CHAPTER 3

CALCULATION OF RISK-BASED PRELIMINARY REMEDIATION GOALS

This chapter presents standardized exposure parameters, the derivation of risk equations, and the corresponding "reduced" equations, for calculating risk-based PRGs at scoping for the media and land-use assumptions discussed in Chapter 2 (i.e., ground water, surface water, and soil for residential land use, and soil for commercial/industrial land use). Both carcinogenic and noncarcinogenic effects are addressed. Standardized default exposure parameters consistent with OSWER Directive 9285.6-03 (EPA 1991b) are used in this chapter; where default parameters are not available in that guidance, the references used are cited. If other media requiring risk-based PRGs are identified during the RI/FS, or other exposure parameters or land uses are assumed, then appropriate equations will need to be modified or new ones developed.

Risk-based equations have been derived in order to reflect the potential risk from exposure to a chemical, given a specific pathway, medium, and land-use combination. By setting the total risk for carcinogenic effects at a target risk level of 10^{-6} (the NCP's point of departure for analysis of remedial alternatives), it is possible to solve for the concentration term (i.e., the risk-based PRG). The total risk for noncarcinogenic effects is set at an HI of 1 for each chemical in a particular medium. Full equations with pathway-specific default exposure factors are presented in boxes with uniformly thin borders. Reduced equations are presented in the standard boxes (i.e., thicker top and bottom borders). At the end of this chapter, the case study that began in Chapter 2 is concluded (by showing how to calculate and present risk-based PRGs).

In general, the equations described in this chapter are sufficient for calculating the risk-based PRGs at the scoping stage of the RI/FS. Note, however, that these equations are based on standard default assumptions that may or may not reflect site-specific conditions. When risk-based PRGs are to be calculated based on site-specific conditions, the risk assessor should modify the full equations, and/or develop additional ones. Risk equations for individual exposure pathways for a given medium are presented in Appendix B of this document, and may be used to develop and/or modify the full equations. (See the introduction to Appendix B for more detailed instructions.)

Before examining the calculation of risk-based PRGs, several important points should be noted:

- Use of toxicity values in the equations as written currently assumes 100 percent absorption effeciency. That is, for the sake of simplicity at scoping, it is assumed that the dose administered to test animals in toxicity studies on which toxicity values are based was fully absorbed. This assumption may need to be revised in cases where toxicity values based on route-to-route extrapolation are used, or there are significant differences in absorption likely between contaminants in site media and the contaminants in the vehicle used in the toxicity study. Chapter 7 and Appendix A in RAGS/HHEM Part A (EPA 1989d) provide additional details on this point.

- The risk-based PRGs should contain at most two significant figures even though some of the parameters used in the reduced equations carry additional significant figures.

- The equations presented in this chapter calculate risk-based concentrations using inhalation reference doses (RfD_is) and inhalation slope factors (SF_is). If only the reference concentration (RfC) and/or inhalation unit risk are available for a particular compound in IRIS, conversion to an RfD_i and/or SF_i will be necessary. Many converted toxicity values are available in HEAST.

- All standard equations presented here incorporate pathway-specific default exposure

factors that generally reflect RME conditions. As detailed in Chapter 8 of RAGS/HHEM Part A (in the discussion on combining pathway risks [Section 8.3]), RME risks from one pathway should be combined with RME risks from another pathway only where there is good reason. Typically, RME from one pathway is not likely to occur with RME from another (unless there is a strong logical dependent relationship between exposures from the two pathways). If risk-based concentrations are developed for both the water and the soil pathways, the risk assessor ultimately may need to adjust exposure assumptions from one pathway (i.e., the one with the lower RME) to less conservative (more typical) values.

3.1 RESIDENTIAL LAND USE

3.1.1 GROUND WATER OR SURFACE WATER

Under residential land use, risk from surface water or ground-water contaminants is assumed to be due primarily to direct ingestion and to inhalation of volatiles from household water use. Therefore, only these exposure pathways are considered in this section. Additional exposure pathways (e.g., dermal absorption) are possible and may be significant at some sites for some contaminants, while perhaps only one exposure pathway (e.g., direct ingestion of water only) may be relevant at others. In any case, the risk-based PRG for each chemical should be calculated by considering all of the relevant exposure pathways.

In the case illustrated here, risks from two exposure pathways from ground water or surface water are combined, and the risk-based concentration is derived to be protective for exposures from both pathways. Default risk from ground water or surface water would be calculated as follows ("total" risk, as used below, refers to the combined risk for a single chemical from all exposure pathways for a given medium):

Total risk from water	=	Risk from ingestion of water (adult)	+	Risk from inhalation of volatiles from household water (adult)

At scoping, risk from indoor inhalation of volatiles is assumed to be relevant only for chemicals that easily volatilize. Thus, the risk equation incorporates a water-air concentration relationship that is applicable only to chemicals with a Henry's Law constant of greater than 1 x 10^{-5} atm-m^3/mole and a molecular weight of less than 200 g/mole. These criteria are not used to screen out chemicals that are not of potential concern for this exposure pathway but only to identify those that generally should be considered for the inhalation pathway when developing risk-based PRGs early in the process. Chemicals that do not meet these criteria may pose significant site risks (and require risk-based goals) through volatiles inhalation. The ultimate decision regarding which contaminants should be considered in the FS must be made on a site-specific basis following completion of the baseline risk assessment.

Based primarily on experimental data on the volatilization of radon from household uses of water, Andelman (1990) derived an equation that defines the relationship between the concentration of a contaminant in household water and the average concentration of the volatilized contaminant in air. In the derivation, all uses of household water were considered (e.g., showering, laundering, dish washing). The equation uses a default "volatilization" constant (K) upper-bound value of 0.0005 x 1000 L/m^3. (The 1000 L/m^3 conversion factor is incorporated into the equation so that the resulting air concentration is expressed in mg/m^3.) Certain assumptions were made in deriving the default constant K (Andelman 1990). For example, it is assumed that the volume of water used in a residence for a family of four is 720 L/day, the volume of the dwelling is 150,000 L and the air exchange rate is 0.25 m^3/hr. Furthermore, it is assumed that the average transfer efficiency weighted by water use is 50 percent (i.e., half of the concentration of each chemical in water will be transfered into air by all water uses [the range extends from 30% for toilets to 90% for dishwashers]). See the Andelman paper for further details.

Concentrations Based on Carcinogenic Effects. Total risk for carcinogenic effects of certain volatile chemicals would be calculated by combining the appropriate inhalation and oral SFs with the two intakes from water:

Total risk	=	SF_o x	Intake from ingestion of water	+	SF_i x	Intake from inhalation of volatiles from water

Adding appropriate parameters, and then rearranging the equation to solve for concentration, results in Equation (1).

Equation (1′) on the next page is the reduced version of Equation (1) using the standard default parameters, and is used to calculate the risk-based PRG at a prespecified cancer risk level of 10^{-6}. It combines the toxicity information of a chemical with standard default exposure parameters for residential land use to generate the concentration of that chemical that corresponds to a 10^{-6} carcinogenic risk level due to that chemical. If either the SF_o or SF_i in Equation (1′) is not available for a particular chemical, the term containing that variable in the equation can be ignored or equated to zero (e.g., for a chemical that does not have SF_i, the term $7.5(SF_i)$ in Equation (1′) is ignored). If any of the default parameter values are changed to reflect site-specific conditions, the reduced equation cannot be used.

RESIDENTIAL WATER — CARCINOGENIC EFFECTS

$$TR = \frac{SF_o \times C \times IR_w \times EF \times ED}{BW \times AT \times 365\ days/yr} + \frac{SF_i \times C \times K \times IR_a \times EF \times ED}{BW \times AT \times 365\ days/yr}$$

$$= \frac{EF \times ED \times C \times [(SF_o \times IR_w) + (SF_i \times K \times IR_a)]}{BW \times AT \times 365\ days/yr}$$

$$C\ (mg/L;\ risk\text{-}based) = \frac{TR \times BW \times AT \times 365\ days/yr}{EF \times ED \times [(SF_i \times K \times IR_a) + (SF_o \times IR_w)]} \quad (1)$$

where:

Parameters	Definition (units)	Default Value
C	chemical concentration in water (mg/L)	—
TR	target excess individual lifetime cancer risk (unitless)	10^{-6}
SF_i	inhalation cancer slope factor ($(mg/kg\text{-}day)^{-1}$)	chemical-specific
SF_o	oral cancer slope factor ($(mg/kg\text{-}day)^{-1}$)	chemical-specific
BW	adult body weight (kg)	70 kg
AT	averaging time (yr)	70 yr
EF	exposure frequency (days/yr)	350 days/yr
ED	exposure duration (yr)	30 yr
IR_a	daily indoor inhalation rate (m^3/day)	15 m^3/day
IR_w	daily water ingestion rate (L/day)	2 L/day
K	volatilization factor (unitless)	0.0005 x 1000 L/m^3 (Andelman 1990)

REDUCED EQUATION: RESIDENTIAL WATER — CARCINOGENIC EFFECTS

$$\text{Risk-based PRG } (mg/L;\ TR = 10^{-6}) = \frac{1.7 \times 10^{-4}}{2(SF_o) + 7.5(SF_i)} \quad (1')$$

where:

SF_o = oral slope factor in $(mg/kg\text{-}day)^{-1}$
SF_i = inhalation slope factor in $(mg/kg\text{-}day)^{-1}$

Concentrations Based on Noncarcinogenic Effects. Total HI would be calculated by combining the appropriate oral and inhalation RfDs with the two intakes from water:

$$HI = \frac{\text{Intake from oral ingestion}}{RfD_o} + \frac{\text{Intake from inhalation}}{RfD_i}$$

Adding appropriate parameters, and then rearranging the equation to solve for concentration, results in Equation (2).

Equation (2′) on the next page is the reduced version of Equation (2) using the standard default parameters, and is used to calculate the risk-based PRG at a prespecified HI of 1. It combines the toxicity information of a chemical with standard exposure parameters for residential land use to generate the concentration of that chemical that corresponds to an HI of 1. If either the RfD_o or RfD_i in Equation (2′) is not available for a particular chemical, the term containing that variable in the equation can be ignored or equated to zero (e.g., for a chemical that does not have RfD_i, the term $7.5/RfD_i$ in Equations (2′) is ignored).

RESIDENTIAL WATER — NONCARCINOGENIC EFFECTS

$$THI = \frac{C \times IR_w \times EF \times ED}{RfD_o \times BW \times AT \times 365\ days/yr} + \frac{C \times K \times IR_a \times EF \times ED}{RfD_i \times BW \times AT \times 365\ days/yr}$$

$$= \frac{EF \times ED \times C \times [(1/RfD_o \times IR_w) + (1/RfD_i \times K \times IR_a)]}{BW \times AT \times 365\ days/yr}$$

$$C\ (mg/L;\ risk\text{-}based) = \frac{THI \times BW \times AT \times 365\ days/yr}{EF \times ED \times [(1/RfD_i \times K \times IR_a) + (1/RfD_o \times IR_w)]} \quad (2)$$

where:

Parameters	Definition	Default Value
C	chemical concentration in water (mg/L)	—
THI	target hazard index (unitless)	1
RfD_o	oral chronic reference dose (mg/kg-day)	chemical-specific
RfD_i	inhalation chronic reference dose (mg/kg-day)	chemical-specific
BW	adult body weight (kg)	70 kg
AT	averaging time (yr)	30 yr (for noncarcinogens, equal to ED)
EF	exposure frequency (days/yr)	350 days/yr
ED	exposure duration (yr)	30 yr
IR_a	daily indoor inhalation rate (m^3/day)	15 m^3/day
IR_w	daily water ingestion rate (L/day)	2 L/day
K	volatilization factor (unitless)	0.0005 x 1000 L/m^3 (Andelman 1990)

REDUCED EQUATION: RESIDENTIAL WATER — NONCARCINOGENIC EFFECTS

$$\text{Risk-based PRG } (mg/L;\ THI = 1) = \frac{73}{[7.5/RfD_i + 2/RfD_o]} \quad (2′)$$

where:

RfD_o = oral chronic reference dose in mg/kg-day
RfD_i = inhalation chronic reference dose in mg/kg-day

3.1.2 SOIL

Under residential land use, risk of the contaminant from soil is assumed to be due to direct ingestion of soil only.

Total risk from soil = Risk from ingestion of soil (child to adult)

Because the soil ingestion rate is different for children and adults, the risk due to direct ingestion of soil is calculated using an age-adjusted ingestion factor. The age-adjusted soil ingestion factor ($IF_{soil/adj}$) takes into account the difference in daily soil ingestion rates, body weights, and exposure durations for two exposure groups — children of one to six years and others of seven to 31 years. Exposure frequency (EF) is assumed to be identical for the two exposure groups. For convenience, this factor is calculated separately as a time-weighted soil intake, normalized to body weight, that can then be substituted in the total intake equation. Calculated in this manner, the factor leads to a more protective risk-based concentration compared to an adult-only assumption. Note that the ingestion factor is in units of mg-yr/kg-day, and therefore is not directly comparable to daily soil intake rate in units of mg/kg-day. See the box containing Equation (3) for the calculation of this factor.

Additional exposure pathways (e.g., inhalation of particulates, inhalation of volatiles, ingestion of foodcrops contaminated through airborne particulate deposits, consumption of ground water contaminated by soil leachate) are possible at some sites. The risk assessor should evaluate whether inhalation or other exposure pathways are significant at the site. Generally, for many undisturbed sites with vegetative cover such as those found in areas of residential land use, air pathways are relatively minor contributors of risk. Greater concern for baseline risk via air pathways exists under commercial/industrial land-use assumptions, given the increased activity levels likely (see Section 3.2.2). Air pathway risks also tend to be major concerns during remedial action (see RAGS/HHEM Part C). If these other pathways are known to be significant at scoping, Appendix B and/or other information should be used to develop site-specific equations for the risk-based PRGs.

Concentrations Based on Carcinogenic Effects. Total risk for carcinogenic effects would be calculated by combining the appropriate oral SF with the intake from soil:

Total risk = SF_o x Intake from ingestion of soil

Adding appropriate parameters, and then rearranging the equation to solve for concentration, results in Equation (4).

Equation (4´) below is the reduced version of Equation (4) using the standard default parameters, and is used to calculate the risk-based PRG at a prespecified cancer risk level of 10^{-6}. It combines the toxicity information of a chemical with standard exposure parameters for residential land use to generate the concentration of that chemical that corresponds to a 10^{-6} carcinogenic risk level due to that chemical.

AGE-ADJUSTED SOIL INGESTION FACTOR

$$IF_{soil/adj}\ (\text{mg-yr/kg-day}) = \frac{IR_{soil/age1\text{-}6} \times ED_{age1\text{-}6}}{BW_{age1\text{-}6}} + \frac{IR_{soil/age7\text{-}31} \times ED_{age7\text{-}31}}{BW_{age7\text{-}31}} \quad (3)$$

Parameter	Definition	Default Value
$IF_{soil/adj}$	age-adjusted soil ingestion factor (mg-yr/kg-day)	114 mg-yr/kg-day
$BW_{age1\text{-}6}$	average body weight from ages 1-6 (kg)	15 kg
$BW_{age7\text{-}31}$	average body weight from ages 7-31 (kg)	70 kg
$ED_{age1\text{-}6}$	exposure duration during ages 1-6 (yr)	6 yr
$ED_{age7\text{-}31}$	exposure duration during ages 7-31 (yr)	24 yr
$IR_{soil/age1\text{-}6}$	ingestion rate of soil age 1 to 6 (mg/day)	200 mg/day
$IR_{soil/age7\text{-}31}$	ingestion rate of soil all other ages (mg/day)	100 mg/day

RESIDENTIAL SOIL — CARCINOGENIC EFFECTS

$$TR = \frac{SF_o \times C \times 10^{-6}\ kg/mg \times EF \times IF_{soil/adj}}{AT \times 365\ days/yr}$$

$$C\ (mg/kg;\ risk\text{-}based) = \frac{TR \times AT \times 365\ days/year}{SF_o \times 10^{-6}\ kg/mg \times EF \times IF_{soil/adj}} \quad (4)$$

where:

Parameters	Definition (units)	Default Value
C	chemical concentration in soil (mg/kg)	—
TR	target excess individual lifetime cancer risk (unitless)	10^{-6}
SF_o	oral cancer slope factor ((mg/kg-day)$^{-1}$)	chemical-specific
AT	averaging time (yr)	70 yr
EF	exposure frequency (days/yr)	350 days/yr
$IF_{soil/adj}$	age-adjusted ingestion factor (mg-yr/kg-day)	114 mg-yr/kg-day (see Equation (3))

REDUCED EQUATION: RESIDENTIAL SOIL — CARCINOGENIC EFFECTS

$$\text{Risk-based PRG } (mg/kg;\ TR = 10^{-6}) = \frac{0.64}{SF_o} \quad (4')$$

where:

SF_o = oral slope factor in (mg/kg-day)$^{-1}$

Concentrations Based on Noncarcinogenic Effects. Total HI would be calculated by combining the appropriate oral RfD with the intake from soil:

$$HI = \frac{\text{Intake from ingestion}}{RfD_o}$$

Adding appropriate parameters, and then rearranging the equation to solve for concentration, results in Equation (5).

Equation (5′) is the reduced version of Equation (5) using the standard default parameters, and is for calculating the risk-based PRG at a prespecified HI of 1. It combines the toxicity information of a chemical with standard exposure parameters for residential land use to generate the concentration of that chemical that corresponds to an HI of 1.

3.2 COMMERCIAL/INDUSTRIAL LAND USE

3.2.1 WATER

Once ground water is determined to be suitable for drinking, risk-based concentrations should be based on residential exposures. This is because the NCP seeks to require protection of ground water to allow for its maximum beneficial use (see Section 2.3). Thus, under the commercial/industrial land-use scenario, risk-based PRGs for ground water are calculated according to procedures detailed in Section 3.1.1. Similarly, for surface water that is to be used for drinking, the risk-based PRGs should be calculated for residential populations, and not simply worker populations.

RESIDENTIAL SOIL — NONCARCINOGENIC EFFECTS

$$THI = \frac{C \times 10^{-6}\ kg/mg \times EF \times IF_{soil/adj}}{RfD_o \times AT \times 365\ days/yr}$$

$$C\ (mg/kg;\ risk\text{-}based) = \frac{THI \times AT \times 365\ days/yr}{1/RfD_o \times 10^{-6}\ kg/mg \times EF \times IF_{soil/adj}} \quad (5)$$

where:

Parameters	Definition (units)	Default Value
C	chemical concentration in soil (mg/kg)	—
THI	target hazard index (unitless)	1
RfD_o	oral chronic reference dose (mg/kg-day)	chemical-specific
AT	averaging time (yr)	30 yr (for noncarcinogens, equal to ED [which is incorporated in $IF_{soil/adj}$])
EF	exposure frequency (days/yr)	350 days/yr
$IF_{soil/adj}$	age-adjusted ingestion factor (mg-yr/kg-day)	114 mg-yr/kg-day (see Equation (3))

REDUCED EQUATION: RESIDENTIAL SOIL — NONCARCINOGENIC EFFECTS

$$\text{Risk-based PRG (mg/kg; THI = 1)} = 2.7 \times 10^{5}\ (RfD_o) \quad (5')$$

where:

RfD_o = oral chronic reference dose in mg/kg-day

3.2.2 SOIL

Under commercial/industrial land use, risk of the contaminant from soil is assumed to be due to direct ingestion, inhalation of volatiles from the soil, and inhalation of particulates from the soil, and is calculated for an adult worker only. For this type of land use, it is assumed for calculating default risk-based PRGs that there is greater potential for use of heavy equipment and related traffic in and around contaminated soils and thus greater potential for soils to be disturbed and produce particulate and volatile emissions than in most residential land-use areas. Additional exposure pathways (e.g., dermal exposure) are possible at some sites, while perhaps only one exposure pathway (e.g., direct ingestion of soil only) may be relevant at others; Appendix B may be used to identify relevant exposure pathways to be combined. In such cases, the risk is calculated by considering all the relevant exposure pathways identified in the RI.

In the default case illustrated below, intakes from the three exposure pathways are combined and the risk-based PRG is derived to be protective for exposures from all three pathways. In this case, the risk for a specific chemical from soil due to the three exposure pathways would be calculated as follows:

Total risk from soil = Risk from ingestion of soil (worker)
+ Risk from inhalation of volatiles from soil (worker)
+ Risk from inhalation of particulates from soil (worker)

It is possible to consider only exposure pathways of site-specific importance by deriving a site-specific risk-based PRG (e.g., using the equations in Appendix B).

Concentrations Based on Carcinogenic Effects. Total risk for carcinogenic effects would be calculated by combining the appropriate inhalation and oral SFs with the three intakes from soil:

$$\text{Total risk} = SF_o \times \text{Intake from ingestion of soil (worker)} + SF_i \times \text{Intake from inhalation of volatiles from soil (worker)} + SF_i \times \text{Intake from inhalation of particulates (worker)}$$

Adding appropriate parameters, and then rearranging the equation to solve for concentration, results in Equation (6). As discussed in more detail in Section 3.3.1, Equation (6a) is used to test the results of Equation (6).

Equation (6´) is the reduced version of Equation (6) using the standard default parameters, and is used to calculate the risk-based PRG at a prespecified cancer risk level of 10^{-6}. It combines the toxicity information of a chemical with standard exposure parameters for commercial/industrial land use to generate the concentration of that chemical that corresponds to a 10^{-6} carcinogenic risk level due to that chemical.

Concentrations Based on Noncarcinogenic Effects. Total HI would be calculated by combining the appropriate oral and inhalation RfDs with the three intakes from soil:

$$HI = \frac{\text{Intake from ingestion}}{RfD_o} + \frac{\text{(Intake from inhalation of volatiles and particulates)}}{RfD_i}$$

Adding appropriate parameters, and then rearranging the equation to solve for concentration, results in Equation (7).

Equation (7´) is the reduced version of Equation (7) using the standard default parameters, and is used to calculate the risk-based PRG at a prespecified HI of 1. It combines the toxicity information of a chemical with standard exposure parameters for commercial/industrial land use to generate the concentration of that chemical that corresponds to an HI of 1.

3.3 VOLATILIZATION AND PARTICULATE EMISSION FACTORS

3.3.1 SOIL-TO-AIR VOLATILIZATION FACTOR

The volatilization factor (VF) is used for defining the relationship between the concentration of contaminants in soil and the volatilized contaminants in air. This relationship was established as a part of the Hwang and Falco (1986) model developed by EPA's Exposure Assessment Group (EAG). Hwang and Falco present a method intended primarily to estimate the permissible residual levels associated with the cleanup of contaminated soils. This method has been used by EPA in estimating exposures to PCBs and 2,3,7,8-TCDD from contaminated soil (EPA 1986; EPA 1988a). One of the pathways considered in this method is the intake by inhalation of volatilized contaminants.

The basic principle of the Hwang and Falco model is applicable only if the soil contaminant concentration is at or below saturation. Saturation is the soil contaminant concentration at which the adsorptive limits of the soil particles and the solubility limits of the available soil moisture have been reached. Above saturation, pure liquid-phase contaminant is present in the soil. Under such conditions, the partial pressure of the pure contaminant and the partial pressure of air in the interstitial soil pore spaces cannot be calculated without first knowing the mole fraction of the contaminant in the soil. Therefore, above saturation, the PRG cannot be accurately calculated based on volatilization. Because of this limitation, the chemical concentration in soil (C) calculated using the VF must be compared with the soil saturation concentration (C_{sat}) calculated using Equation (6a) or (7a). If C is greater than C_{sat}, then the PRG is set equal to C_{sat}.

The VF presented in this section assumes that the contaminant concentration in the soil is homogeneous from the soil surface to the depth of concern and that the contaminated material is not covered by contaminant-free soil material. For the purpose of calculating VF, depth of concern is defined as the depth at which a near impenetrable layer or the permanent ground-water level is reached.

COMMERCIAL/INDUSTRIAL SOIL — CARCINOGENIC EFFECTS

$$TR = \frac{SF_o \times C \times 10^{-6}\ kg/mg \times EF \times ED \times IR_{soil}}{BW \times AT \times 365\ days/yr} + \frac{SF_i \times C \times EF \times ED \times IR_{air} \times (1/VF + 1/PEF)}{BW \times AT \times 365\ days/yr}$$

$$C\ (mg/kg;\ risk\text{-}based) = \frac{TR \times BW \times AT \times 365\ days/yr}{EF \times ED \times [(SF_o \times 10^{-6}\ kg/mg \times IR_{soil}) + (SF_i \times IR_{air} \times [1/VF + 1/PEF])]} \quad (6)$$

where:

Parameters	Definition (units)	Default Value
C	chemical concentration in soil (mg/kg)	—
TR	target excess individual lifetime cancer risk (unitless)	10^{-6}
SF_i	inhalation cancer slope factor ((mg/kg-day)$^{-1}$)	chemical-specific
SF_o	oral cancer slope factor ((mg/kg-day)$^{-1}$)	chemical-specific
BW	adult body weight (kg)	70 kg
AT	averaging time (yr)	70 yr
EF	exposure frequency (days/yr)	250 days/yr
ED	exposure duration (yr)	25 yr
IR_{soil}	soil ingestion rate (mg/day)	50 mg/day
IR_{air}	workday inhalation rate (m^3/day)	20 m^3/day
VF	soil-to-air volatilization factor (m^3/kg)	chemical-specific (see Section 3.3.1)
PEF	particulate emission factor(m^3/kg)	4.63×10^9 m^3/kg (see Section 3.3.2)

$$C_{sat} = (K_d \times s \times n_m) + (s \times \Theta_m) \quad (6a)$$

where:

Parameters	Definition (units)	Default Value
C_{sat}	soil saturation concentration (mg/kg)	—
K_d	soil-water partition coefficient (L/kg)	chemical-specific, or K_{oc} x OC
K_{oc}	organic carbon partition coefficient (L/kg)	chemical-specific
OC	organic carbon content of soil (fraction)	site-specific, or 0.02
s	solubility (mg/L-water)	chemical-specific
n_m	soil moisture content, expressed as a weight fraction	site-specific
Θ_m	soil moisture content, expressed as L-water/kg-soil	site-specific

REDUCED EQUATION: COMMERCIAL/INDUSTRIAL SOIL — CARCINOGENIC EFFECTS

$$\text{Risk-based PRG } (mg/kg;\ TR = 10^{-6}) = \frac{2.9 \times 10^{-4}}{[((5 \times 10^{-5}) \times SF_o) + (SF_i \times ((20/VF) + (4.3 \times 10^{-9})))]} \quad (6')$$

where:

SF_o = oral slope factor in (mg/kg-day)$^{-1}$
SF_i = inhalation slope factor in (mg/kg-day)$^{-1}$
VF = chemical-specific soil-to-air volatilization factor in m^3/kg (see Section 3.3.1)

If PRG > C_{sat}, then set PRG = C_{sat} (where C_{sat} = soil saturation concentration (mg/kg); see Equation (6a) and Section 3.3.1).

COMMERCIAL/INDUSTRIAL SOIL — NONCARCINOGENIC EFFECTS

$$THI = \frac{C \times 10^{-6}\ kg/mg \times EF \times ED \times IR_{soil}}{RfD_o \times BW \times AT \times 365\ days/yr} + \frac{C \times EF \times ED \times IR_{air} \times (1/VF + 1/PEF)}{RfD_i \times BW \times AT \times 365\ days/yr}$$

$$C\ (mg/kg;\ risk\text{-}based) = \frac{THI \times BW \times AT \times 365\ days/yr}{ED \times EF \times [((1/RfD_o) \times 10^{-6}\ kg/mg \times IR_{soil}) + ((1/RfD_i) \times IR_{air} \times (1/VF + 1/PEF))]} \quad (7)$$

where:

Parameters	Definition (units)	Default Value
C	chemical concentration in soil (mg/kg)	—
THI	target hazard index (unitless)	1
RfD_o	oral chronic reference dose (mg/kg-day)	chemical-specific
RfD_i	inhalation chronic reference dose (mg/kg-day)	chemical-specific
BW	adult body weight (kg)	70 kg
AT	averaging time (yr)	25 yr (always equal to ED)
EF	exposure frequency (days/yr)	250 days/yr
ED	exposure duration (yr)	25 yr
IR_{soil}	soil ingestion rate (mg/day)	50 mg/day
IR_{air}	workday inhalation rate (m^3/day)	20 m^3/day
VF	soil-to-air volatilization factor (m^3/kg)	chemical-specific (see Section 3.3.1)
PEF	particulate emission factor (m^3/kg)	4.63×10^9 m^3/kg (see Section 3.3.2)

$$C_{sat} = (K_d \times s \times n_m) + (s \times \Theta_m) \quad (7a)$$

where:

Parameters	Definition (units)	Default Value
C_{sat}	soil saturation concentration (mg/kg)	—
K_d	soil-water partition coefficient (L/kg)	chemical-specific, or K_{oc} x OC
K_{oc}	organic carbon partition coefficient (L/kg)	chemical-specific
OC	organic carbon content of soil (fraction)	site-specific, or 0.02
s	solubility (mg/L-water)	chemical-specific
n_m	soil moisture content, expressed as a weight fraction	site-specific
Θ_m	soil moisture content, expressed as L-water/kg-soil	site-specific

REDUCED EQUATION: COMMERCIAL/INDUSTRIAL SOIL — NONCARCINOGENIC EFFECTS

$$\text{Risk-based PRG (mg/kg; THI = 1)} = \frac{102}{[(5 \times 10^{-5}/RfD_o) + ((1/RfD_i) \times ((20/VF) + (4.3 \times 10^{-9})))]} \quad (7')$$

where:

RfD_o = oral chronic reference dose in mg/kg-day
RfD_i = inhalation chronic reference dose in mg/kg-day
VF = chemical-specific soil-to-air volatilization factor in m^3/kg (see Section 3.3.1)

If PRG > C_{sat}, then set PRG = C_{sat} (where C_{sat} = soil saturation concentration (mg/kg); see Equation (7a) and Section 3.3.1).

A chemical-specific value for VF is used in the standard default equations (Equations (6), (6′), (7), and (7′) in Section 3.2.2) and is developed in Equation (8). The VF value calculated using Equation (8) has been developed for specific use in the other equations in this guidance; it may not be applicable in other technical contexts. Equation (8) lists the standard default parameters for calculating VF. If site-specific information is available, Equation (8) may be modified to calculate a VF that is more appropriate for the particular site. Supporting references should be consulted when substituting site-specific data to ensure that the model and specific parameters can be appropriately applied to the given site.

3.3.2 PARTICULATE EMISSION FACTOR

The particulate emission factor (PEF) relates the contaminant concentration in soil with the concentration of respirable particles (PM_{10}) in the air due to fugitive dust emissions from surface contamination sites. This relationship is derived by Cowherd (1985) for a rapid assessment procedure applicable to a typical hazardous waste site where the surface contamination provides a relatively continuous and constant potential for emission over an extended period of time (e.g., years). The particulate emissions from contaminated sites are due to wind erosion and, therefore, depend on the erodibility of the surface

SOIL-TO-AIR VOLATILIZATION FACTOR

$$VF\ (m^3/kg) = \frac{(LS \times V \times DH)}{A} \times \frac{(3.14 \times \alpha \times T)^{1/2}}{(2 \times D_{ei} \times E \times K_{as} \times 10^{-3}\ kg/g)} \quad (8)$$

where:

$$\alpha\ (cm^2/s) = \frac{(D_{ei} \times E)}{E + (\rho_s)(1-E)/K_{as}}$$

Standard default parameter values that can be used to reduce Equation (8) are listed below. These represent "typical" values as identified in a number of sources. For example, when site-specific values are not available, the length of a side of the contaminated area (LS) is assumed to be 45 m; this is based on a contaminated area of 0.5 acre which approximates the size of an average residential lot. The "typical" values LS, DH, and V are from EPA 1986. "Typical" values for E, OC, and ρ_s are from EPA 1984, EPA 1988b, and EPA 1988f. Site-specific data should be substituted for the default values listed below wherever possible. Standard values for chemical-specific D_i, H, and K_{oc} can be obtained by calling the Superfund Health Risk Technical Support Center.

Parameter	Definition (units)	Default
VF	volatilization factor (m^3/kg)	—
LS	length of side of contaminated area (m)	45 m
V	wind speed in mixing zone (m/s)	2.25 m/s
DH	diffusion height (m)	2 m
A	area of contamination (cm^2)	20,250,000 cm^2
D_{ei}	effective diffusivity (cm^2/s)	$D_i \times E^{0.33}$
E	true soil porosity (unitless)	0.35
K_{as}	soil/air partition coefficient (g soil/cm^3 air)	(H/K_d) x 41, where 41 is a units conversion factor
ρ_s	true soil density or particulate density (g/cm^3)	2.65 g/cm^3
T	exposure interval (s)	7.9×10^8 s
D_i	molecular diffusivity (cm^2/s)	chemical-specific
H	Henry's law constant (atm-m^3/mol)	chemical-specific
K_d	soil-water partition coefficient (cm^3/g)	chemical-specific, or $K_{oc} \times OC$
K_{oc}	organic carbon partition coefficient (cm^3/g)	chemical-specific
OC	organic carbon content of soil (fraction)	site-specific, or 0.02

material. The equation presented below, Equation (9), is representative of a surface with "unlimited erosion potential," which is characterized by bare surfaces of finely divided material such as sandy agricultural soil with a large number ("unlimited reservoir") of erodible particles. Such surfaces erode at low wind speeds, and particulate emission rates are relatively time-independent at a given wind speed.

This model was selected for use in RAGS/HHEM Part B because it represents a conservative estimate for intake of particulates; it is used to derive Equations (6) and (7) in Section 3.2.2.

Using the default parameter values given in the box for Equation (9), the default PEF is equal to 4.63×10^9 m^3/kg. The default values necessary to calculate the flux rate for an "unlimited reservoir" surface (i.e., G, U_m, U_t, and F(x)) are provided by Cowherd (1985), and the remaining default values (i.e., for LS, V, and DH) are "typical" values (EPA 1986). If site-specific information is available, Equation (9) may be modified to calculate a PEF that is more appropriate for the particular site. Again, the original reference should be consulted when substituting site-specific data to ensure applicability of the model to specific site conditions.

PARTICULATE EMISSION FACTOR

$$PEF\ (m^3/kg) = \frac{LS \times V \times DH \times 3600\ s/hr}{A} \times \frac{1000\ g/kg}{0.036 \times (1-G) \times (U_m/U_t)^3 \times F(x)} \quad (9)$$

where:

Parameter	Definition (units)	Default
PEF	particulate emission factor (m^3/kg)	4.63×10^9 m^3/kg
LS	width of contaminated area (m)	45 m
V	wind speed in mixing zone (m/s)	2.25 m/s
DH	diffusion height (m)	2 m
A	area of contamination (m^2)	2025 m^2
0.036	respirable fraction (g/m^2-hr)	0.036 g/m^2-hr
G	fraction of vegetative cover (unitless)	0
U_m	mean annual wind speed (m/s)	4.5 m/s
U_t	equivalent threshold value of wind speed at 10 m (m/s)	12.8 m/s
F(x)	function dependent on U_m/U_t (unitless)	0.0497 (determined using Cowherd 1985)

3.4 CALCULATION AND PRESENTATION OF RISK-BASED PRGs

The equations presented in this chapter can be used to calculate risk-based PRGs for both carcinogenic and noncarcinogenic effects. If both a carcinogenic and a noncarcinogenic risk-based PRG are calculated for a particular chemical, then the lower of the two values is considered the appropriate risk-based PRG for any given contaminant. The case-study box below illustrates a calculation of a risk-based PRG. A summary table — such as that in the final case-study box — should be developed to present both the risk-based PRGs and the ARAR-based PRGs. The table should be labeled as to whether it presents the concentrations that were developed during scoping or after the baseline risk assessment.

CASE STUDY: CALCULATE RISK-BASED PRGs[a]

Risk-based PRGs for ground water for isophorone, one of the chemicals detected in ground-water monitoring wells at the site, are calculated below. Initial risk-based PRGs for isophorone (carcinogenic and noncarcinogenic effects) are derived using Equations (1′) and (2′) in Section 3.1.1. Equations (1′) and (2′) combine the toxicity information of the chemical (oral RfD of 0.2 mg/kg-day and oral SF of 0.0039 $[mg/kg\text{-}day]^{-1}$; inhalation values are not available and, therefore, only the oral exposure route is considered) with standard exposure parameters. The calculated concentrations in mg/L correspond to a target risk of 10^{-6} and a target HQ of 1, as follows:

$$\text{Carcinogenic risk-based PRG} = \frac{1.7 \times 10^{-4}}{2(SF_o)} = \frac{1.7 \times 10^{-4}}{2(0.0039)} = 0.022 \text{ mg/L}$$

$$\text{Noncarcinogenic risk-based PRG} = \frac{73}{2/RfD_o} = \frac{73}{2/0.2} = 7.3 \text{ mg/L}$$

The lower of the two values (i.e., 0.022 mg/L) is selected as the appropriate risk-based PRG. Risk-based PRGs are calculated similarly for the other chemicals of concern.

[a] All information in this example is for illustration purposes only.

CASE STUDY: PRESENT PRGs DEVELOPED DURING SCOPING[a]

Site: XYZ Co.
Location: Anytown, Anystate
Medium: Ground Water

Land Use: Residential
Exposure Routes: Water Ingestion, Inhalation of Volatiles

Chemical	Risk-based PRGs (mg/L)*		ARAR-based PRG	
	10^{-6}	HQ = 1	Type	Concentration (mg/L)
Benzene	—	—	MCL	0.005
Carbon Tetrachloride	—	—	MCL	0.005
Ethylbenzene	—	—	MCLG MCL	0.7*** 0.7
Hexane	—	0.33	—	—
Isophorone	0.022**	7.3	—	—
Triallate	—	0.47	—	—
1,1,2-Trichloroethane	—	—	MCLG MCL	0.003*** 0.005
Vinyl chloride	—	—	MCL	0.002

[a] All information in this example is for illustration purposes only.
* These concentrations were calculated using the standard default equations in Chapter 3.
** Of the two potential risk-based PRGs for this chemical, this concentration is the selected risk-based PRG.
*** Of the two potential ARAR-based PRGs for this chemical, this concentration is selected as the ARAR-based PRG.