Schedule B7
Appendix B

Equations for derivation of soil HILs

Contents

Equations for derivation of soil HILs

1.1 Introduction

This appendix presents the equations used in the derivation of soil HILs. The derivation of HILs requires the consideration of a number of exposure pathways. With respect to the soil HILs, the following pathways are considered (as relevant for the exposure scenarios and compounds considered):

- Ingestion of soil and/or dust (indoors). The ingestion rate adopted for the characterisation of this pathway is a combined value reflecting both sources; hence, the calculation undertaken is a combined calculation.
- Dermal absorption during contact with soil and/or dust (indoors that may be derived from outdoor soil). As with the calculation of ingestion, the calculation of dermal absorption is based on absorption from both sources combined.
- Inhalation of dust generated from outdoor soil (where surface cover is poor) both outdoors and indoors (including re-suspension of dust indoors).
- Inhalation of volatile chemicals in soil indoors and outdoors.

1.2 General equations

The approach adopted in the derivation of soil HILs is consistent with the approach adopted in the derivation of previous HILs (NEPM 1999) and in other jurisdictions including the US EPA (in the derivation of preliminary remediation goals (US EPA 1992, 2002) and regional screening levels (US EPA 2009)) and the UK and New Zealand (in the derivation of soil guideline values [MfE 2010; UK 2009]).

Very generally, a soil health investigation level (HIL) for an exposure pathway (x), where a threshold approach is adopted, can be back calculated by setting the estimated intake for a chemical (i) to the acceptable intake allowable from soil for that chemical (i), then rearranging the equation as follows:

$$HIL_{x,i} \ (mg/kg) = \frac{acceptable\ intake}{intake\ from\ contamination} = \frac{(acceptable\ intake_i\ from\ soil) \times (body\ weight) \times (averaging\ time)}{(contact\ rate_i) \times (exposure\ frequency) \times (exposure\ duration)}$$

Equation 1

Similarly, HILs can be derived for other pathways of exposure and for non-threshold carcinogenic effects as relevant. The final HIL is calculated by combining the pathway specific HILs as noted below:

$$HIL\,(mg/kg) = \frac{1}{\left[\dfrac{1}{HIL_{ingestion}}\right] + \left[\dfrac{1}{HIL_{dermal}}\right] + \left[\dfrac{1}{HIL_{plant\ uptake}}\right] + \left[\dfrac{1}{HIL_{dust}}\right] + \left[\dfrac{1}{HIL_{vapours}}\right]}$$

Equation 2

where:

$HIL_{ingestion}$ = derived soil guideline associated with the ingestion of soil and dust by young child and/or adult, refer to **Equations 3, 4 and 5**

HIL_{dermal} = derived soil guideline associated with dermal absorption of contaminant in soil/dust by young child and/or adult, refer to **Equations 6, 7 and 8**

$HIL_{plant\ uptake}$ = derived soil guideline associated with ingestion of contaminant in home-grown fruit and vegetable produce by young child and/or adult (where relevant), refer to **Equations 18 to 21**

HIL_{dust} = derived soil guideline associated with inhalation of contaminants in dust by young child and/or adult, refer to **Equations 9, 10 and 11**

$HIL_{volatile}$ = derived soil guideline associated with inhalation of volatile contaminants in air by young child and/or adult, refer to **Equations 12 to 17**

This approach assumes that the pathways of exposure are all complete and are additive, and that the toxicological end-point considered for all pathways of exposure are the same or additive.

1.3 Pathway specific equations

1.3.1 Ingestion of soil/dust

Threshold contaminants

$$HIL_{ingestion} \ (mg/kg) = \frac{(TRV_o - B) \times BW \times AT_T}{IR_S \times B_o \times CF \times EF \times ED}$$ **Equation 3**

where:

TRV_o	= Toxicity reference value relevant for the quantification of oral intakes, (as mg/kg/day for threshold contaminants)
B	= Background intakes relevant to oral/dermal exposures (from sources other than soil which include food, water, air and consumer products where relevant) (fraction relevant to the % allocated to background intakes)
IR_s	= Ingestion rate of soil/dust (mg/day)
B_o	= Oral bioavailability (unitless)
CF	= Conversion factor of 1×10^{-6} to convert mg to kg
EF	= Exposure frequency (days/year)
ED	= Exposure duration (years)
BW	= Body weight (kg)
AT_T	= Averaging time for threshold contaminants (days, = ED x 365 days)

Non-threshold contaminants

$$HIL_{ingestion} \ (mg/kg) = \frac{TR}{Intake_o \times TRV_o}$$ **Equation 4**

$$Intake_o \ (kg/kg/day) = \sum \left(\frac{IRs_x \times Bo \times CF \times EF_x \times ED_x}{BW_x \times AT_{NT}} \right)$$ **Equation 5**

where:

TRV_o	= Toxicity reference value relevant for the quantification of oral intakes, (as $(mg/kg/day)^{-1}$ for non-threshold contaminants)
TR	= Target risk for non-threshold contaminants (unitless)
$\sum$	= signifies the sum over all receptor groups x considered (in the HILs derived these groups include a child (C) and adult (A))
IRs_X	= Ingestion rate of soil/dust by each receptor group x (mg/day)
Bo	= Oral bioavailability (unitless)
CF	= Conversion factor of 1×10^{-6} to convert mg to kg
EF_x	= Exposure frequency relevant to exposures by each receptor group x (days/year)
ED_x	= Exposure duration relevant to exposures by each receptor group x (years)
BW_x	= Body weight relevant to exposures by each receptor group x (kg)
AT_{NT}	= Averaging time (days, which for non-threshold compounds = 70 years x 365 days)

1.3.2 Dermal contact with soil/dust

Threshold contaminants

$$HIL_{dermal} \ (mg/kg) = \frac{(TRV_D - B) \times BW \times AT_T}{SA \times AF \times DAF \times CF \times EF \times ED}$$

Equation 6

where:

TRV_D = Toxicity reference value relevant for the quantification of dermal intakes, (as mg/kg/day for threshold contaminants);

B = Background intakes relevant to oral/dermal exposures (from sources other than soil which include food, water, air and consumer products where relevant) (fraction relevant to the % allocated to background intakes)

SA = Exposed skin surface area (cm²)

AF = Soil to skin adherence factor (mg/cm²/day)

B = Bioavailability (unitless)

DAF = Dermal absorption factor, chemical specific (unitless)

CF = Conversion factor of 1x10⁻⁶ to convert mg to kg

EF = Exposure frequency (days/year)

ED = Exposure duration (years)

BW = Body weight (kg)

AT_T = Averaging time for threshold contaminants (days, = ED x 365 days)

Non-threshold contaminants

$$HIL_{ingestion} \ (mg/kg) = \frac{TR}{Intake_D \times TRV_D}$$

Equation 7

$$Intake_D \ (kg/kg/day) = \sum \left(\frac{SA_x \times AF \times DAF \times B \times CF \times EF_x \times ED_x}{BW_x \times AT_{NT}} \right)$$

Equation 8

where:

TRV_D = Toxicity reference value relevant for the quantification of dermal intakes, (as (mg/kg/day)⁻¹ for non-threshold contaminants)

TR = Target risk for non-threshold contaminants (unitless)

$\sum$ = signifies the sum over all receptor groups x considered (in the HILs derived these groups include a child (C) and adult (A))

SA_x = Exposed skin surface area for all receptor groups x (cm²)

AF = Soil to skin adherence factor (mg/cm²/day)

DAF = Dermal absorption factor, chemical specific (unitless)

CF = Conversion factor of 1x10⁻⁶ to convert mg to kg

EF_x = Exposure frequency relevant to exposures by all receptor groups x (days/year)

ED_x = Exposure duration relevant to exposures by all receptor groups x (years)

BW_x = Body weight relevant to exposures by all receptor groups x (kg)

AT_{NT} = Averaging time (days, which for non-threshold compounds = 70 years x 365 days)

1.3.3 Inhalation of dust

Threshold contaminants

$$\text{HIL}_{dust} \, (mg/kg) = \frac{(TRV_i - B) \times BW \times AT_T}{\left[\left[\frac{1}{PEF_o} \times InhR_o \times ET_o\right] + \left[\frac{1}{PEF_i} \times TR \times InhR_i \times ET_i\right]\right] \times RF \times EF \times ED}$$ **Equation 9**

where:

TRV_i = Toxicity reference value relevant for the quantification of inhalation intakes, (as mg/kg/day for threshold contaminants)

B = Background intakes relevant to inhalation exposures (from sources other than soil which include food, water, air and consumer products where relevant) (fraction relevant to the % allocated to background intakes)

$PEF_{i,o}$ = Particulate emission factor (or dust loading) for outdoor (O) or indoor (I) air (m³/kg)

$InhR_{i,o}$ = Inhalation rate outdoors (O) or indoors (I) (m³/hour)

$ET_{i,o}$ = Exposure time outdoors (O) or indoors (I) (hours/day)

TR = Indoor dust transport factor (unitless)

RF = Lung retention factor relevant for the inhalation of dust from site (unitless)

EF = Exposure frequency (days/year)

ED = Exposure duration (years)

BW = Body weight (kg)

AT_T = Averaging time for threshold contaminants (days, = ED x 365 days)

Non-threshold contaminants

$$\text{HIL}_{dust} \, (mg/kg) = \frac{TR}{Intake_{dust} \times TRV_i}$$ **Equation 10**

$$\text{Intake}_{dust} \, (kg/kg/day) = \sum \left(\frac{\left[\left[\frac{1}{PEF_o} \times InhR_{ox} \times ET_o\right] + \left[\frac{1}{PEF_i} \times TR \times InhR_{ix} \times ET_i\right]\right] \times RF \times EF_x \times ED_x}{BW_x \times AT_{NT}} \right)$$ **Equation 11**

where:

TRV_i = Toxicity reference value relevant for the quantification of inhalation intakes, (as (mg/kg/day)$^{-1}$ for non-threshold contaminants)

TR = Target risk for non-threshold contaminants (unitless)

$\sum$ = signifies the sum over all receptor groups x considered (in the HILs derived these groups include a child (C) and adult (A))

$PEF_{i,o}$ = Particulate emission factor (or dust loading) for outdoor (O) or indoor (I) air (m³/kg)

$InhR_{ix}$ = Inhalation rate indoors (I) for all receptor groups x (m³/hour)

$InhR_{ox}$ = Inhalation rate outdoors (O) for all receptor groups x (m³/hour)

$ET_{i,o}$ = Exposure time indoors (I) and outdoors (O) (hours/day)

TR = indoor dust transport factor (unitless)

RF = Lung retention factor relevant for the inhalation of dust from site (unitless)

EF_x = Exposure frequency for all receptor groups x (days/year)

ED_x = Exposure duration for all receptor groups x (years)

BW_x = Body weight for all receptor groups x (kg)

AT_{NT} = Averaging time for non-threshold contaminants (days, = 70 years x 365 days)

1.3.4 Inhalation of volatiles

Threshold contaminants

$$HIL_{volatile} \ (mg/kg) = \frac{(TRV_i - B) \times BW \times AT_T}{\left[\left[\frac{1}{VF_o} \times InhR_o \times ET_o\right] + \left[\frac{1}{VF_i} \times InhR_i \times ET_i\right]\right] \times EF \times ED}$$

Equation 12

where:

TRV_i = Toxicity reference value relevant for the quantification of inhalation intakes, (as mg/kg/day for threshold contaminants);

B = Background intakes relevant to inhalation exposures (from sources other than soil which include food, water, air and consumer products where relevant) (fraction relevant to the % allocated to background intakes)

$VF_{i,o}$ = Volatilisation factor (based on vapour modelling) for outdoor (O) or indoor (I) air (m³/kg)

$InhR_{i,o}$ = Inhalation rate outdoors (O) or indoors (I) (m³/hour)

$ET_{i,o}$ = Exposure time outdoors (O) or indoors (I) (hours/day)

EF = Exposure frequency (days/year)

ED = Exposure duration (years)

BW = Body weight (kg)

AT_T = Averaging time for threshold contaminants (days, = ED x 365 days)

Non-threshold contaminants

$$HIL_{volatile} \ (mg/kg) = \frac{TR}{Intake_{volatile} \times TRV_i}$$

Equation 13

$$Intake_{volatile} \ (kg/kg/day) = \sum \left(\frac{\left[\left[\frac{1}{VF_o} \times InhR_{ox} \times ET_o\right] + \left[\frac{1}{VF_i} \times InhR_{ix} \times ET_i\right]\right] \times EF_x \times ED_x}{BW_x \times AT_{NT}} \right)$$

Equation 14

where:

TRV_i = Toxicity reference value relevant for the quantification of inhalation intakes, (as (mg/kg/day)$^{-1}$ for non-threshold contaminants)

TR = Target risk for non-threshold contaminants (unitless)

$\sum$ = signifies the sum over all receptor groups x considered (in the HILs derived these groups include a child (C) and adult (A))

$VF_{i,o}$ = Volatilisation factor (based on vapour modelling) for outdoor (O) or indoor (I) air (m³/kg)

$InhR_{ix}$ = Inhalation rate indoors (I) for all receptor groups (m³/hour)

$InhR_{ox}$ = Inhalation rate outdoors (O) for all receptor groups (m³/hour)

$ET_{i,o}$ = Exposure time outdoors (O) or indoors (I) (hours/day)

EF_x = Exposure frequency for all receptor groups (days/year)

ED_x = Exposure duration for all receptor groups (years)

BW_x = Body weight for all receptor groups (kg)

AT_{NT} = Averaging time for non-threshold contaminants (days, = 70 years x 365 days)

Note that for the derivation of soil gas HILs, an attenuation factor has been adopted that relates the indoor air concentration to the soil vapour concentration.

The interim soil vapour HIL (based on indoor air exposures) has then been derived on the basis of the following equations:

$$\text{Interim soil vapour HIL}\,(mg/m^3) = \frac{(TRV_i - B) \times BW \times AT_T}{\alpha \times InhR_i \times ET_i \times EF \times ED}$$ **Equation 15**

where:

TRV_i = Toxicity reference value relevant for the quantification of inhalation intakes, (as mg/kg/day for threshold contaminants);

B = Background intakes relevant to inhalation exposures (from sources other than soil which include food, water, air and consumer products where relevant) (fraction relevant to the % allocated to background intakes)

$InhR_i$ = Inhalation rate indoors (I) (m³/hour)

ET_i = Exposure time indoors (I) (hours/day)

EF = Exposure frequency (days/year)

ED = Exposure duration (years)

BW = Body weight (kg)

AT_T = Averaging time for threshold contaminants (days, = ED x 365 days)

Non-threshold contaminants

$$\text{Interim soil vapour HIL}\,(mg/m^3) = \frac{TR}{Intake_{volatile} \times TRV_i}$$ **Equation 16**

$$\text{Intake}_{volatile}\,(m^3/kg/day) = \sum \left(\frac{\alpha \times InhR_i x \times ET_{ix} \times EF_x \times ED_x}{BW_x \times AT_{NT}} \right)$$ **Equation 17**

where:

TRV_i = Toxicity reference value relevant for the quantification of inhalation intakes, (as (mg/kg/day)$^{-1}$ for non-threshold contaminants)

TR = Target Risk for non-threshold contaminants (unitless)

$\sum$ = signifies the sum over all receptor groups x considered (in the HILs derived these groups include a child (C) and adult (A))

$InhR_ix$ = Inhalation rate indoors (I) for all receptor groups (m³/hour)

ET_i = Exposure time indoors (I) (hours/day)

EF_x = Exposure frequency for all receptor groups (days/year)

ED_x = Exposure duration for all receptor groups (years)

BW_x = Body weight for all receptor groups (kg)

AT_{NT} = Averaging time for non-threshold contaminants (days, = 70 years x 365 days)

1.3.5 Ingestion of produce

Intake factors relevant to the estimation of exposures associated with the ingestion of contaminants following uptake into home-grown fruit and vegetable crops (considered as below ground tuber vegetables (tuber) and root vegetables (root) and above ground green vegetables (green) and tree fruit (fruit)) are as follows:

Threshold contaminants

$$\text{HIL}_{\text{plant uptake}} \, (\text{mg}/\text{kg}) = \frac{(\text{TRV}_o - B) \times BW \times AT_T}{UF_V \times F_{HG} \times EF \times ED} \qquad \textbf{Equation 18}$$

$$UF_V \, (\text{kg}/\text{day}) = (CF_{\text{tuber}} \times C_{\text{tuber}}) + (CF_{\text{root}} \times C_{\text{root}}) + (CF_{\text{green}} \times C_{\text{green}}) + (CF_{\text{fruit}} \times C_{\text{fruit}}) \qquad \textbf{Equation 19}$$

where:

TRV_o = Toxicity reference value relevant for the quantification of oral intakes, (as mg/kg/day for threshold contaminants);

B = Background intakes relevant to oral/dermal exposures (from sources other than soil which include food, water, air and consumer products where relevant) (fraction relevant to the % allocated to background intakes)

CF_y = plant concentration factors relevant for produce type (y), chemical specific value mg/kg fresh with produce to mg/kg dry weight soil)

C_y = Consumption rate of each produce type (y) (kg/day)

F_{HG} = Fraction of all fruit and vegetable produce consumed that is home-grown (unitless)

EF = Exposure frequency (days/year)

ED = Exposure duration (years)

BW = Body weight (kg)

AT_T = Averaging time for threshold contaminants (days, = ED x 365 days)

Non-threshold contaminants

$$\text{HIL}_{\text{plant uptake}} \, (\text{mg}/\text{kg}) = \frac{TR}{\text{Intake}_{\text{plant}} \times TRVo} \qquad \textbf{Equation 20}$$

$$\text{Intake}_{\text{plant}} \, (\text{kg}/\text{kg}/\text{day}) = \sum \left(\frac{UF_V \times F_{HG} \times EF_x \times ED_x}{BW_x \times AT_{NT}} \right) \qquad \textbf{Equation 21}$$

where:

TRV_o = Toxicity reference value relevant for the quantification of oral intakes, (as (mg/kg/day)$^{-1}$ for non-threshold contaminants)

TR = Target risk for non-threshold contaminants (unitless)

$\sum$ = signifies the sum over all receptor groups x considered (in the HILs derived these groups include a child (C) and adult (A))

CF_y = plant concentration factors relevant for produce type (y), chemical specific value mg/kg fresh with produce to mg/kg dry weight soil)

C_{yx} = Consumption rate of each produce type (y) for all receptor groups x (kg/day)

F_{HG} = Fraction of fruit and vegetable produce consumed that is home-grown (unitless)

EF_x = Exposure frequency for all receptor groups x (days/year)

ED_x = Exposure duration for all receptor groups x (years)

BW_x = Body weight for all receptor groups x (kg)

AT_{NT} = Averaging time for non-threshold contaminants (days, = 70 years x 365 days)

Note that the calculation of intakes derived from home-grown produce has been included in the derivation of HIL A where relevant. However, it is noted that for some compounds such as metals, the assessment of intakes derived from the consumption of home-grown produce as well as intakes derived from the diet (as estimated from total diet surveys) results in double counting of intakes that may be derived from produce.

To address the potential for double counting of these intakes it is assumed that 50% of the intake derived from home grown produce (10% of total intake) is already accounted for in the data available on intakes derived from all dietary sources. Hence, the derivation of the HIL for plant uptake for metals has been adjusted to address this issue (refer to Appendix A for compound-specific data).

1.4 Calculation of particulate emission factor

Soil-derived dust concentrations in outdoor air have been estimated using a particulate emission factor (PEF) using the approach outlines by the US EPA (1996 and 2002) and UK (2009). The PEF represents an estimate of the relationship between the concentration of a contaminant in soil and its concentration in air as a consequence of dust re-suspension. Dust particles considered in the PEF are assumed to be less than 10 μm is diameter. This has been calculated using the following equation:

$$PEF_o \ (m^3 / kg) = \frac{Q/C \bullet 3600}{0.036 \bullet (1-V) \bullet (\frac{U_m}{U_t})^3 \bullet F_x}$$
Equation 22

where:

PEF_O	= particulate emission factor outdoors (mg/kg soil per mg/m³ air)
Q/C	= air dispersion factor which describes the dispersion of soil particles in the atmosphere of a theoretical outdoor box. A value of 90.8 (g/m²/s per kg/m³) has been used in the derivation of HILs. The value is a default value recommended by the USEPA (2002) for small sites (0.5 acres).
V	= the fraction of outdoor surface cover (0= bare soil), dimensionless
Um	= mean annual wind speed at a height of 10m (m/s), assumed to be 8.75 km/hr based on the average 9am and 3 pm winds from Canberra
Ut	= threshold value of wind speed at a height of 10m (m/s), which is how much wind is required to generate dust at a given site from an erodible surface. A default value of 7.2 m/s has been used in the derivation of HILs (EA, 2009)
Fx	=empirical function calculated based on the ratio of mean and threshold windspeeds as noted by EA (2009). For the derivation of HILs the following was used:

$$Fx = 0.18 \times (8x^3 + 12x) \exp(-x^2), \quad \text{where} \quad x = 0.886 \frac{U_t}{U_m}$$
Equation 23

The PEF calculated for indoor air (and outdoors for HIL C) is based on a dust loading factor. The PEF is calculated as follows:

$$PEF_i \ (m^3 / kg) = \frac{1}{DL \times 10^{-6}}$$
Equation 24

where:

DL = dust loading factor (mg dust/m³ air)

10^{-6} = conversion factor for mg to kg

1.5 Calculation of plant concentration factors

The concentration of contaminants in edible portions of fruit and vegetables is estimated from the relationship between soil and plant and described using a soil-to-plant concentration factor (CFx).

For inorganic contaminants, the CFx values are derived from available literature (relevant to below or above ground crops).

For organic contaminants, there is a range of equations available that based on experimental data. Where relevant, plant uptake of organic compounds has been estimated in the derivation of HILs using the equations presented by EA (2009) which are detailed as follows (refer to EA [2009] for further explanation on the basis for these equations):

Root Crops

$$CF_{root} \text{ (mg/kg fw plant per mg/kg dw soil)} = \frac{\left(\dfrac{Q}{K_{oc} \times F_{oc}}\right)}{\dfrac{Q}{\left[\dfrac{W}{\rho_p} + \dfrac{L}{\rho_p} \times 1.22 K_{ow}^{0.77}\right]} + (k_g + K_m)\,\rho_p\,RV}$$

Equation 25

Where:

Q = transpiration stream flow rate, cm^3/day (assumed to be equal to default of 1000)
Koc = organic carbon-water partition coefficient for the contaminant, cm^3/g (compound-specific)
Foc = fraction of organic carbon in the soil, dimensionless
Kow = octanol-water partition coefficient, dimensionless (compound-specific)
W = root water content, g/g (assumed equal to the default of 0.89)
L = root lipid content on a mass basis, g/g (assumed equal to the default of 0.025)
ρ_P = plant root density, g/cm^3 (assumed equal to the default of 1)
k_g = first order growth rate constant, per day (assumed equal to the default of 0.1)
K_m = first order metabolism rate constant, per day (assumed equal to the default of 0)
RV = root volume, cm^3 (assumed equal to the default of 1000)

Tuber Crops

$$CF_{tuber} \text{ (mg/kg fw plant per mg/kg dw soil)} = \frac{k_1}{k_2 + k_g}$$

Equation 26

where:

$$k_1 = k_2\left(\frac{K_{pw}}{K_{oc}}\right)$$

Equation 27

$$K_{pw} = \left(\frac{W}{\rho_p}\right) + (f_{ch}K_{ch}) + \left(\frac{L}{\rho_p}\right)1.22 K_{ow}^{0.77}$$

Equation 28

$$k_2 = \frac{23\left(\dfrac{3600 D_{water}(W^{7/3}/\rho_p)}{K_{pw}}\right)}{R^2}$$

Equation 29

k_1 = rate of chemical flux into the potato, per hour (Equation 27)
k_2 = rate of chemical flux out of the potato, per hour (Equation 29)
k_g = exponential rate of growth of the potato, per hour (assumed equal to the default of 0.0014)
D_{water} = chemical diffusion coefficient in water, m^2/s (compound-specific)
ρ_P = potato tissue density, g/cm^3 (assumed equal to the default of 1)
R = radius of the potato, m (assumed equal to the default of 0.04)
W = water content of potato, g/g (assumed equal to the default of 0.79)
K_{pw} = equilibrium partition coefficient between potato and water, cm^3/g (Equation 28)
Koc = organic carbon-water partition coefficient for the contaminant, cm^3/g (compound-specific)
f_{ch} = fraction of carbohydrates in the potato, unitless (assumed equal to the default of 0.209)
L = lipid content of potato on a mass basis, g/g (assumed equal to the default of 0.001)
A = density correction factor between water and octanol, unitless (assumed equal to default of 1.22)
Kow = octanol-water partition coefficient, dimensionless (compound-specific)
B = correction coefficient of roots, unitless (assumed equal to the default of 0.77)
Kch = carbohydrate-water partition coefficient, cm^3/g (calculated from chemical lipophilicity according to the following table)
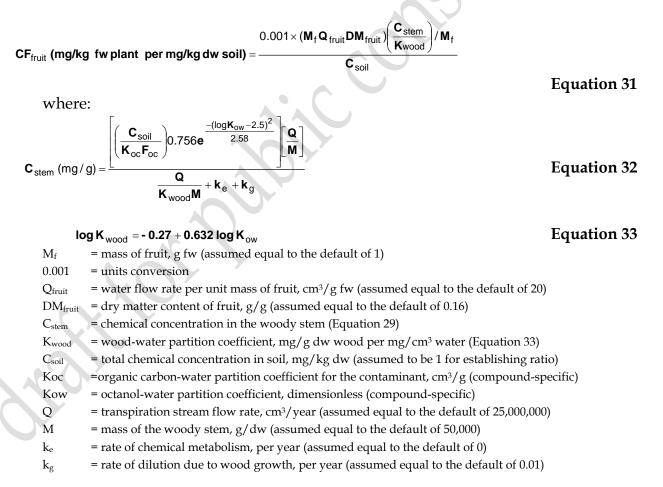
Chemical Log Kow	Chemical K_{ch} (cm³/g)
<0	0.1
≥0 but <1	0.2
≥1 but <2	0.5
≥2 but <3	1
≥3 but <4	2
≥4	3

Green Vegetables

☒ EMBED Equation.3 ☒☒☒

(mg/kg fw plant per mg/kg dw soil)   **Equation 30**

where:

Koc   = organic carbon-water partition coefficient for the contaminant, cm³/g (compound-specific)

foc   = fraction of organic carbon in the soil, dimensionless

Kow   = octanol-water partition coefficient, dimensionless (compound-specific)

ρ_s = dry soil bulk density, g/cm³

θws   = soil-water content by volume, cm³/cm³

Tree Fruit

$$CF_{fruit} \text{ (mg/kg fw plant per mg/kg dw soil)} = \frac{0.001 \times \left(M_f Q_{fruit} DM_{fruit}\right)\left(\dfrac{C_{stem}}{K_{wood}}\right)/M_f}{C_{soil}}$$

Equation 31

where:

$$C_{stem} \text{ (mg/g)} = \frac{\left[\left(\dfrac{C_{soil}}{K_{oc}F_{oc}}\right) 0.756 e^{\frac{-(\log K_{ow} - 2.5)^2}{2.58}}\right]\left[\dfrac{Q}{M}\right]}{\dfrac{Q}{K_{wood}M} + k_e + k_g}$$

Equation 32

$$\log K_{wood} = -0.27 + 0.632 \log K_{ow}$$

Equation 33

M_f = mass of fruit, g fw (assumed equal to the default of 1)

0.001   = units conversion

Q_{fruit} = water flow rate per unit mass of fruit, cm³/g fw (assumed equal to the default of 20)

DM_{fruit} = dry matter content of fruit, g/g (assumed equal to the default of 0.16)

C_{stem} = chemical concentration in the woody stem (Equation 29)

K_{wood} = wood-water partition coefficient, mg/g dw wood per mg/cm³ water (Equation 33)

C_{soil} = total chemical concentration in soil, mg/kg dw (assumed to be 1 for establishing ratio)

Koc   = organic carbon-water partition coefficient for the contaminant, cm³/g (compound-specific)

Kow   = octanol-water partition coefficient, dimensionless (compound-specific)

Q   = transpiration stream flow rate, cm³/year (assumed equal to the default of 25,000,000)

M   = mass of the woody stem, g/dw (assumed equal to the default of 50,000)

k_e = rate of chemical metabolism, per year (assumed equal to the default of 0)

k_g = rate of dilution due to wood growth, per year (assumed equal to the default of 0.01)

1.6 Calculation of volatilisation factors

1.6.1 Indoor air models/approaches

General

The steady-state vapour-phase concentration of a contaminant inside a building ($C_{building}$), where an infinite source is present, can be calculated on the basis of the following equation (US EPA, 2004a)

$$C_{indoor} = C_{source} \bullet \alpha$$

Equation 34

Where

C_{indoor} = the steady-state vapor-phase concentration of a contaminant inside a building (mg/m³)

α = attenuation coefficient [unitless], can be estimated or calculates as per Equation 36

C_{source} = vapour concentration at the source (mg/m³), refer to Equation 35.

Source phase partitioning

For a soil source, it is assumed that the vapour phase concentration directly above the soil is in equilibrium with the source and the concentration is related to the soil concentration by the following (which can be rearranged to evaluate the soil gas (vapour) to soil ratio):

$$C_{source}\,(mg/m^3) = C_{soil} \times PC \quad \text{where } PC = \frac{H' \times \rho_S}{\theta_{ws} + k_d \times \rho_S + H' \times \theta_{as}} \times 10^9$$

Equation 35

where:

C_{soil}	= Concentration in soil source zone (mg/kg)
PC	= phase partitioning coefficient (kg/m³)
10^9	= Units conversion
H'	= Henry's Law constant (unitless)
ρ_S	= Soil bulk density (g soil/cm³ soil)
θ_{ws}	= Volumetric water content in soil source zone (cm³ water/cm³ soil)
θ_{as}	= Volumetric air content in soil source zone (cm³ air/cm³ soil)
K_d	= Soil-water partition coefficient (cm³ air/g soil) = K_{oc} x f_{oc}
K_{oc}	= Soil organic carbon partition coefficient, chemical specific (cm³/g)
f_{oc}	= Soil organic carbon fraction (unitless)

Modelled attenuation factor

The steady-state attenuation factor describes the diffusive transport of contaminant vapours through the unsaturated zone and through building foundation and advective transport of contaminant vapours through the building foundation. The attenuation factor is calculated as follows (US EPA, 2004a):

$$\alpha = \frac{\left[\dfrac{D_T^{eff} \bullet A_B}{Q_{building} \bullet L_T}\right] \bullet \exp\left[\dfrac{Q_{soil} \bullet L_{crack}}{D^{crack} \bullet A_{crack}}\right]}{\left[\exp\left[\dfrac{Q_{soil} \bullet L_{crack}}{D^{crack} \bullet A_{crack}}\right] + \left[\dfrac{D_T^{eff} \bullet A_B}{Q_{building} \bullet L_T}\right] + \left[\dfrac{D_T^{eff} \bullet A_B}{Q_{soil} \bullet L_T}\right] \bullet \exp\left[\dfrac{Q_{soil} \bullet L_{crack}}{D^{crack} \bullet A_{crack}}\right]^{-1}\right]}$$

Equation 36

where:

D_T^{eff}. = total overall effective diffusion coefficient. Refer to Equations 39 and 40.

A_B = area of the enclosed space below the ground level which will vary depending on whether the building has a basement below the ground or not (cm²).

$Q_{building}$. = building ventilation rate which is calculated using building parameters and air exchange rate (cm³/s). Refer to Equation 37.

L_T = separation distance between the source and the building (cm).

Q_{soil}. = volumetric flowrate of soil gas into the enclosed space. This represents the convective flow of vapours into a building though cracks in the floor and walls. It incorporates pressure driven flows and a default value of 5 L/min is recommended (2003), however it can also be calculated (refer to US EPA, 2004a for equation).

L_{crack} = enclosed space foundation or slab thickness (cm).

D^{crack} = effective diffusion coefficient through the cracks (cm²/s).

A_{crack} = area of total cracks which varies depending on whether there is a basement or not (cm²), refer to Equation 38.

The building ventilation rate is calculated using Equation 37 for the building dimensions representing the living space of the building. It assumes that the total air volume entering the structure is mixed and that the vapour entering the structure is instantaneously and homogeneously distributed.

$$Q_{building} = \frac{(L_B \bullet W_B \bullet H_B \bullet ER)}{3600}$$

Equation 37

where:

L_B = length of building, (cm)

W_B = width of building, (cm)

H_B = height of building, (cm)

ER = air exchange rate, (per hour)

3600 = conversion from hours to seconds

$$A_{crack} = n \bullet AB$$
$$AB = L_B \bullet W_B + (2 \bullet L_B \bullet L_h + 2 \bullet W_B \bullet L_h)$$

Equation 38

where:

AB = area of enclosed space below ground, (cm²)

n = ratio of crack area to total area (unitless)

A_{crack} = total crack area, (cm²)

L_h = depth below ground, (cm)

The total overall effective diffusion coefficient can be calculated for n different soil layers between the source and the enclosed floor (including the capillary fringe where relevant). This is estimated using Equation 39.

$$D_T^{eff} = \frac{L_T}{\sum\limits_{i=1}^{n} L_i / D_i^{eff}}$$

Equation 39

L_T = separation distance between the source and the building (cm)

L_i = thickness of the soil layer i (cm)

D_i^{eff} = effective diffusion coefficient across soil layer i (cm²/s) – refer to Equation D2

$$D_i^{eff} = D_a \bullet \left[\frac{\theta_{ai}^{3.33}}{n_i^2}\right] + \left[\frac{D_w}{H'}\right] \bullet \left[\frac{\theta_{wi}^{3.33}}{n_i^2}\right]$$

Equation 40

D_a = diffusivity in air, chemical specific (cm²/s)

θ_{ai} = soil air-filled volume of layer i (cm³/cm³)

n_i = soil total porosity of layer i (cm³/cm³)

  = $1 - \rho_b / \rho_s$

  ρ_b = soil dry bulk density, (g/cm³)

  ρ_s = soil particle density, (g/cm³) - typically 2.65

D_w = diffusivity in water, chemical specific (cm²/s)

θ_{wi} = soil water-filled volume of layer i, (cm³/cm³)

Indoor air volatilisation factor

On the basis of the above an indoor air volatilisation factor has been calculated for use if the derivation of HILs. The indoor air volatilisation factor is as follows:

$$VF_i \text{ (mg/kg soil per mg/m}^3 \text{ vapour)} = \frac{1}{PC \times \alpha}$$

Equation 41

1.6.2 Outdoor air model

An estimate of vapour phase concentration in outdoor air derived from a soil source hasbeen estimated assuming an infinite soil source, equilibrium partitioning between vapour, liquid and adsorbed phases and no degradation. The model adopted is a box model where emissions to air from the surface of the ground are mixed with ambient air within a box that is used to define the exposure concentration.

The calculation of an outdoor air volatilisation factor is described in ASTM (2002) as follows:

$$
VF_o \ (mg/kg\,soil \ per \ mg/m^3 \ vapour) = 1 \Bigg/ \left[\dfrac{H \bullet \rho_s}{\left[\theta_{ws} + k_d \bullet \rho_s + H \bullet \theta_{as} \right] \left[1 + \dfrac{U_{air} \bullet \delta_{air} \bullet L_s}{D^{eff} \bullet W} \right]} \right]
$$

Equation 42

where:

W	= Length of source area parallel to wind direction [cm]
ρ_s	= Dry soil bulk density [g-soil/cm³-soil]
U_{air}	= Wind speed at δ_a above ground [cm/s]
δ_{air}	= Breathing zone height [cm]
L_s	= Depth to source (cm)
D^{eff}	= Effective diffusion coefficient in soil based on vapour-phase concentration [cm²/s], Equation 39
H	= Chemical-specific Henry's Law constant [(L-H_2O)/(L-air)]
θ_{ws}	= Volumetric water content in vadose zone soils [cm³-H_2O/cm³- soil]
K_d	= $f_{oc} \bullet K_{oc}$
	= Chemical-specific soil-water sorption coefficient [cm³-H_2O/g-soil]
θ_{as}	= Volumetric air content in the vadose zone soils [cm³-air/cm³-soil]
τ	= Averaging time for vapor flux [s]
	= $ED \ (yr) \bullet 365 \ (day/yr) \bullet 86400 \ (sec/day)$
10^3	= Conversion factor [(cm³-kg)/(m³-g)]