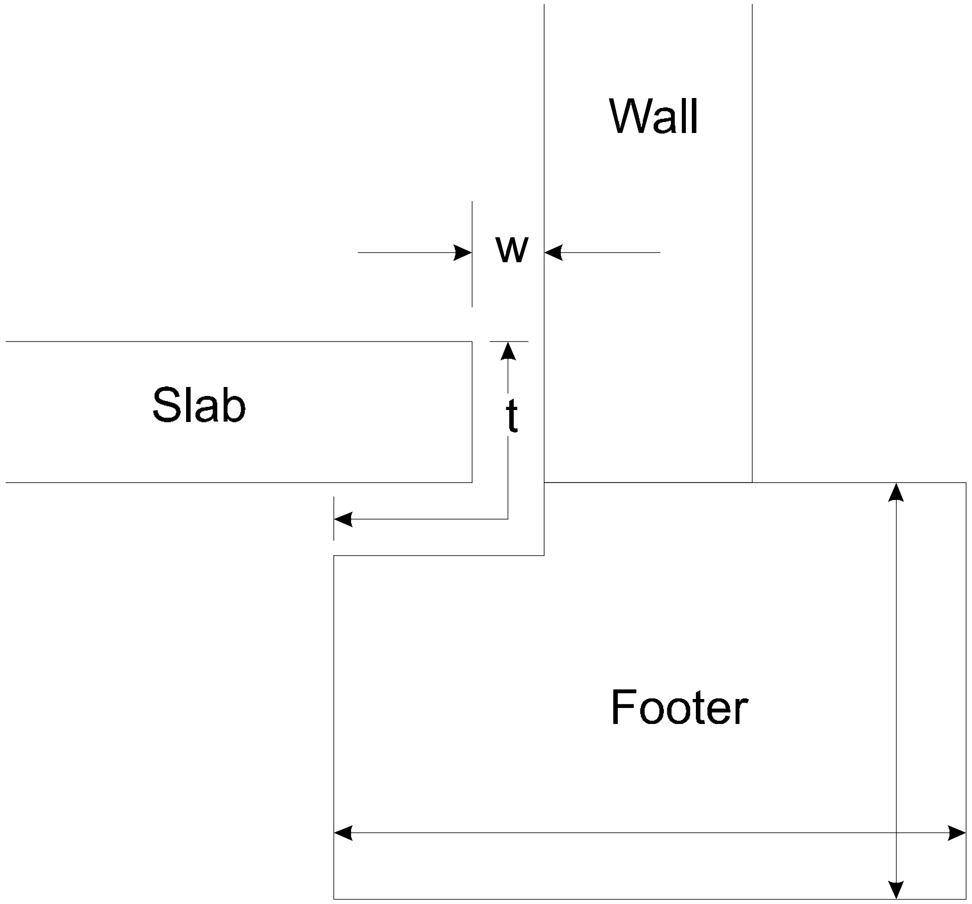


Figure 9. Floor Slab and Foundation

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

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

32. *Averaging Time for Noncarcinogens* (All Models)

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)

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)

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 Models)

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

36. *Target Hazard quotient for Noncarcinogens* (All Models)

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

# SECTION 4

# THE RESULTS SHEET AND ANCILLARY SHEETS

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).

## 4.1 THE RESULTS SHEET (RESULTS)

Once all data are entered in the data entry sheet, the model results may be viewed on the RESULTS sheet. Model 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 tier-2 models, the user should check the 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. All data in the results sheet are protected.

## 4.2 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.

## 4.3 THE INTERMEDIATE CALCULATIONS SHEET (INTERCALCS)

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.

## 4.4 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 Carsel and Parrish (1988) (see Tables 2 and 4) and the mean grain diameter data of Nielson and Rogers (1990) (see Table 3) by SCS soil type. The second table contains all of the chemical and toxicological data for all of the chemicals included with each model.

Data for any chemical may be edited, new chemicals added, or existing chemicals deleted from the Chemical Properties Lookup Table. To begin an editing session, the user must unprotect (unseal) the worksheet (the password is "ABC" in capital letters); editing of individual elements or deletion of chemicals may then proceed. Space has been allocated for up to 150 chemicals in the lookup table. Row number 171 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 5

# MODEL ASSUMPTIONS AND LIMITATIONS

The following is a discussion of the major assumptions and limitations of the Johnson and Ettinger vapor intrusion model as well as the ancillary models for estimating the vapor concentration at the source of contamination, soil vapor permeability, the rise of the capillary zone, and the effective diffusion coefficient across the capillary zone.

## 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) and will overpredict vapor concentrations in such cases. 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. Therefore, use of these models to calculate incremental risks under inappropriate conditions will cause erroneous results.

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, the final soil concentration will be set equal to the soil saturation concentration. This tends to eliminate the possibility of allowing a residual phase to exist within the soil column.

Likewise, the groundwater models will compare the calculated risk-based groundwater concentration to the aqueous solubility limit of the compound and will limit the allowed concentration to a value less than or equal to the solubility limit.

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 pump 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.

## 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 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 is 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 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 episodic rises 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 Johnson and Ettinger 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 differential (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 transport by convection (e.g., water infiltration) and by mechanical dispersion are neglected. Transformation processes (e.g., biodegradation, hydrolysis, etc.) are also neglected.

A recent empirical field study (Fitzpatrick and Fitzgerald, 1997) indicates that the model may be overly conservative for nonchlorinated species (e.g., benzene, toluene, ethybenzene 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 Johnson and Ettinger 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

# VALUES FOR INPUT VARIABLES

The Johnson and Ettinger model as constructed within the accompanying spreadsheets requires a range of input variables depending on whether a screening-level or tier-2 model is chosen.

Table 5 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 5 also includes references for each value or range of values.

Table 6 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.

# TABLE 5. RANGE OF VALUES, SENSITIVITY, AND UNCERTAINTY OF MODEL INPUT PARAMETERS

| Input parameter | Practical range of values | Default value | Relative model sensitivity | Relative uncertainty |
|---|---|---|---|---|
| Soil water-filled porosity ($\theta_w$) | 0.02 -0.43 $cm^3/cm^3$[a] | 0.30 $cm^3/cm^3$[a] | High | High |
| Soil vapor permeability ($k_v$) | $10^{-6}$ - $10^{-12}$ $cm^2$[b,c] | $10^{-8}$ $cm^2$[d] | High | High |
| Soil-building pressure differential ($\Delta P$) | 0 - 20 Pa[e] | 4 Pa[f] | High | High |
| Media initial concentration ($C_R$, $C_w$) | User-defined | NA | High | Moderate |
| Depth to bottom of soil contamination ($L_b$) | User-defined | NA | High | Moderate |
| Depth to top of contamination ($L_T$) | User-defined | NA | High | Low |
| Floor-wall seam gap (w) | 0.05 - 1.0 cm[e] | 0.1 cm[e] | Moderate | High |
| Soil organic carbon fraction ($f_{oc}$) | 0.001 - 0.006[a] | 0.002[a] | Moderate | Moderate |
| Building air exchange rate (ER) | 0.18 - 1.26 ($h^{-1}$)[g] | 0.45 ($h^{-1}$)[g,h] | Moderate | Moderate |
| Building volume | 147 - 672 $m^3$[i] | 451 $m^3$[I] | Moderate | Low |
| Soil total porosity (n) | 0.34 - 0.53 $cm^3/cm^3$[a] | 0.43 $cm^3/cm^3$[a] | Moderate | Low |
| Soil dry bulk density ($\rho_b$) | 1.25 - 1.75 $g/cm^3$[a] | 1.5 $g/cm^3$[a] | Low | Low |

[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 6. 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 ($\theta_w$) | Increase | Decrease |
| Soil vapor permeability ($k_v$) | Increase | Increase |
| Soil-building pressure differential ($\Delta P$) | 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 contamination ($L_t$) | Increase | Decrease |
| Floor-wall seam gap (w) | Increase | Increase |
| Soil organic carbon fraction ($f_{oc}$) | Increase | Decrease |
| Building air exchange rate (ER) | Increase | Decrease |
| Building volume[c] | Increase | Decrease |
| Soil total porosity (n) | Increase | Increase |
| Soil dry bulk density ($\rho_b$) | Increase | Decrease |

[a] This parameter is applicable only when forward-calculating risk.
[b] Applicable only to tier-2 model for soil contamination.
[c] Used with building air exchange rate to calculate building ventilation rate.

## SECTION 7

## 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 Johnson and Ettinger 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 monitoring 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 an actual or hypothetical structure. Once a representative average concentration is determined, all vapor directly below the areal extent of the building is presumed to enter the structure. This concentration, along with the building ventilation rate, will determine the indoor concentration. When using soil gas measurements, it must be remembered that no analysis has been made concerning the source of contamination. Therefore, the calculated indoor concentration must be assumed to be steady-state. Soil gas monitoring may also be used to help calibrate the theoretical equilibrium partitioning and diffusion transport considerations of the model. The reader is 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 has been limited to radon studies 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.

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# APPENDIX A

# EXAMPLE WORKSHEETS FOR THE TIER-2 SOIL CONTAMINATION MODEL

# DATA ENTRY SHEET

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 |

| **ENTER** Average soil temperature, $T_S$ ($^{\circ}$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 D28) 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 | SCL | | |

| **ENTER** Stratum A soil dry bulk density, $\rho_b^A$ (g/cm$^3$) | **ENTER** Stratum A soil total porosity, $n^A$ (unitless) | **ENTER** Stratum A soil water-filled porosity, $\theta_w^A$ (cm$^3$/cm$^3$) | **ENTER** Stratum A soil organic carbon fraction, $f_{oc}^A$ (unitless) | **ENTER** Stratum B soil dry bulk density, $\rho_b^B$ (g/cm$^3$) | **ENTER** Stratum B soil total porosity, $n^B$ (unitless) | **ENTER** Stratum B soil water-filled porosity, $\theta_w^B$ (cm$^3$/cm$^3$) | **ENTER** Stratum B soil organic carbon fraction, $f_{oc}^B$ (unitless) | **ENTER** Stratum C soil dry bulk density, $\rho_b^C$ (g/cm$^3$) | **ENTER** Stratum C soil total porosity, $n^C$ (unitless) | **ENTER** Stratum C soil water-filled porosity, $\theta_w^C$ (cm$^3$/cm$^3$) | **ENTER** Stratum C soil organic carbon fraction, $f_{oc}^C$ (unitless) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.5 | 0.43 | 0.15 | 0.006 | 1.5 | 0.43 | 0.25 | 0.003 | 1.7 | 0.34 | 0.26 | 0.002 |

| **ENTER** Enclosed space floor thickness, $L_{crack}$ (cm) | **ENTER** Soil-bldg. pressure differential, $\Delta P$ (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) |
|---|---|---|---|---|---|---|
| 15 | 40 | 961 | 961 | 488 | 0.1 | 0.45 |

| **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. | |

## 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 ($mg/m^3$) |
|---|---|---|---|---|---|---|---|---|---|---|
| 8.80E-02 | 9.80E-06 | 5.56E-03 | 25 | 7,342 | 353.24 | 562.16 | 5.89E+01 | 1.75E+03 | 8.3E-06 | 0.0E+00 |

INTERMEDIATE CALCULATIONS SHEET

| Exposure duration, $\tau$ (sec) | Source-building separation, $L_T$ (cm) | Stratum A soil air-filled porosity, $\theta_a^A$ (cm$^3$/cm$^3$) | Stratum B soil air-filled porosity, $\theta_a^B$ (cm$^3$/cm$^3$) | Stratum C soil air-filled porosity, $\theta_a^C$ (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, $C_R$ (µg/kg) | Bldg. ventilation rate, $Q_{building}$ (cm$^3$/s) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 9.46E+08 | 200 | 0.280 | 0.180 | 0.080 | 0.152 | 4.85E-09 | 0.919 | 4.46E-09 | 3,844 | 1 | 5.63E+04 |

| Area of enclosed space below grade, $A_B$ (cm$^2$) | Crack-to-total area ratio, $\eta$ (unitless) | Crack depth below grade, $Z_{crack}$ (cm) | Enthalpy of vaporization at ave. groundwater temperature, $\Delta H_{v,TS}$ (cal/mol) | Henry's law constant at ave. groundwater temperature, $H_{TS}$ (atm-m$^3$/mol) | Henry's law constant at ave. groundwater temperature, $H'_{TS}$ (unitless) | Vapor viscosity at ave. soil temperature, $\mu_{TS}$ (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) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.69E+06 | 2.27E-04 | 200 | 8,122 | 2.69E-03 | 1.16E-01 | 1.75E-04 | 6.86E-03 | 1.58E-03 | 1.78E-04 | 3.19E-04 | 200 | 200 |

| Soil-water partition coefficient, $K_d$ (cm$^3$/g) | Source vapor conc., $C_{source}$ (µg/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, $\alpha$ (unitless) | Infinite source bldg. conc., $C_{building}$ (µg/m$^3$) | Finite source $\beta$ term (unitless) | Finite source $\psi$ term (sec)$^{-1}$ | Time for source depletion, $\tau_D$ (sec) | Exposure duration > time for source depletion (YES/NO) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.18E-01 | 4.19E+02 | 0.10 | 2.96E+00 | 6.86E-03 | 3.84E+02 | 2.07E+07 | NA | NA | 1.91E+00 | 1.97E-09 | 1.23E+09 | NO |

| Finite source indoor attenuation coefficient, $<\alpha>$ (unitless) | Mass limit bldg. conc., $C_{building}$ (µg/m$^3$) | Finite source bldg. conc., $C_{building}$ (µg/m$^3$) | Final finite source bldg. conc., $C_{building}$ (µg/m$^3$) | Unit risk factor, URF (µg/m$^3$)$^{-1}$ | Reference conc., RfC (mg/m$^3$) |
|---|---|---|---|---|---|
| 2.07E-05 | NA | 8.69E-03 | 8.69E-03 | 8.3E-06 | NA |

## 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) |
|---|---|---|---|---|
| 3.37E+01 | NA | 3.37E+01 | 4.83E+05 | 3.37E+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 |

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

# VLOOKUP TABLES

Soil Properties Lookup Table

| SCS Soil Type | $K_s$ (cm/h) | $\alpha$ (1/cm) | N (unitless) | M (unitless) | $\theta_s$ ($cm^3/cm^3$) | $\theta_r$ ($cm^3/cm^3$) | Mean Grain Diameter (cm) |
|---|---|---|---|---|---|---|---|
| C | 0.20 | 0.008 | 1.09 | 0.083 | 0.38 | 0.068 | 0.0092 |
| CL | 0.26 | 0.019 | 1.31 | 0.237 | 0.41 | 0.095 | 0.016 |
| L | 1.04 | 0.036 | 1.56 | 0.359 | 0.43 | 0.078 | 0.020 |
| LS | 14.59 | 0.124 | 2.28 | 0.561 | 0.41 | 0.057 | 0.040 |
| S | 29.70 | 0.145 | 2.68 | 0.627 | 0.43 | 0.045 | 0.044 |
| SC | 0.12 | 0.027 | 1.23 | 0.187 | 0.38 | 0.100 | 0.025 |
| SCL | 1.31 | 0.059 | 1.48 | 0.324 | 0.39 | 0.100 | 0.029 |
| SI | 0.25 | 0.016 | 1.37 | 0.270 | 0.46 | 0.034 | 0.0046 |
| SIC | 0.02 | 0.005 | 1.09 | 0.083 | 0.26 | 0.070 | 0.0039 |
| SICL | 0.07 | 0.010 | 1.23 | 0.187 | 0.43 | 0.089 | 0.0056 |
| SIL | 0.45 | 0.020 | 1.41 | 0.291 | 0.45 | 0.067 | 0.011 |
| SL | 4.42 | 0.075 | 1.89 | 0.471 | 0.41 | 0.065 | 0.030 |

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 ($mg/m^3$) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 50293 | DDT | 2.63E+06 | 1.37E-02 | 4.95E-06 | 2.50E-02 | 3.32E-04 | 8.10E-06 | 25 | 533.15 | 720.75 | 11,000 | 9.7E-05 | 0.0E+00 |
| 50328 | Benzo(a)pyrene | 1.02E+06 | 4.30E-02 | 9.00E-06 | 1.62E-03 | 4.63E-05 | 1.13E-06 | 25 | 715.90 | 969.27 | 15,000 | 2.1E-03 | 0.0E+00 |
| 51285 | 2,4-Dinitrophenol | 1.00E-02 | 2.73E-02 | 9.06E-06 | 2.79E+03 | 1.82E-05 | 4.44E-07 | 25 | 605.28 | 827.85 | 15,000 | 0.0E+00 | 7.0E-03 |
| 53703 | Dibenz(a,h)anthracene | 3.80E+06 | 2.02E-02 | 5.18E-06 | 2.49E-03 | 6.03E-07 | 1.47E-08 | 25 | 743.24 | 990.41 | 16,000 | 2.1E-03 | 0.0E+00 |
| 56235 | Carbon tetrachloride | 1.74E+02 | 7.80E-02 | 8.80E-06 | 7.93E+02 | 1.25E+00 | 3.05E-02 | 25 | 349.90 | 556.60 | 7,127 | 1.5E-05 | 0.0E+00 |
| 56553 | Benz(a)anthracene | 3.98E+05 | 5.10E-02 | 9.00E-06 | 9.40E-03 | 1.37E-04 | 3.34E-06 | 25 | 708.15 | 1004.79 | 15,000 | 2.1E-04 | 0.0E+00 |
| 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 | 13,000 | 3.7E-04 | 0.0E+00 |
| 58899 | gamma-HCH (Lindane) | 1.07E+03 | 1.42E-02 | 7.34E-06 | 6.80E+00 | 5.74E-04 | 1.40E-05 | 25 | 596.55 | 839.36 | 13,000 | 3.7E-04 | 0.0E+00 |
| 60571 | Dieldrin | 2.14E+04 | 1.25E-02 | 4.74E-06 | 1.95E-01 | 6.19E-04 | 1.51E-05 | 25 | 613.32 | 842.25 | 13,000 | 4.6E-03 | 0.0E+00 |
| 65850 | Benzoic Acid | 6.00E-01 | 5.36E-02 | 7.97E-06 | 3.50E+03 | 6.31E-05 | 1.54E-06 | 25 | 720.00 | 751.00 | 10,000 | 0.0E+00 | 1.4E+01 |
| 67641 | Acetone | 5.75E-01 | 1.24E-01 | 1.14E-05 | 1.00E+06 | 1.59E-03 | 3.88E-05 | 25 | 329.20 | 508.10 | 6,955 | 0.0E+00 | 3.5E-01 |
| 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 |
| 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 | 0.0E+00 |
| 71363 | Butanol | 6.92E+00 | 8.00E-02 | 9.30E-06 | 7.40E+04 | 3.61E-04 | 8.80E-06 | 25 | 390.88 | 563.05 | 10,346 | 0.0E+00 | 3.5E-01 |
| 71432 | Benzene | 5.89E+01 | 8.80E-02 | 9.80E-06 | 1.75E+03 | 2.28E-01 | 5.56E-03 | 25 | 353.24 | 562.16 | 7,342 | 8.3E-06 | 0.0E+00 |
| 71556 | 1,1,1-Trichloroethane | 1.10E+02 | 7.80E-02 | 8.80E-06 | 1.33E+03 | 7.05E-01 | 1.72E-02 | 25 | 347.24 | 545.00 | 7,136 | 0.0E+00 | 1.0E+00 |
| 72208 | Endrin | 1.23E+04 | 1.25E-02 | 4.74E-06 | 2.50E-01 | 3.08E-04 | 7.51E-06 | 25 | 718.15 | 986.20 | 12,000 | 0.0E+00 | 1.1E-03 |
| 72435 | Methoxychlor | 9.77E+04 | 1.56E-02 | 4.46E-06 | 4.50E-02 | 6.48E-04 | 1.58E-05 | 25 | 651.02 | 848.49 | 14,000 | 0.0E+00 | 1.8E-02 |
| 72548 | DDD | 1.00E+06 | 1.69E-02 | 4.76E-06 | 9.00E-02 | 1.64E-04 | 4.00E-06 | 25 | 639.90 | 863.77 | 14,000 | 6.9E-05 | 0.0E+00 |
| 72559 | DDE | 4.47E+06 | 1.44E-02 | 5.87E-06 | 1.20E-01 | 8.61E-04 | 2.10E-05 | 25 | 636.44 | 860.38 | 13,000 | 9.7E-05 | 0.0E+00 |
| 74839 | Methyl bromide | 1.05E+01 | 7.28E-02 | 1.21E-05 | 1.52E+04 | 2.56E-01 | 6.24E-03 | 25 | 276.71 | 467.00 | 5,714 | 0.0E+00 | 5.0E-03 |
| 75014 | Vinyl chloride (chloroethene) | 1.86E+01 | 1.06E-01 | 1.23E-06 | 2.76E+03 | 1.11E+00 | 2.71E-02 | 25 | 259.25 | 432.00 | 5,250 | 8.4E-05 | 0.0E+00 |
| 75092 | Methylene chloride | 1.17E+01 | 1.01E-01 | 1.17E-05 | 1.30E+04 | 8.98E-02 | 2.19E-03 | 25 | 313.00 | 510.00 | 6,706 | 4.7E-07 | 3.0E+00 |
| 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 |
| 75252 | Bromoform | 8.71E+01 | 1.49E-02 | 1.03E-05 | 3.10E+03 | 2.19E-02 | 5.34E-04 | 25 | 422.35 | 696.00 | 9,479 | 1.1E-06 | 0.0E+00 |
| 75274 | Bromodichloromethane | 5.50E+01 | 2.98E-02 | 1.06E-05 | 6.74E+03 | 6.56E-02 | 1.60E-03 | 25 | 363.15 | 585.85 | 7,000 | 1.8E-05 | 0.0E+00 |
| 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 |
| 75354 | 1,1-Dichloroethylene | 5.89E+01 | 9.00E-02 | 1.04E-05 | 2.25E+03 | 1.07E+00 | 2.61E-02 | 25 | 304.75 | 576.05 | 6,247 | 5.0E-05 | 0.0E+00 |
| 76448 | Heptachlor | 1.41E+06 | 1.12E-02 | 5.69E-06 | 1.80E-01 | 4.47E-02 | 1.09E-03 | 25 | 603.69 | 846.31 | 13,000 | 1.3E-03 | 0.0E+00 |
| 77474 | Hexachlorocyclopentadiene | 2.00E+05 | 1.61E-02 | 7.21E-06 | 1.80E+00 | 1.11E+00 | 2.71E-02 | 25 | 512.15 | 746.00 | 10,931 | 0.0E+00 | 7.0E-05 |
| 78591 | Isophorone | 4.68E+01 | 6.23E-02 | 6.76E-06 | 1.20E+04 | 2.72E-04 | 6.63E-06 | 25 | 488.35 | 715.00 | 10,271 | 2.7E-07 | 0.0E+00 |
| 78875 | 1,2-Dichloropropane | 4.37E+01 | 7.82E-02 | 8.73E-06 | 2.80E+03 | 1.15E-01 | 2.80E-03 | 25 | 369.52 | 572.00 | 7,590 | 0.0E+00 | 4.0E-03 |
| 79005 | 1,1,2-Trichloroethane | 5.01E+01 | 7.80E-02 | 8.80E-06 | 4.42E+03 | 3.74E-02 | 9.12E-04 | 25 | 386.15 | 602.00 | 8,322 | 1.6E-05 | 0.0E+00 |
| 79016 | Trichloroethylene | 1.66E+02 | 7.90E-02 | 9.10E-06 | 1.10E+03 | 4.22E-01 | 1.03E-02 | 25 | 360.36 | 544.20 | 7,505 | 1.7E-06 | 0.0E+00 |
| 79345 | 1,1,2,2-Tetrachloroethane | 9.33E+01 | 7.10E-02 | 7.90E-06 | 2.97E+03 | 1.41E-02 | 3.44E-04 | 25 | 419.60 | 661.15 | 8,996 | 5.8E-05 | 0.0E+00 |
| 83329 | Acenaphthene | 7.08E+03 | 4.21E-02 | 7.69E-06 | 4.24E+00 | 6.36E-03 | 1.55E-04 | 25 | 550.54 | 803.15 | 12,155 | 0.0E+00 | 2.1E-01 |
| 84662 | Diethylphthalate | 2.88E+02 | 2.56E-02 | 6.35E-06 | 1.08E+03 | 1.85E-05 | 4.51E-07 | 25 | 567.15 | 757.00 | 13,733 | 0.0E+00 | 2.8E+00 |
| 84742 | Di-n-butyl phthalate | 3.39E+04 | 4.38E-02 | 7.86E-06 | 1.12E+01 | 3.85E-08 | 9.39E-10 | 25 | 613.15 | 798.67 | 14,751 | 0.0E+00 | 3.5E-01 |
| 85687 | Butyl benzyl phthalate | 5.75E+04 | 1.74E-02 | 4.83E-06 | 2.69E+00 | 5.17E-05 | 1.26E-06 | 25 | 660.60 | 839.68 | 13,000 | 0.0E+00 | 7.0E-01 |
| 86306 | N-Nitrosodiphenylamine | 1.29E+03 | 3.12E-02 | 6.35E-06 | 3.51E+01 | 2.05E-04 | 5.00E-06 | 25 | 632.28 | 890.45 | 13,000 | 1.4E-06 | 0.0E+00 |
| 86737 | Fluorene | 1.38E+04 | 3.63E-02 | 7.88E-06 | 1.98E+00 | 2.61E-03 | 6.37E-05 | 25 | 570.44 | 870.00 | 12,666 | 0.0E+00 | 1.4E-01 |
| 86748 | Carbazole | 3.39E+03 | 3.90E-02 | 7.03E-06 | 7.48E+00 | 6.26E-07 | 1.53E-08 | 25 | 627.87 | 899.00 | 13,977 | 5.7E-06 | 0.0E+00 |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 87683 | Hexachloro-1,3-butadiene | 5.37E+04 | 5.61E-02 | 6.16E-06 | 3.23E+00 | 3.34E-01 | 8.15E-03 | 25 | 486.15 | 738.00 | 10,206 | 2.2E-05 | 0.0E+00 |
| 87865 | Pentachlorophenol | 5.92E+02 | 5.60E-02 | 6.10E-06 | 1.95E+03 | 1.00E-06 | 2.44E-08 | 25 | 582.15 | 813.20 | 14,000 | 3.4E-05 | 0.0E+00 |
| 88062 | 2,4,6-Trichlorophenol | 3.81E+02 | 3.18E-02 | 6.25E-06 | 8.00E+02 | 3.19E-04 | 7.78E-06 | 25 | 519.15 | 749.03 | 12,000 | 3.1E-06 | 0.0E+00 |
| 91203 | Naphthalene | 2.00E+03 | 5.90E-02 | 7.50E-06 | 3.10E+01 | 1.98E-02 | 4.83E-04 | 25 | 491.14 | 748.40 | 10,373 | 0.0E+00 | 1.4E-01 |
| 91941 | 3,3-Dichlorobenzidine | 7.24E+02 | 1.94E-02 | 6.74E-06 | 3.11E+00 | 1.64E-07 | 4.00E-09 | 25 | 560.26 | 754.03 | 13,000 | 1.3E-04 | 0.0E+00 |
| 95476 | o-Xylene | 3.63E+02 | 8.70E-02 | 1.00E-05 | 1.78E+02 | 2.13E-01 | 5.20E-03 | 25 | 417.60 | 630.30 | 8,661 | 0.0E+00 | 7.0E+00 |
| 95487 | 2-Methylphenol (o-cresol) | 9.12E+01 | 7.40E-02 | 8.30E-06 | 2.60E+04 | 4.92E-05 | 1.20E-06 | 25 | 464.19 | 697.60 | 10,800 | 0.0E+00 | 1.8E-01 |
| 95501 | 1,2-Dichlorobenzene | 6.17E+02 | 6.90E-02 | 7.90E-06 | 1.56E+02 | 7.79E-02 | 1.90E-03 | 25 | 453.57 | 705.00 | 9,700 | 2.0E-01 | 0.0E+00 |
| 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 |
| 95954 | 2,4,5-Trichlorophenol | 1.60E+03 | 2.91E-02 | 7.03E-06 | 1.20E+03 | 1.78E-04 | 4.34E-06 | 25 | 526.15 | 759.13 | 13,000 | 0.0E+00 | 3.5E-01 |
| 98953 | Nitrobenzene | 6.46E+01 | 7.60E-02 | 8.60E-06 | 2.09E+03 | 9.84E-04 | 2.40E-05 | 25 | 483.95 | 719.00 | 10,566 | 0.0E+00 | 2.0E-03 |
| 100414 | Ethylbenzene | 3.63E+02 | 7.50E-02 | 7.80E-06 | 1.69E+02 | 3.23E-01 | 7.88E-03 | 25 | 409.34 | 617.20 | 8,501 | 0.0E+00 | 1.0E+00 |
| 100425 | Styrene | 7.76E+02 | 7.10E-02 | 8.00E-06 | 3.10E+02 | 1.13E-01 | 2.76E-03 | 25 | 418.31 | 636.00 | 8,737 | 0.0E+00 | 1.0E+00 |
| 105679 | 2,4-Dimethylphenol | 2.09E+02 | 5.84E-02 | 8.69E-06 | 7.87E+03 | 8.20E-05 | 2.00E-06 | 25 | 484.13 | 707.60 | 11,329 | 0.0E+00 | 7.0E-02 |
| 106423 | p-Xylene | 3.89E+02 | 7.69E-02 | 8.44E-06 | 1.85E+02 | 3.14E-01 | 7.66E-03 | 26 | 411.52 | 616.20 | 8,525 | 0.0E+00 | 7.0E+00 |
| 106467 | 1,4-Dichlorobenzene | 6.17E+02 | 6.90E-02 | 7.90E-06 | 7.38E+01 | 9.96E-02 | 2.43E-03 | 25 | 447.21 | 684.75 | 9,271 | 8.0E-01 | 0.0E+00 |
| 106478 | p-Chloroaniline | 6.61E+01 | 4.83E-02 | 1.01E-05 | 5.30E+03 | 1.36E-05 | 3.32E-07 | 25 | 503.65 | 754.00 | 11,689 | 0.0E+00 | 1.4E-02 |
| 107062 | 1,2-Dichloroethane | 1.74E+01 | 1.04E-01 | 9.90E-06 | 8.52E+03 | 4.01E-02 | 9.78E-04 | 25 | 356.65 | 561.00 | 7,643 | 2.6E-05 | 0.0E+00 |
| 108054 | Vinyl acetate | 5.25E+00 | 8.50E-02 | 9.20E-06 | 2.00E+04 | 2.10E-02 | 5.12E-04 | 25 | 345.65 | 519.13 | 7,800 | 0.0E+00 | 2.0E-01 |
| 108383 | m-Xylene | 4.07E+02 | 7.00E-02 | 7.80E-06 | 1.61E+02 | 3.01E-01 | 7.34E-03 | 25 | 412.27 | 617.05 | 8,523 | 0.0E+00 | 7.0E+00 |
| 108883 | Toluene | 1.82E+02 | 8.70E-02 | 8.60E-06 | 5.26E+02 | 2.72E-01 | 6.63E-03 | 25 | 383.78 | 591.79 | 7,930 | 0.0E+00 | 4.0E-01 |
| 108907 | Chlorobenzene | 2.19E+02 | 7.30E-02 | 8.70E-06 | 4.72E+02 | 1.52E-01 | 3.71E-03 | 25 | 404.87 | 632.40 | 8,410 | 0.0E+00 | 2.0E-02 |
| 108952 | Phenol | 2.88E+01 | 8.20E-02 | 9.10E-06 | 8.28E+04 | 1.63E-05 | 3.98E-07 | 25 | 455.02 | 694.20 | 10,920 | 0.0E+00 | 2.1E+00 |
| 111444 | Bis(2-chloroethyl)ether | 1.55E+01 | 6.92E-02 | 7.53E-06 | 1.72E+04 | 7.38E-04 | 1.80E-05 | 25 | 451.15 | 659.79 | 9,000 | 3.3E-04 | 0.0E+00 |
| 115297 | Endosulfan | 2.14E+03 | 1.15E-02 | 4.55E-06 | 5.10E-01 | 4.59E-04 | 1.12E-05 | 25 | 674.43 | 942.94 | 14,000 | 0.0E+00 | 2.1E-02 |
| 117817 | Bis(2-ethylhexyl)phthalate | 1.51E+07 | 3.51E-02 | 3.66E-06 | 3.40E-01 | 4.18E-06 | 1.02E-07 | 25 | 657.15 | 806.00 | 15,999 | 4.0E-06 | 0.0E+00 |
| 117840 | Di-n-octyl phthalate | 8.32E+07 | 1.51E-02 | 3.58E-06 | 2.00E-02 | 2.74E-03 | 6.68E-05 | 25 | 704.09 | 862.22 | 15,000 | 0.0E+00 | 7.0E-02 |
| 118741 | Hexachlorobenzene | 5.50E+04 | 5.42E-02 | 5.91E-06 | 6.20E+00 | 5.41E-02 | 1.32E-03 | 25 | 582.55 | 825.00 | 14,447 | 4.6E-04 | 0.0E+00 |
| 120127 | Anthracene | 2.95E+04 | 3.24E-02 | 7.74E-06 | 4.34E-02 | 2.67E-03 | 6.51E-05 | 25 | 615.18 | 873.00 | 13,121 | 0.0E+00 | 1.1E+00 |
| 120821 | 1,2,4-Trichlorobenzene | 1.78E+03 | 3.00E-02 | 8.23E-06 | 3.00E+02 | 5.82E-02 | 1.42E-03 | 25 | 486.15 | 725.00 | 10,471 | 0.0E+00 | 2.0E-01 |
| 120832 | 2,4-Dichlorophenol | 1.47E+02 | 3.46E-02 | 8.77E-06 | 4.50E+03 | 1.30E-04 | 3.17E-06 | 25 | 482.15 | 708.17 | 11,000 | 0.0E+00 | 1.1E-02 |
| 121142 | 2,4-Dinitrotoluene | 9.55E+01 | 2.03E-01 | 7.06E-06 | 2.70E+02 | 3.80E-06 | 9.27E-08 | 25 | 590.00 | 814.00 | 13,467 | 1.9E-04 | 0.0E+00 |
| 124481 | Chlorodibromomethane | 6.31E+01 | 1.96E-02 | 1.05E-05 | 2.60E+03 | 3.21E-02 | 7.83E-04 | 25 | 416.14 | 678.20 | 8,000 | 2.4E-05 | 0.0E+00 |
| 127184 | Tetrachloroethylene | 1.55E+02 | 7.20E-02 | 8.20E-06 | 2.00E+02 | 7.54E-01 | 1.84E-02 | 25 | 394.40 | 620.20 | 8,288 | 5.8E-07 | 0.0E+00 |
| 129000 | Pyrene | 1.05E+05 | 2.72E-02 | 7.24E-06 | 1.35E-01 | 4.51E-04 | 1.10E-05 | 25 | 667.95 | 936.00 | 14,370 | 0.0E+00 | 1.1E-01 |
| 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 | 544.00 | 7,192 | 0.0E+00 | 3.5E-02 |
| 156605 | trans-1,2-Dichloroethylene | 5.25E+01 | 7.07E-02 | 1.19E-05 | 6.30E+03 | 3.85E-01 | 9.39E-03 | 25 | 320.85 | 516.50 | 6,717 | 0.0E+00 | 7.0E-02 |
| 193395 | Indeno(1,2,3-cd)pyrene | 3.47E+06 | 1.90E-02 | 5.66E-06 | 2.20E-05 | 6.56E-05 | 1.60E-06 | 25 | 809.15 | 1078.24 | 17,000 | 2.1E-04 | 0.0E+00 |
| 205992 | Benzo(b)fluoranthene | 1.23E+06 | 2.26E-02 | 5.56E-06 | 1.50E-03 | 4.55E-03 | 1.11E-04 | 25 | 715.90 | 969.27 | 15,000 | 2.1E-04 | 0.0E+00 |
| 206440 | Fluoranthene | 1.07E+05 | 3.02E-02 | 6.35E-06 | 2.06E-01 | 6.60E-04 | 1.61E-05 | 25 | 655.95 | 905.00 | 13,815 | 0.0E+00 | 1.4E-01 |
| 207089 | Benzo(k)fluoranthene | 1.23E+06 | 2.26E-02 | 5.56E-06 | 8.00E-04 | 3.40E-05 | 8.29E-07 | 25 | 753.15 | 1019.70 | 16,000 | 2.1E-05 | 0.0E+00 |
| 218019 | Chrysene | 3.98E+05 | 2.48E-02 | 6.21E-06 | 1.60E-03 | 3.88E-03 | 9.46E-05 | 25 | 714.15 | 979.00 | 16,455 | 2.1E-06 | 0.0E+00 |
| 309002 | Aldrin | 2.45E+06 | 1.32E-02 | 4.86E-06 | 1.80E-01 | 6.97E-03 | 1.70E-04 | 25 | 603.01 | 839.37 | 13,000 | 4.9E-03 | 0.0E+00 |
| 319846 | alpha-HCH (alpha-BHC) | 1.23E+03 | 1.42E-02 | 7.34E-06 | 2.00E+00 | 4.35E-04 | 1.06E-05 | 25 | 596.55 | 839.36 | 13,000 | 1.8E-03 | 0.0E+00 |
| 319857 | beta-HCH (beta-BHC) | 1.26E+03 | 1.42E-02 | 7.34E-06 | 2.40E-01 | 3.05E-05 | 7.44E-07 | 25 | 596.55 | 839.36 | 13,000 | 5.3E-04 | 0.0E+00 |
| 542756 | 1,3-Dichloropropene | 4.57E+01 | 6.26E-02 | 1.00E-05 | 2.80E+03 | 7.26E-01 | 1.77E-02 | 25 | 381.15 | 587.38 | 7,000 | 3.7E-05 | 2.0E-02 |
| 606202 | 2,6-Dinitrotoluene | 6.92E+01 | 3.27E-02 | 7.26E-06 | 1.82E+02 | 3.06E-05 | 7.46E-07 | 25 | 558.00 | 770.00 | 12,938 | 1.9E-04 | 0.0E+00 |
| 621647 | N-Nitrosodi-n-propylamine | 2.40E+01 | 5.45E-02 | 8.17E-06 | 9.89E+03 | 9.23E-05 | 2.25E-06 | 25 | 509.60 | 746.87 | 11,000 | 2.0E-03 | 0.0E+00 |
| 1024573 | Heptachlor epoxide | 8.32E+04 | 1.32E-02 | 4.23E-06 | 2.00E-01 | 3.90E-04 | 9.51E-06 | 25 | 613.96 | 848.76 | 13,000 | 2.6E-03 | 0.0E+00 |
| 7439976 | Mercury (elemental) | 5.20E+01 | 3.07E-02 | 6.30E-06 | 5.62E-02 | 4.67E-01 | 1.14E-02 | 25 | 629.88 | 1750.00 | 14,127 | 0.0E+00 | 3.0E-04 |
| 8001352 | Toxaphene | 2.57E+05 | 1.16E-02 | 4.34E-06 | 7.40E-01 | 2.46E-04 | 6.00E-06 | 25 | 657.15 | 873.31 | 14,000 | 3.2E-04 | 0.0E+00 |
| 11096825 | Aroclor 1260 (PCB-1260) | 2.90E+05 | 1.38E-02 | 4.32E-06 | 8.00E-02 | 1.89E-01 | 4.60E-03 | 25 | 402.50 | 539.37 | 19,000 | 1.0E-04 | 0.0E+00 |
| 11097691 | Aroclor 1254 (PCB-1254) | 2.00E+05 | 1.56E-02 | 5.00E-06 | 5.70E-02 | 8.20E-02 | 2.00E-03 | 25 | 377.50 | 512.27 | 19,000 | 1.0E-04 | 0.0E+00 |
| 12674112 | Aroclor 1016 (PCB-1016) | 3.30E+04 | 2.22E-02 | 5.42E-06 | 4.20E-01 | 1.19E-02 | 2.90E-04 | 25 | 340.50 | 475.22 | 18,000 | 1.0E-04 | 0.0E+00 |
| 53469219 | Aroclor 1242 (PCB-1242) | 3.30E+04 | 2.14E-02 | 5.31E-06 | 3.40E-01 | 2.13E-02 | 5.20E-04 | 25 | 345.50 | 482.20 | 18,000 | 1.0E-04 | 0.0E+00 |

# APPENDIX B

# SAMPLE DATA ENTRY SHEETS FOR EACH MODEL

## DATA ENTRY SHEET (SLSCREEN)

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 |

| **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, $T_S$ (°C) | **ENTER** Vadose zone SCS soil type (used to estimate soil vapor permeability) | | **ENTER** User-defined vadose zone soil vapor permeability, $k_v$ (cm$^2$) |
|---|---|---|---|---|---|
| | | | | OR | |
| 200 | 400 | 10 | SCL | | |

| **ENTER** Vadose zone soil dry bulk density, $\rho_b^A$ (g/cm$^3$) | **ENTER** Vadose zone soil total porosity, $n^V$ (unitless) | **ENTER** Vadose zone soil water-filled porosity, $\theta_w^V$ (cm$^3$/cm$^3$) | **ENTER** Vadose zone soil organic carbon fraction, $f_{oc}^V$ (unitless) |
|---|---|---|---|
| 1.5 | 0.43 | 0.3 | 0.002 |

| **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. | |

# DATA ENTRY SHEET (GWSCREEN)

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 |

| **ENTER** Depth below grade to bottom of enclosed space floor, $L_F$ (15 or 200 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) |
|---|---|---|---|
| 200 | 400 | SC | 10 |

| **ENTER** Vadose zone SCS soil type (used to estimate soil vapor permeability) | | **ENTER** User-defined vadose zone soil vapor permeability, $k_v$ (cm$^2$) | **ENTER** Vadose zone soil dry bulk density, $\rho_b^V$ (g/cm$^3$) | **ENTER** Vadose zone soil total porosity, $n^V$ (unitless) | **ENTER** Vadose zone soil water-filled porosity, $\theta_w^V$ (cm$^3$/cm$^3$) |
|---|---|---|---|---|---|
| | OR | | | | |
| SCL | | | 1.5 | 0.43 | 0.3 |

| **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 (SLTIER2)

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 |

| **ENTER** Average soil temperature, $T_S$ ($^\circ$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 D28)<br>Thickness of soil stratum A, $h_A$ (cm) | **ENTER**<br>Thickness of soil stratum B, (Enter value or 0) $h_B$ (cm) | **ENTER**<br>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 | SCL | | |

| **ENTER** Stratum A soil dry bulk density, $\rho_b^A$ (g/cm$^3$) | **ENTER** Stratum A soil total porosity, $n^A$ (unitless) | **ENTER** Stratum A soil water-filled porosity, $\theta_w^A$ (cm$^3$/cm$^3$) | **ENTER** Stratum A soil organic carbon fraction, $f_{oc}^A$ (unitless) | **ENTER** Stratum B soil dry bulk density, $\rho_b^B$ (g/cm$^3$) | **ENTER** Stratum B soil total porosity, $n^B$ (unitless) | **ENTER** Stratum B soil water-filled porosity, $\theta_w^B$ (cm$^3$/cm$^3$) | **ENTER** Stratum B soil organic carbon fraction, $f_{oc}^B$ (unitless) | **ENTER** Stratum C soil dry bulk density, $\rho_b^C$ (g/cm$^3$) | **ENTER** Stratum C soil total porosity, $n^C$ (unitless) | **ENTER** Stratum C soil water-filled porosity, $\theta_w^C$ (cm$^3$/cm$^3$) | **ENTER** Stratum C soil organic carbon fraction, $f_{oc}^C$ (unitless) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.5 | 0.43 | 0.15 | 0.006 | 1.5 | 0.43 | 0.25 | 0.003 | 1.7 | 0.34 | 0.26 | 0.002 |

| **ENTER** Enclosed space floor thickness, $L_{crack}$ (cm) | **ENTER** Soil-bldg. pressure differential, $\Delta P$ (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) |
|---|---|---|---|---|---|---|
| 15 | 40 | 961 | 961 | 488 | 0.1 | 0.45 |

| **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.

DATA ENTRY SHEET (GWTIER2)

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 | ENTER | |
|---|---|---|
| Chemical CAS No. (numbers only, no dashes) | Initial groundwater conc., $C_W$ ($\mu g/L$) | Chemical |
| 71432 | | Benzene |

| ENTER | ENTER | ENTER | ENTER | ENTER | ENTER | ENTER | ENTER | ENTER | | ENTER |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Totals must add up to value of $L_{WT}$ (cell D28) | | | | | | | |
| Average soil/ groundwater temperature, $T_S$ (°C) | Depth below grade to bottom of enclosed space floor, $L_F$ (cm) | Depth below grade to water table, $L_{WT}$ (cm) | Thickness of soil stratum A, $h_A$ (cm) | Thickness of soil stratum B, (Enter value or 0) $h_B$ (cm) | Thickness of soil stratum C, (Enter value or 0) $h_C$ (cm) | Soil stratum directly above water table, (Enter A, B, or C) | SCS soil type directly above water table | Soil stratum A SCS soil type (used to estimate soil vapor permeability) | OR | User-defined stratum A soil vapor permeability, $k_v$ ($cm^2$) |
| 10 | 200 | 400 | 300 | 50 | 50 | C | SC | L | | |

| ENTER | ENTER | ENTER | ENTER | ENTER | ENTER | ENTER | ENTER | ENTER |
|---|---|---|---|---|---|---|---|---|
| Stratum A soil dry bulk density, $\rho_b^A$ ($g/cm^3$) | Stratum A soil total porosity, $n^A$ (unitless) | Stratum A soil water-filled porosity, $\theta_w^A$ ($cm^3/cm^3$) | Stratum B soil dry bulk density, $\rho_b^B$ ($g/cm^3$) | Stratum B soil total porosity, $n^B$ (unitless) | Stratum B soil water-filled porosity, $\theta_w^B$ ($cm^3/cm^3$) | Stratum C soil dry bulk density, $\rho_b^C$ ($g/cm^3$) | Stratum C soil total porosity, $n^C$ (unitless) | Stratum C soil water-filled porosity, $\theta_w^C$ ($cm^3/cm^3$) |
| 1.5 | 0.43 | 0.2 | 1.7 | 0.42 | 0.27 | 1.7 | 0.43 | 0.3 |

| ENTER | ENTER | ENTER | ENTER | ENTER | ENTER | ENTER |
|---|---|---|---|---|---|---|
| Enclosed space floor thickness, $L_{crack}$ (cm) | Soil-bldg. pressure differential, $\Delta P$ ($g/cm\text{-}s^2$) | Enclosed space floor length, $L_B$ (cm) | Enclosed space floor width, $W_B$ (cm) | Enclosed space height, $H_B$ (cm) | Floor-wall seam crack width, w (cm) | Indoor air exchange rate, ER (1/h) |
| 15 | 40 | 961 | 961 | 488 | 0.1 | 0.45 |

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

# APPENDIX C

# CHEMICAL PROPERTIES LOOKUP TABLE AND REFERENCES

# CHEMICAL PROPERTIES 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 ($atm\text{-}m^3/mol$) | | 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 ($mg/m^3$) | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 50293 | DDT | 2.63E+06 | 1 | 1.37E-02 | 1 | 4.95E-06 | 1 | 2.50E-02 | 1 | 3.32E-04 | 1 | 8.10E-06 | 5 | 25 | 1 | 533.15 | 7 | 720.75 | 11 | 11,000 | 12 | 9.7E-05 | 1 | | |
| 50328 | Benzo(a)pyrene | 1.02E+06 | 1 | 4.30E-02 | 1 | 9.00E-06 | 1 | 1.62E-03 | 1 | 4.63E-05 | 1 | 1.13E-06 | 5 | 25 | 1 | 715.90 | 8 | 969.27 | 11 | 15,000 | 12 | 2.1E-03 | 13 | | |
| 51285 | 2,4-Dinitrophenol | 1.00E-02 | 1 | 2.73E-02 | 1 | 9.06E-06 | 1 | 2.79E+03 | 1 | 1.82E-05 | 1 | 4.44E-07 | 5 | 25 | 1 | 605.28 | 8 | 827.85 | 11 | 15,000 | 12 | | | 7.0E-03 | 13 |
| 53703 | Dibenz(a,h)anthracene | 3.80E+06 | 1 | 2.02E-02 | 1 | 5.18E-06 | 1 | 2.49E-03 | 1 | 6.03E-07 | 1 | 1.47E-08 | 5 | 25 | 1 | 743.24 | 8 | 990.41 | 11 | 16,000 | 12 | 2.1E-03 | 13 | | |
| 56235 | Carbon tetrachloride | 1.74E+02 | 1 | 7.80E-02 | 1 | 8.80E-06 | 1 | 7.93E+02 | 1 | 1.25E+00 | 1 | 3.05E-02 | 5 | 25 | 1 | 349.90 | 9 | 556.60 | 9 | 7,127 | 9 | 1.5E-05 | 1 | | |
| 56553 | Benz(a)anthracene | 3.98E+05 | 1 | 5.10E-02 | 1 | 9.00E-06 | 1 | 9.40E-03 | 1 | 1.37E-04 | 1 | 3.34E-06 | 5 | 25 | 1 | 708.15 | 8 | 1004.79 | 11 | 15,000 | 12 | 2.1E-04 | 13 | | |
| 57749 | Chlordane | 1.20E+05 | 1 | 1.18E-02 | 1 | 4.37E-06 | 1 | 5.60E-02 | 1 | 1.99E-03 | 1 | 4.85E-05 | 5 | 25 | 1 | 624.24 | 8 | 885.73 | 11 | 13,000 | 12 | 3.7E-04 | 1 | | |
| 58899 | gamma-HCH (Lindane) | 1.07E+03 | 1 | 1.42E-02 | 1 | 7.34E-06 | 1 | 6.80E+00 | 1 | 5.74E-04 | 1 | 1.40E-05 | 5 | 25 | 1 | 596.55 | 7 | 839.36 | 11 | 13,000 | 12 | 3.7E-04 | 13 | | |
| 60571 | Dieldrin | 2.14E+04 | 1 | 1.25E-02 | 1 | 4.74E-06 | 1 | 1.95E-01 | 1 | 6.19E-04 | 1 | 1.51E-05 | 5 | 25 | 1 | 613.32 | 8 | 842.25 | 11 | 13,000 | 12 | 4.6E-03 | 1 | | |
| 65850 | Benzoic Acid | 6.00E-01 | 1 | 5.36E-02 | 1 | 7.97E-06 | 1 | 3.50E+03 | 1 | 6.31E-05 | 1 | 1.54E-06 | 5 | 25 | 1 | 720.00 | 10 | 751.00 | 10 | 10,000 | 12 | | | 1.4E+01 | 13 |
| 67641 | Acetone | 5.75E-01 | 1 | 1.24E-01 | 1 | 1.14E-05 | 1 | 1.00E+06 | 1 | 1.59E-03 | 1 | 3.88E-05 | 5 | 25 | 1 | 329.20 | 9 | 508.10 | 9 | 6,955 | 9 | | | 3.5E-01 | 13 |
| 67663 | Chloroform | 3.98E+01 | 1 | 1.04E-01 | 1 | 1.00E-05 | 1 | 7.92E+03 | 1 | 1.50E-01 | 1 | 3.66E-03 | 5 | 25 | 1 | 334.32 | 9 | 536.40 | 9 | 6,988 | 9 | 2.3E-05 | 1 | | |
| 67721 | Hexachloroethane | 1.78E+03 | 1 | 2.50E-03 | 1 | 6.80E-06 | 1 | 5.00E+01 | 1 | 1.59E-01 | 1 | 3.88E-03 | 5 | 25 | 1 | 458.00 | 10 | 695.00 | 10 | 9,510 | 10 | 4.0E-06 | 1 | | |
| 71363 | Butanol | 6.92E+00 | 1 | 8.00E-02 | 1 | 9.30E-06 | 1 | 7.40E+04 | 1 | 3.61E-04 | 1 | 8.80E-06 | 5 | 25 | 1 | 390.88 | 9 | 563.05 | 9 | 10,346 | 9 | | | 3.5E-01 | 13 |
| 71432 | Benzene | 5.89E+01 | 1 | 8.80E-02 | 1 | 9.80E-06 | 1 | 1.75E+03 | 1 | 2.28E-01 | 1 | 5.56E-03 | 5 | 25 | 1 | 353.24 | 9 | 562.16 | 9 | 7,342 | 9 | 8.3E-06 | 1 | | |
| 71556 | 1,1,1-Trichloroethane | 1.10E+02 | 1 | 7.80E-02 | 1 | 8.80E-06 | 1 | 1.33E+03 | 1 | 7.05E-01 | 1 | 1.72E-02 | 5 | 25 | 1 | 347.24 | 9 | 545.00 | 9 | 7,136 | 9 | | | 1.0E+00 | 1 |
| 72208 | Endrin | 1.23E+04 | 1 | 1.25E-02 | 1 | 4.74E-06 | 1 | 2.50E-01 | 1 | 3.08E-04 | 1 | 7.51E-06 | 5 | 25 | 1 | 718.15 | 9 | 986.20 | 11 | 12,000 | 12 | | | 1.1E-03 | 13 |
| 72435 | Methoxychlor | 9.77E+04 | 1 | 1.56E-02 | 1 | 4.46E-06 | 1 | 4.50E-02 | 1 | 6.48E-04 | 1 | 1.58E-05 | 5 | 25 | 1 | 651.02 | 8 | 848.49 | 11 | 14,000 | 12 | | | 1.8E-02 | 13 |
| 72548 | DDD | 1.00E+06 | 1 | 1.69E-02 | 1 | 4.76E-06 | 1 | 9.00E-02 | 1 | 1.64E-04 | 1 | 4.00E-06 | 5 | 25 | 1 | 639.90 | 8 | 863.77 | 11 | 14,000 | 12 | 6.9E-05 | 13 | | |
| 72559 | DDE | 4.47E+06 | 1 | 1.44E-02 | 1 | 5.87E-06 | 1 | 1.20E-01 | 1 | 8.61E-04 | 1 | 2.10E-05 | 5 | 25 | 1 | 636.44 | 8 | 860.38 | 11 | 13,000 | 12 | 9.7E-05 | 13 | | |
| 74839 | Methyl bromide | 1.05E+01 | 1 | 7.28E-02 | 1 | 1.21E-05 | 1 | 1.52E+04 | 1 | 2.56E-01 | 1 | 6.24E-03 | 5 | 25 | 1 | 276.71 | 9 | 467.00 | 10 | 5,714 | 9 | | | 5.0E-03 | 1 |
| 75014 | Vinyl chloride (chloroethene) | 1.86E+01 | 1 | 1.06E-01 | 1 | 1.23E-06 | 1 | 2.76E+03 | 1 | 1.11E+00 | 1 | 2.71E-02 | 5 | 25 | 1 | 259.25 | 10 | 432.00 | 10 | 5,250 | 10 | 8.4E-05 | 1 | | |
| 75092 | Methylene chloride | 1.17E+01 | 1 | 1.01E-01 | 1 | 1.17E-05 | 1 | 1.30E+04 | 1 | 8.98E-02 | 1 | 2.19E-03 | 5 | 25 | 1 | 313.00 | 9 | 510.00 | 9 | 6,706 | 9 | 4.7E-07 | 1 | 3.0E+00 | 1 |
| 75150 | Carbon disulfide | 4.57E+01 | 1 | 1.04E-01 | 1 | 1.00E-05 | 1 | 1.19E+03 | 1 | 1.24E+00 | 1 | 3.02E-02 | 5 | 25 | 1 | 319.00 | 9 | 552.00 | 9 | 6,391 | 9 | | | 7.0E-01 | 1 |
| 75252 | Bromoform | 8.71E+01 | 1 | 1.49E-02 | 1 | 1.03E-05 | 1 | 3.10E+03 | 1 | 2.19E-02 | 1 | 5.34E-04 | 5 | 25 | 1 | 422.35 | 10 | 696.00 | 10 | 9,479 | 9 | 1.1E-06 | 1 | | |
| 75274 | Bromodichloromethane | 5.50E+01 | 1 | 2.98E-02 | 1 | 1.06E-05 | 1 | 6.74E+03 | 1 | 6.56E-02 | 1 | 1.60E-03 | 5 | 25 | 1 | 363.15 | 7 | 585.85 | 11 | 7,000 | 12 | 1.8E-05 | 13 | | |
| 75343 | 1,1-Dichloroethane | 3.16E+01 | 1 | 7.42E-02 | 1 | 1.05E-05 | 1 | 5.06E+03 | 1 | 2.30E-01 | 1 | 5.61E-03 | 5 | 25 | 1 | 330.55 | 9 | 523.00 | 9 | 6,895 | 9 | | | 5.0E-01 | 1 |
| 75354 | 1,1-Dichloroethylene | 5.89E+01 | 1 | 9.00E-02 | 1 | 1.04E-05 | 1 | 2.25E+03 | 1 | 1.07E+00 | 1 | 2.61E-02 | 5 | 25 | 1 | 304.75 | 9 | 576.05 | 9 | 6,247 | 9 | 5.0E-05 | 1 | | |
| 76448 | Heptachlor | 1.41E+06 | 1 | 1.12E-02 | 1 | 5.69E-06 | 1 | 1.80E-01 | 1 | 4.47E-02 | 1 | 1.09E-03 | 5 | 25 | 1 | 603.69 | 8 | 846.31 | 11 | 13,000 | 12 | 1.3E-03 | 1 | | |
| 77474 | Hexachlorocyclopentadiene | 2.00E+05 | 1 | 1.61E-02 | 1 | 7.21E-06 | 1 | 1.80E+00 | 1 | 1.11E+00 | 1 | 2.71E-02 | 5 | 25 | 1 | 512.15 | 10 | 746.00 | 10 | 10,931 | 10 | | | 7.0E-05 | 1 |
| 78591 | Isophorone | 4.68E+01 | 1 | 6.23E-02 | 1 | 6.76E-06 | 1 | 1.20E+04 | 1 | 2.72E-04 | 1 | 6.63E-06 | 5 | 25 | 1 | 488.35 | 10 | 715.00 | 10 | 10,271 | 10 | 2.7E-07 | 13 | | |
| 78875 | 1,2-Dichloropropane | 4.37E+01 | 1 | 7.82E-02 | 1 | 8.73E-06 | 1 | 2.80E+03 | 1 | 1.15E-01 | 1 | 2.80E-03 | 5 | 25 | 1 | 369.52 | 10 | 572.00 | 10 | 7,590 | 10 | | | 4.0E-03 | 1 |
| 79005 | 1,1,2-Trichloroethane | 5.01E+01 | 1 | 7.80E-02 | 1 | 8.80E-06 | 1 | 4.42E+03 | 1 | 3.74E-02 | 1 | 9.12E-04 | 5 | 25 | 1 | 386.15 | 9 | 602.00 | 10 | 8,322 | 9 | 1.6E-05 | 1 | | |
| 79016 | Trichloroethylene | 1.66E+02 | 1 | 7.90E-02 | 1 | 9.10E-06 | 1 | 1.10E+03 | 1 | 4.22E-01 | 1 | 1.03E-02 | 5 | 25 | 1 | 360.36 | 9 | 544.20 | 9 | 7,505 | 9 | 1.7E-06 | 1 | | |
| 79345 | 1,1,2,2-Tetrachloroethane | 9.33E+01 | 1 | 7.10E-02 | 1 | 7.90E-06 | 1 | 2.97E+03 | 1 | 1.41E-02 | 1 | 3.44E-04 | 5 | 25 | 1 | 419.60 | 9 | 661.15 | 9 | 8,996 | 9 | 5.8E-05 | 1 | | |
| 83329 | Acenaphthene | 7.08E+03 | 1 | 4.21E-02 | 1 | 7.69E-06 | 1 | 4.24E+00 | 1 | 6.36E-03 | 1 | 1.55E-04 | 5 | 25 | 1 | 550.54 | 10 | 803.15 | 10 | 12,155 | 10 | | | 2.1E-01 | 13 |
| 84662 | Diethylphthalate | 2.88E+02 | 1 | 2.56E-02 | 1 | 6.35E-06 | 1 | 1.08E+03 | 1 | 1.85E-05 | 1 | 4.51E-07 | 5 | 25 | 1 | 567.15 | 10 | 757.00 | 10 | 13,733 | 10 | | | 2.8E+00 | 13 |
| 84742 | Di-n-butyl phthalate | 3.39E+04 | 1 | 4.38E-02 | 1 | 7.86E-06 | 1 | 1.12E+01 | 1 | 3.85E-08 | 1 | 9.39E-10 | 5 | 25 | 1 | 613.15 | 9 | 798.67 | 11 | 14,751 | 9 | | | 3.5E-01 | 13 |
| 85687 | Butyl benzyl phthalate | 5.75E+04 | 1 | 1.74E-02 | 1 | 4.83E-06 | 1 | 2.69E+00 | 1 | 5.17E-05 | 1 | 1.26E-06 | 5 | 25 | 1 | 660.60 | 8 | 839.68 | 11 | 13,000 | 12 | | | 7.0E-01 | 13 |
| 86306 | N-Nitrosodiphenylamine | 1.29E+03 | 1 | 3.12E-02 | 1 | 6.35E-06 | 1 | 3.51E+01 | 1 | 2.05E-04 | 1 | 5.00E-06 | 5 | 25 | 1 | 632.28 | 8 | 890.45 | 11 | 13,000 | 12 | 1.4E-06 | 13 | | |
| 86737 | Fluorene | 1.38E+04 | 1 | 3.63E-02 | 1 | 7.88E-06 | 1 | 1.98E+00 | 1 | 2.61E-03 | 1 | 6.37E-05 | 5 | 25 | 1 | 570.44 | 10 | 870.00 | 10 | 12,666 | 10 | | | 1.4E-01 | 13 |
| 86748 | Carbazole | 3.39E+03 | 1 | 3.90E-02 | 1 | 7.03E-06 | 1 | 7.48E+00 | 1 | 6.26E-07 | 1 | 1.53E-08 | 5 | 25 | 1 | 627.87 | 10 | 899.00 | 10 | 13,977 | 10 | 5.7E-06 | 13 | | |
| 87683 | Hexachloro-1,3-butadiene | 5.37E+04 | 1 | 5.61E-02 | 1 | 6.16E-06 | 1 | 3.23E+00 | 1 | 3.34E-01 | 1 | 8.15E-03 | 5 | 25 | 1 | 486.15 | 10 | 738.00 | 10 | 10,206 | 10 | 2.2E-05 | 1 | | |
| 87865 | Pentachlorophenol | 5.92E+02 | 1 | 5.60E-02 | 1 | 6.10E-06 | 1 | 1.95E+03 | 1 | 1.00E-06 | 1 | 2.44E-08 | 5 | 25 | 1 | 582.15 | 9 | 813.20 | 11 | 14,000 | 12 | 3.4E-05 | 13 | | |
| 88062 | 2,4,6-Trichlorophenol | 3.81E+02 | 1 | 3.18E-02 | 1 | 6.25E-06 | 1 | 8.00E+02 | 1 | 3.19E-04 | 1 | 7.78E-06 | 5 | 25 | 1 | 519.15 | 9 | 749.03 | 11 | 12,000 | 12 | 3.1E-06 | 1 | | |
| 91203 | Naphthalene | 2.00E+03 | 1 | 5.90E-02 | 1 | 7.50E-06 | 1 | 3.10E+01 | 1 | 1.98E-02 | 1 | 4.83E-04 | 5 | 25 | 1 | 491.14 | 10 | 748.40 | 10 | 10,373 | 10 | | | 1.4E-01 | 13 |
| 91941 | 3,3-Dichlorobenzidine | 7.24E+02 | 1 | 1.94E-02 | 1 | 6.74E-06 | 1 | 3.11E+00 | 1 | 1.64E-07 | 1 | 4.00E-09 | 5 | 25 | 1 | 560.26 | 8 | 754.03 | 11 | 13,000 | 12 | 1.3E-04 | 13 | | |
| 95476 | o-Xylene | 3.63E+02 | 1 | 8.70E-02 | 1 | 1.00E-05 | 1 | 1.78E+02 | 1 | 2.13E-01 | 1 | 5.20E-03 | 5 | 25 | 1 | 417.60 | 9 | 630.30 | 9 | 8,661 | 9 | | | 7.0E+00 | 13 |
| 95487 | 2-Methylphenol (o-cresol) | 9.12E+01 | 1 | 7.40E-02 | 1 | 8.30E-06 | 1 | 2.60E+04 | 1 | 4.92E-05 | 1 | 1.20E-06 | 5 | 25 | 1 | 464.19 | 9 | 697.60 | 9 | 10,800 | 9 | | | 1.8E-01 | 13 |
| 95501 | 1,2-Dichlorobenzene | 6.17E+02 | 1 | 6.90E-02 | 1 | 7.90E-06 | 1 | 1.56E+02 | 1 | 7.79E-02 | 1 | 1.90E-03 | 5 | 25 | 1 | 453.57 | 10 | 705.00 | 10 | 9,700 | 10 | 2.0E-01 | 1 | | |
| 95578 | 2-Chlorophenol | 3.88E+02 | 1 | 5.01E-02 | 1 | 9.46E-06 | 1 | 2.20E+04 | 1 | 1.60E-02 | 1 | 3.90E-04 | 5 | 25 | 1 | 447.53 | 10 | 675.00 | 10 | 9,572 | 10 | | | 1.8E-02 | 13 |
| 95954 | 2,4,5-Trichlorophenol | 1.60E+03 | 1 | 2.91E-02 | 1 | 7.03E-06 | 1 | 1.20E+03 | 1 | 1.78E-04 | 1 | 4.34E-06 | 5 | 25 | 1 | 526.15 | 9 | 759.13 | 11 | 13,000 | 12 | | | 3.5E-01 | 13 |
| 98953 | Nitrobenzene | 6.46E+01 | 1 | 7.60E-02 | 1 | 8.60E-06 | 1 | 2.09E+03 | 1 | 9.84E-04 | 1 | 2.40E-05 | 5 | 25 | 1 | 483.95 | 10 | 719.00 | 10 | 10,566 | 10 | | | 2.0E-03 | 1 |
| 100414 | Ethylbenzene | 3.63E+02 | 1 | 7.50E-02 | 1 | 7.80E-06 | 1 | 1.69E+02 | 1 | 3.23E-01 | 1 | 7.88E-03 | 5 | 25 | 1 | 409.34 | 9 | 617.20 | 9 | 8,501 | 9 | | | 1.0E+00 | 1 |
| 100425 | Styrene | 7.76E+02 | 1 | 7.10E-02 | 1 | 8.00E-06 | 1 | 3.10E+02 | 1 | 1.13E-01 | 1 | 2.76E-03 | 5 | 25 | 1 | 418.31 | 10 | 636.00 | 10 | 8,737 | 10 | | | 1.0E+00 | 1 |
| 105679 | 2,4-Dimethylphenol | 2.09E+02 | 1 | 5.84E-02 | 1 | 8.69E-06 | 1 | 7.87E+03 | 1 | 8.20E-05 | 1 | 2.00E-06 | 5 | 25 | 1 | 484.13 | 10 | 707.60 | 10 | 11,329 | 10 | | | 7.0E-02 | 13 |
| 106423 | p-Xylene | 3.89E+02 | 1 | 7.69E-02 | 1 | 8.44E-06 | 1 | 1.85E+02 | 1 | 3.14E-01 | 1 | 7.66E-03 | 5 | 26 | 1 | 411.52 | 9 | 616.20 | 9 | 8,525 | 9 | | | 7.0E+00 | 13 |
| 106467 | 1,4-Dichlorobenzene | 6.17E+02 | 1 | 6.90E-02 | 1 | 7.90E-06 | 1 | 7.38E+01 | 1 | 9.96E-02 | 1 | 2.43E-03 | 5 | 25 | 1 | 447.21 | 10 | 684.75 | 10 | 9,271 | 10 | 8.0E-01 | 1 | | |

# CHEMICAL PROPERTIES 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, $T_R$ ($^oC$) | | 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/$m^3$) | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 106478 | p-Chloroaniline | 6.61E+01 | 1 | 4.83E-02 | 1 | 1.01E-05 | 1 | 5.30E+03 | 1 | 1.36E-05 | 1 | 3.32E-07 | 5 | 25 | 1 | 503.65 | 10 | 754.00 | 10 | 11,689 | 10 | | | 1.4E-02 | 13 |
| 107062 | 1,2-Dichloroethane | 1.74E+01 | 1 | 1.04E-01 | 1 | 9.90E-06 | 1 | 8.52E+03 | 1 | 4.01E-02 | 1 | 9.78E-04 | 5 | 25 | 1 | 356.65 | 9 | 561.00 | 9 | 7,643 | 9 | 2.6E-05 | 1 | | |
| 108054 | Vinyl acetate | 5.25E+00 | 1 | 8.50E-02 | 1 | 9.20E-06 | 1 | 2.00E+04 | 1 | 2.10E-02 | 1 | 5.12E-04 | 5 | 25 | 1 | 345.65 | 10 | 519.13 | 10 | 7,800 | 10 | | | 2.0E-01 | 1 |
| 108383 | m-Xylene | 4.07E+02 | 1 | 7.00E-02 | 1 | 7.80E-06 | 1 | 1.61E+02 | 1 | 3.01E-01 | 1 | 7.34E-03 | 5 | 25 | 1 | 412.27 | 9 | 617.05 | 9 | 8,523 | 9 | | | 7.0E+00 | 13 |
| 108883 | Toluene | 1.82E+02 | 1 | 8.70E-02 | 1 | 8.60E-06 | 1 | 5.26E+02 | 1 | 2.72E-01 | 1 | 6.63E-03 | 5 | 25 | 1 | 383.78 | 9 | 591.79 | 9 | 7,930 | 9 | | | 4.0E-01 | 1 |
| 108907 | Chlorobenzene | 2.19E+02 | 1 | 7.30E-02 | 1 | 8.70E-06 | 1 | 4.72E+02 | 1 | 1.52E-01 | 1 | 3.71E-03 | 5 | 25 | 1 | 404.87 | 9 | 632.40 | 9 | 8,410 | 9 | | | 2.0E-02 | 1 |
| 108952 | Phenol | 2.88E+01 | 1 | 8.20E-02 | 1 | 9.10E-06 | 1 | 8.28E+04 | 1 | 1.63E-05 | 1 | 3.98E-07 | 5 | 25 | 1 | 455.02 | 9 | 694.20 | 9 | 10,920 | 9 | | | 2.1E+00 | 13 |
| 111444 | Bis(2-chloroethyl)ether | 1.55E+01 | 1 | 6.92E-02 | 1 | 7.53E-06 | 1 | 1.72E+04 | 1 | 7.38E-04 | 1 | 1.80E-05 | 5 | 25 | 1 | 451.15 | 9 | 659.79 | 11 | 9,000 | 12 | 3.3E-04 | 1 | | |
| 115297 | Endosulfan | 2.14E+03 | 1 | 1.15E-02 | 1 | 4.55E-06 | 1 | 5.10E-01 | 1 | 4.59E-04 | 1 | 1.12E-05 | 5 | 25 | 1 | 674.43 | 8 | 942.94 | 11 | 14,000 | 12 | | | 2.1E-02 | 13 |
| 117817 | Bis(2-ethylhexyl)phthalate | 1.51E+07 | 1 | 3.51E-02 | 1 | 3.66E-06 | 1 | 3.40E-01 | 1 | 4.18E-06 | 1 | 1.02E-07 | 5 | 25 | 1 | 657.15 | 10 | 806.00 | 10 | 15,999 | 10 | 4.0E-06 | 13 | | |
| 117840 | Di-n-octyl phthalate | 8.32E+07 | 1 | 1.51E-02 | 1 | 3.58E-06 | 1 | 2.00E-02 | 1 | 2.74E-03 | 1 | 6.68E-05 | 5 | 25 | 1 | 704.09 | 8 | 862.22 | 11 | 15,000 | 12 | | | 7.0E-02 | 13 |
| 118741 | Hexachlorobenzene | 5.50E+04 | 1 | 5.42E-02 | 1 | 5.91E-06 | 1 | 6.20E+00 | 1 | 5.41E-02 | 1 | 1.32E-03 | 5 | 25 | 1 | 582.55 | 10 | 825.00 | 10 | 14,447 | 10 | 4.6E-04 | 1 | | |
| 120127 | Anthracene | 2.95E+04 | 1 | 3.24E-02 | 1 | 7.74E-06 | 1 | 4.34E-02 | 1 | 2.67E-03 | 1 | 6.51E-05 | 5 | 25 | 1 | 615.18 | 10 | 873.00 | 10 | 13,121 | 10 | | | 1.1E+00 | 13 |
| 120821 | 1,2,4-Trichlorobenzene | 1.78E+03 | 1 | 3.00E-02 | 1 | 8.23E-06 | 1 | 3.00E+02 | 1 | 5.82E-02 | 1 | 1.42E-03 | 5 | 25 | 1 | 486.15 | 10 | 725.00 | 10 | 10,471 | 10 | | | 2.0E-01 | 1 |
| 120832 | 2,4-Dichlorophenol | 1.47E+02 | 1 | 3.46E-02 | 1 | 8.77E-06 | 1 | 4.50E+03 | 1 | 1.30E-04 | 1 | 3.17E-06 | 5 | 25 | 1 | 482.15 | 9 | 708.17 | 11 | 11,000 | 12 | | | 1.1E-02 | 13 |
| 121142 | 2,4-Dinitrotoluene | 9.55E+01 | 1 | 2.03E-01 | 1 | 7.06E-06 | 1 | 2.70E+02 | 1 | 3.80E-06 | 1 | 9.27E-08 | 5 | 25 | 1 | 590.00 | 10 | 814.00 | 10 | 13,467 | 10 | 1.9E-04 | 13 | | |
| 124481 | Chlorodibromomethane | 6.31E+01 | 1 | 1.96E-02 | 1 | 1.05E-05 | 1 | 2.60E+03 | 1 | 3.21E-02 | 1 | 7.83E-04 | 5 | 25 | 1 | 416.14 | 8 | 678.20 | 11 | 8,000 | 12 | 2.4E-05 | 13 | | |
| 127184 | Tetrachloroethylene | 1.55E+02 | 1 | 7.20E-02 | 1 | 8.20E-06 | 1 | 2.00E+02 | 1 | 7.54E-01 | 1 | 1.84E-02 | 5 | 25 | 1 | 394.40 | 9 | 620.20 | 9 | 8,288 | 9 | 5.8E-07 | 1 | | |
| 129000 | Pyrene | 1.05E+05 | 1 | 2.72E-02 | 1 | 7.24E-06 | 1 | 1.35E-01 | 1 | 4.51E-04 | 1 | 1.10E-05 | 5 | 25 | 1 | 667.95 | 10 | 936.00 | 10 | 14,370 | 10 | | | 1.1E-01 | 13 |
| 156592 | cis-1,2-Dichloroethylene | 3.55E+01 | 1 | 7.36E-02 | 1 | 1.13E-05 | 1 | 3.50E+03 | 1 | 1.67E-01 | 1 | 4.07E-03 | 5 | 25 | 1 | 333.65 | 10 | 544.00 | 10 | 7,192 | 10 | | | 3.5E-02 | 13 |
| 156605 | trans-1,2-Dichloroethylene | 5.25E+01 | 1 | 7.07E-02 | 1 | 1.19E-05 | 1 | 6.30E+03 | 1 | 3.85E-01 | 1 | 9.39E-03 | 5 | 25 | 1 | 320.85 | 10 | 516.50 | 10 | 6,717 | 10 | | | 7.0E-02 | 13 |
| 193395 | Indeno(1,2,3-cd)pyrene | 3.47E+06 | 1 | 1.90E-02 | 1 | 5.66E-06 | 1 | 2.20E-05 | 1 | 6.56E-05 | 1 | 1.60E-06 | 5 | 25 | 1 | 809.15 | 7 | 1078.24 | 11 | 17,000 | 12 | 2.1E-04 | 13 | | |
| 205992 | Benzo(b)fluoranthene | 1.23E+06 | 1 | 2.26E-02 | 1 | 5.56E-06 | 1 | 1.50E-03 | 1 | 4.55E-03 | 1 | 1.11E-04 | 5 | 25 | 1 | 715.90 | 8 | 969.27 | 11 | 15,000 | 12 | 2.1E-04 | 13 | | |
| 206440 | Fluoranthene | 1.07E+05 | 1 | 3.02E-02 | 1 | 6.35E-06 | 1 | 2.06E-01 | 1 | 6.60E-04 | 1 | 1.61E-05 | 5 | 25 | 1 | 655.95 | 10 | 905.00 | 10 | 13,815 | 10 | | | 1.4E-01 | 13 |
| 207089 | Benzo(k)fluoranthene | 1.23E+06 | 1 | 2.26E-02 | 1 | 5.56E-06 | 1 | 8.00E-04 | 1 | 3.40E-05 | 1 | 8.29E-07 | 5 | 25 | 1 | 753.15 | 7 | 1019.70 | 11 | 16,000 | 12 | 2.1E-05 | 13 | | |
| 218019 | Chrysene | 3.98E+05 | 1 | 2.48E-02 | 1 | 6.21E-06 | 1 | 1.60E-03 | 1 | 3.88E-03 | 1 | 9.46E-05 | 5 | 25 | 1 | 714.15 | 10 | 979.00 | 10 | 16,455 | 10 | 2.1E-06 | 13 | | |
| 309002 | Aldrin | 2.45E+06 | 1 | 1.32E-02 | 1 | 4.86E-06 | 1 | 1.80E-01 | 1 | 6.97E-03 | 1 | 1.70E-04 | 5 | 25 | 1 | 603.01 | 8 | 839.37 | 11 | 13,000 | 12 | 4.9E-03 | 1 | | |
| 319846 | alpha-HCH (alpha-BHC) | 1.23E+03 | 1 | 1.42E-02 | 1 | 7.34E-06 | 1 | 2.00E+00 | 1 | 4.35E-04 | 1 | 1.06E-05 | 5 | 25 | 1 | 596.55 | 7 | 839.36 | 11 | 13,000 | 12 | 1.8E-03 | 1 | | |
| 319857 | beta-HCH (beta-BHC) | 1.26E+03 | 1 | 1.42E-02 | 1 | 7.34E-06 | 1 | 2.40E-01 | 1 | 3.05E-05 | 1 | 7.44E-07 | 5 | 25 | 1 | 596.55 | 7 | 839.36 | 11 | 13,000 | 12 | 5.3E-04 | 1 | | |
| 542756 | 1,3-Dichloropropene | 4.57E+01 | 1 | 6.26E-02 | 1 | 1.00E-05 | 1 | 2.80E+03 | 1 | 7.26E-01 | 1 | 1.77E-02 | 5 | 25 | 1 | 381.15 | 9 | 587.38 | 11 | 7,000 | 12 | 3.7E-05 | 1 | 2.0E-02 | 1 |
| 606202 | 2,6-Dinitrotoluene | 6.92E+01 | 1 | 3.27E-02 | 1 | 7.26E-06 | 1 | 1.82E+02 | 1 | 3.06E-05 | 1 | 7.46E-07 | 5 | 25 | 1 | 558.00 | 10 | 770.00 | 10 | 12,938 | 10 | 1.9E-04 | 13 | | |
| 621647 | N-Nitrosodi-n-propylamine | 2.40E+01 | 1 | 5.45E-02 | 1 | 8.17E-06 | 1 | 9.89E+03 | 1 | 9.23E-05 | 1 | 2.25E-06 | 5 | 25 | 1 | 509.60 | 8 | 746.87 | 11 | 11,000 | 12 | 2.0E-03 | 13 | | |
| 1024573 | Heptachlor epoxide | 8.32E+04 | 1 | 1.32E-02 | 1 | 4.23E-06 | 1 | 2.00E-01 | 1 | 3.90E-04 | 1 | 9.51E-06 | 5 | 25 | 1 | 613.96 | 8 | 848.76 | 11 | 13,000 | 12 | 2.6E-03 | 1 | | |
| 7439976 | Mercury (elemental) | 5.20E+01 | 2 | 3.07E-02 | 1 | 6.30E-06 | 1 | 5.62E-02 | 14 | 4.67E-01 | 1 | 1.14E-02 | 5 | 25 | 1 | 629.88 | 9 | 1750.00 | 9 | 14,127 | 9 | | | 3.0E-04 | 1 |
| 8001352 | Toxaphene | 2.57E+05 | 1 | 1.16E-02 | 1 | 4.34E-06 | 1 | 7.40E-01 | 1 | 2.46E-04 | 1 | 6.00E-06 | 5 | 25 | 1 | 657.15 | 9 | 873.31 | 11 | 14,000 | 12 | 3.2E-04 | 1 | | |
| 11096825 | Aroclor 1260 (PCB-1260) | 2.90E+05 | 3 | 1.38E-02 | 4 | 4.32E-06 | 4 | 8.00E-02 | 3 | 1.89E-01 | 6 | 4.60E-03 | 3 | 25 | 3 | 402.50 | 3 | 539.37 | 11 | 19,000 | 12 | 1.0E-04 | 3 | | |
| 11097691 | Aroclor 1254 (PCB-1254) | 2.00E+05 | 3 | 1.56E-02 | 4 | 5.00E-06 | 4 | 5.70E-02 | 3 | 8.20E-02 | 6 | 2.00E-03 | 3 | 25 | 3 | 377.50 | 3 | 512.27 | 11 | 19,000 | 12 | 1.0E-04 | 3 | | |
| 12674112 | Aroclor 1016 (PCB-1016) | 3.30E+04 | 3 | 2.22E-02 | 4 | 5.42E-06 | 4 | 4.20E-01 | 3 | 1.19E-02 | 6 | 2.90E-04 | 3 | 25 | 3 | 340.50 | 3 | 475.22 | 11 | 18,000 | 12 | 1.0E-04 | 3 | | |
| 53469219 | Aroclor 1242 (PCB-1242) | 3.30E+04 | 3 | 2.14E-02 | 4 | 5.31E-06 | 4 | 3.40E-01 | 3 | 2.13E-02 | 6 | 5.20E-04 | 3 | 25 | 3 | 345.50 | 3 | 482.20 | 11 | 18,000 | 12 | 1.0E-04 | 3 | | |

**LEGEND:**

1 = Soil Screening Level (SSL) Guidance Documents, U. S. EPA (1996a and b).
2 = SSL Guidance Documents (U. S. EPA, 1996a and b); value is the soil-water partition coefficient ($K_d$) at pH = 6.8.
3 = ATSDR draft Toxicity Profile for PCBs, August 1995.
4 = Estimation using the U. S. EPA WATER8 model.
5 = Unitless Henry's law constant divided by 41.
6 = Henry's law constant in units of atm-$m^3$/mol multiplied by 41.
7 = U. S. EPA Superfund Chemical Data Matrix.
8 = Estimation based on the Quantitative Structure Activity Relationship method of Stein and Brown (1994).
9 = CRC Handbook of Chemistry and Physics, CRC Press (1994).
10 = Design Institute for Physical Property Data, The American Institute for Chemical Engineers, on-line data search, 1997.
11 = Estimation based on Lyman et al. (1990), Equations 12-4 and 12-5.
12 = Estimation based on Lyman et al. (1990), Equation 13-16; Antoine coefficients estimated by boiling point using the U. S. EPA CHEMDAT8 model.
13 = Route-to-Route extrapolation based on the procedures in U. S. EPA (1996b).
14 = The Merck Index, Eleventh Edition, Merck & Co., Inc. 1989.