CalTOX, A Multimedia Total Exposure Model for Hazardous Waste Sites

Part III: The Multiple Pathway Exposure Model

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FOREWORD

This is the third of a series of three reports describing the technical and scientific basis of the CalTOX risk assessment model. The major objective of CalTOX is to improve the accuracy of risk assessment information presented to risk managers. In the development of CalTOX, the Department of Toxic Substance Control (DTSC) has given great weight to scientific credibility. A recognized international expert in the field of environmental chemical transport and risk assessment developed the model based on publications in the peer-reviewed scientific literature. These CalTOX reports have undergone three review and revision cycles focusing exclusively on the technical and scientific issues.

DTSC has intentionally avoided issues relating to the application of the model to assess risk for regulatory action in these three documents. This is because the models basis needed to be formed primarily on credible science, not regulatory need. CalTOX introduces a number of approaches which differ form current forms of risk assessment including a stochastic means of estimating risk and a source depleting transport model. Therefore, existing risk assessment policy will not be adequate to guide the use of CalTOX. Additional policy will have to be determined before the model can be implemented for regulatory decision making. Therefore, these technical documents should be viewed as describing the technical basis around which a policy will be developed. These reports do not contain that policy context. Therefore, **do not cite, quote or use these documents to support any regulatory action**.

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CalTOX, A Multimedia Total Exposure Model for Hazardous Waste Sites

Part III: The Multiple Pathway Exposure Model

ABSTRACT

Part III of the CalTOX model manual is a description of the multimedia, multiple pathway, multiple route exposure model used to estimate the daily intake of a chemical of concern by an exposed person at a hazardous waste site. The model assumes that soil is the primary environmental medium contaminated at a hazardous waste site (also called hazardous substances release site). Air, water and food may also become contaminated from soil. The model assumes that a person may be exposed to a chemical by as many as thirteen potential pathways at a hazardous waste site. The multiple pathway exposure model determines the daily intake from all relevant pathways, can relate a soil concentration of a chemical to that daily intake, and calculates the risks and hazards associated with the intake. Part III describes the methods, assumptions, and inputs used in the model for making these exposure and dose assessments. The multiple pathway exposure model requires either measured concentrations or the concentrations provided by the transport and transformation model (described in Part II) for chemicals in the environmental compartments of ambient air (gas and particle phases), surface water, ground water, surface soil, and root-zone soil at a site. From the chemical concentration in these environmental compartments, the model first provides estimates of the chemical concentration in each exposure medium (the medium with which a person has contact, such as, personal air, tap water, foods, household dusts, and soils). Then, the model determines the daily intake as the product of the concentrations in these exposure media, contact rate factors (such as, breathing rate, ingestion rate), and time factors (exposure duration and frequency, and averaging time). Finally, the model provides an estimate of the distribution of potential intake among people associated with that site. The variance in this distribution is attributable both to inter-individual variability among the members of the exposed population and to uncertainties that result from estimation errors in models and from the limits of precision in measurements.

A. INTRODUCTION

The objective of the CalTOX model is to quantitatively relate a soil concentration of a chemical of concern with a person's risk of experiencing an adverse health effect. This relationship permits computation of theoretical risk for a given soil concentration or computation of a human health-based soil target clean up level given an acceptable level of risk.

The CalTOX model is made up of two major models, within which several other models exist. Part I of this manual provides the overall description of the CalTOX model. Part II describes the first model, the dynamic multimedia transport and transformation model. This model determines how the chemical moves from the soil into other environmental compartments and provides the concentration of the chemical in the relevant compartments. In Part III, the theoretical basis of the multiple pathway exposure model is described. The exposure model is comprised of equations which describe the intake of the chemical of concern by ingestion, inhalation, and dermal contact with potentially contaminated water, air, soil, and food. Appendix A of Part III provides the terminology, definitions, and abbreviations used in the body of Part III. A supplement to the CalTOX model, "Parameter Values and Ranges for CalTOX", provides the default parameter values for the equations described in Parts II and III and the scientific rationale for those values. More importantly, "Parameter Values and Ranges for CalTOX" gives information on how estimates of parameter values are to be obtained.

Exposure has been previously defined by the U.S. Environmental Protection Agency (EPA) (1988) in terms of contact with "exchange boundaries" where contaminant absorption takes place (skin, lung, gastrointestinal tract). However, the more recent consensus of the scientific community (National Research Council, 1991a, 1991b; U.S. EPA 1992b) is that exposure should be defined in terms of contact with the visible exterior of the person. Under this definition, we view the human body as having a hypothetical outer boundary separating internal living tissues from the outside surfaces. This outer boundary is the skin and openings to the body (the mouth, the nose, and skin punctures and lesions). The multiple pathway exposure model described here is based on this latter definition.

The equations used in the CalTOX multiple pathway exposure model are modified from or extensions of equations described by the U.S. EPA in Chapter 6 of Risk Assessment Guidance for

Superfund, Volume 1. Human Health Evaluation Manual, Part A (RAGS/HHEM, U.S. EPA 1989b).

B. THE BASIC EXPOSURE MODEL

The equations for estimating exposures to chemicals in the environment are described and discussed below.

1. THE EXPOSURE EQUATION AS DESCRIBED IN THE RISK ASSESSMENT GUIDANCE FOR SUPERFUND/HUMAN HEALTH EVALUATION MANUAL

In RAGS/HHEM (U.S. EPA 1989b, pg. 6-21), the following generic equation is shown:

$$I = C \; x \; \frac{CR \; x \; EFD}{BW} \; x \; \frac{1}{AT} \qquad [1]$$

Where:

I = intake of a chemical via an exposure route (inhalation, ingestion, dermal contact) in mg chemical per kg body weight per day, abbreviated as mg/kg/d

C = chemical concentration in the exposure medium (such as, personal air, tap water, milk, food, soil); equal to $C_{exposure}$ in equations 3 and 4

CR = contact rate; the amount of contaminated medium contacted per unit time or event (such as, liters per day (L/day))

EFD = exposure frequency and duration; describes how long and how often exposure occurs. May be calculated using two terms as follows:

EF = exposure frequency (days/year)

ED = exposure duration (years)

BW = body weight; the average body weight over the exposure period (kg)

AT = averaging time; period over which exposure is averaged (days)

The pathway specific intake equations described in Chapter 6 of RAGS/HHEM (ingestion of drinking water, inhalation of contaminated air, etc.) are based on this generic intake equation.

2. THE CALTOX EXPOSURE MODEL

The RAGS/HHEM equation is rearranged slightly to derive an alternative generic exposure equation which is used in the CalTOX exposure model:

$$I = C \ x \left[\frac{CR}{BW}\right] x \ FI \ x \ EFD \ x \ \frac{1}{AT} \quad [2]$$

where:

FI = fractional intake from the contaminated source

The other variables have the same meaning as in equation 1.

Equation 2 differs from equation 1 in three ways. First, fractional intake (FI) is considered only in the soil and food ingestion pathways in RAGS/HHEM (U.S. EPA 1989b), whereas, fractional intake is considered in all the CalTOX exposure equations. Fractional intake corrects the intake for the fraction of the contact medium that is contaminated. For example, if only fifty percent of the daily fluid intake is likely to come from contaminated tap water, a FI of 0.5 would be used to adjust for that circumstance. Second, RAGS/HHEM assumes that all parameters in the equation are independent from one another, whereas, the CalTOX exposure model assumes a correlation of contact rate with body weight and requires a ratio of contact rate to body weight (CR/BW) be used. For example, heavyweight people consume more food than lightweight people. CR/BW ratios have been calculated for various contact rates and age groups (see "Parameter Values and Ranges for CalTOX", Table II). The third and most important difference between equations 1 and 2 is the way the chemical concentration in the exposure medium (C) is considered in RAGS/HHEM (U.S. EPA 1989b) and by the CalTOX exposure model. RAGS/HHEM (U.S. EPA 1989b) in Section 6.5 provides narrative general guidance for the estimation of concentrations in exposure media (called "exposure concentrations" in RAGS/HHEM), whereas, the CalTOX exposure model describes an explicit method for computing the concentrations in inhaled air, ingested water, foods and soil, and the water and soil that come into contact with the skin. These media are defined as exposure media, because they are the media with which people have contact. Exposure media are distinct from environmental compartment media. Environmental compartment media are outdoor ambient air above the site, surface soil on the site, and root-zone soil, surface water, and ground water below the site.

The advantage of estimating the concentration of chemical in an exposure medium and using that concentration instead of the concentration of that chemical in an environmental medium is that the exposure medium concentration provides the more reasonable, realistic basis for exposure. In the CalTOX exposure model, if the concentration of chemical in an exposure medium is not measured, it is calculated from the chemical concentration in the environmental compartment. This explicit approach is consistent with RAGS/HHEM (U.S. EPA 1989b). For example, RAGS/HHEM, Section 6.5.7, discusses methods for estimating the amount of chemical in fish tissue, the exposure medium, from the concentration of that chemical in the environmental media of sediment and water, and estimating the amount of chemical in plants from air and soil using modeling approaches or various partition coefficients. In the CalTOX exposure model, first, the dynamic multimedia transport and transformation model (described in Part II) provides the concentration of the chemical of concern in the environmental compartments: air, surface soil, root-zone soil, surface water, and ground water. (In the transport and transformation model, the vadose zone leachate is the surrogate for ground water.) Second, an inter-media transfer factor (TF), defined as the ratio of the chemical concentration in the exposure medium to the chemical concentration in the environmental compartment, is used to estimate the chemical concentration in the exposure or contact medium relative to the chemical concentration in the environmental compartment or medium. The equations are expressed as follows:

$$TF = \frac{C_{exposure}}{C_{environm}}$$

[3]

where:

TF = the inter-media transfer factor from an environmental compartment to an exposure medium

$C_{exposure}$ = chemical concentration in the exposure medium; equal to C in equations 1 and 2

$C_{environm}$ = chemical concentration in the environmental compartment,

and, therefore:

$$C_{exposure} = TF \ x \ C_{environm} \qquad [4]$$

As equation 4 shows, the concentration of the chemical in the exposure medium is easily computed when the concentration of the chemical in the environmental compartment and the inter-media TF are known. The concentration of the chemical in several environmental compartments might contribute to the chemical concentration in a single exposure medium. For example, a chemcial in the air, irrigation water, and soil may contaminate homegrown vegetables. In this circumstance, the products of the appropriate inter-media TFs and concentrations of the chemical in those environmental compartments are summed to compute the concentration of the chemical in the vegetables (the exposure medium).

The inter-media TF is usually represented by an appropriate chemical-specific partition coefficient (a K value, see Table V, "Parameter Values and Ranges for CalTOX" for examples) which describes the relative physiochemical attraction of the chemical for the environmental and exposure media or is calculated from compartment models described in the following sections.

3. EXPOSURE PATHWAY OVERVIEW

In the CalTOX exposure model the concentrations of the chemical in multiple exposure media contaminated by the chemical in multiple environmental media are used to compute the intake of that chemical by the ingestion, inhalation, and dermal routes. The matrix of exposure pathways linking environmental media, exposure scenarios, and exposure routes is shown in Table I, page 17 of Part I. The CalTOX model is designed to consider the following exposure pathways linking environmental compartment concentrations to ultimate intake by different routes:

Ingestion Intake:

1) ingestion of <u>ground water</u> or <u>surface water</u> as drinking water

2) ingestion of produce contaminated by chemicals transferred from air (either as vapor or particles)

3) ingestion of produce contaminated by chemicals transferred from surface or root-zone soil

4) ingestion of produce contaminated by chemicals transferred from irrigation water

5) ingestion of meat, dairy products, and eggs contaminated by inhalation of chemicals in air (either as vapor or particles) by meat, dairy, and egg-producing animals or by ingestion by these animals of feed contaminated by chemicals transferred from air

6) ingestion of meat, dairy products, and eggs contaminated by chemicals in surface or root-zone soil by direct ingestion of soil by these animals and by ingestion of feed contaminated by chemicals transferred from soil

7) ingestion of meat, dairy products, and eggs contaminated by ingestion of chemicals in ground or surface water by meat, dairy and egg-producing animals

8) ingestion of fish and seafood contaminated by chemicals in surface water

9) ingestion of surface water during swimming and other water recreation

10) incidental ingestion of surface soil

Inhalation Intake:

1) inhalation of gases and particles in outdoor and indoor air

2) inhalation of surface soil resuspended in air as dust

3) inhalation of vapors from root-zone soil

4) inhalation of chemicals volatilizing from ground water or from surface water used for bathing, showering, washing dishes, etc.

Dermal Uptake:

1) dermal contact with surface soil

2) dermal contact with ground or surface water while bathing, showering or swimming

The CalTOX model provides for the exclusion of exposure pathways that are not relevant to the site (see Section C. Multiple Pathway Exposures and Total Intake, 5. Excluding an Exposure Pathway from Quantitative Analysis).

4. CONDITIONS OF THE CALTOX EXPOSURE MODEL

The exposure assessment provided by the CalTOX multimedia multiple pathway exposure model has several important conditions. First, as discussed in Part II, the CalTOX model looks at fate and transport processes months and years rather than days and weeks after contamination has occurred and thus assumes that the original spill or contamination of soil has taken place more than one year before the chemical concentration in soil was measured. This assumption is consistent with the historical record of contamination at most hazardous waste sites. Second, the current version of the CalTOX model assumes the potentially exposed individual to be on site, because no dispersion models are now used within the overall CalTOX model. Finally, since this model is based on the RAGS/HHEM intake equations and risk characterization (U.S.EPA 1989b), CalTOX is subject to all the same limitations described for those equations.

In contrast to RAGS/HHEM (U.S. EPA 1989b), default exposure parameter values are not listed with the intake equations for each pathway in this manual. Instead, default exposure parameter values are given in a supplemental report, Parameter Values and Ranges for CalTOX. In this way, the theoretical basis for estimating the potential exposures discussed in this manual is separated from the issue of the appropriateness of specific default values. Exposure parameter values recommended by RAGS/HHEM (U.S. EPA 1989b, Section 6) may be specified in the CalTOX exposure model equations in order to determine exposure intake values. Alternatively, mean exposure parameter values with their associated coefficients of variation may be used to calculate typical uptake values and to perform statistical analysis of uncertainty. The supplemental report, "Parameter Values and Ranges for CalTOX", provides an in-depth discussion of how parameter values are to be obtained and how they may be used in the CalTOX model.

C. MULTIPLE PATHWAY EXPOSURES AND TOTAL INTAKE

In this section, the equations for estimating intakes using the CalTOX exposure model are given. Concentrations of chemicals in each environmental compartment ($C_{environm}$) listed below are used in conjunction with inter-media transfer factors to compute the concentration of chemicals in each exposure medium:

(1) C_a in mg/m^3 - the chemical concentration in ambient air gases;

(2) C_{ap} in mg/m^3 - the concentration of chemical bound to all air particles (dust);

(3) C_g in mg/kg - chemical concentration in ground-surface soil (to a depth of 1 cm or 0.4 inches);

(4) C_s in mg/kg - chemical concentration in root-zone soil below the surface layer (1 cm to approximately 1 m in depth or 0.4 inches to 39 inches);

(5) C_q in mg/L - chemical concentration in ground water;

(6) C_w in mg/L - chemical concentration in surface water.

1. THE INGESTION ROUTE

In the multiple-pathway approach of the CalTOX exposure model, contaminated air, water, and soil may contribute to ingestion exposure. Total ingestion intake includes potential doses from the ingestion of contaminated exposure media, such as tap water; soil; local or homegrown fruits, vegetables, grains, milk, meat, and eggs; locally caught fish; and surface water while swimming. For each exposure pathway an inter-media transfer factor, TF, is derived to express the ratio of chemical concentration in the exposure medium to chemical concentration in an environmental compartment. The TF is then used to calculate the chemical concentration ($C_{exposure}$) in the exposure medium for input to the intake equation. For the contact rate of the exposure medium per unit body weight, (CR/BW), we use the daily average ingestion rates per unit body weight as listed in Table II in the supplemental report, Parameter Values and Ranges for

CalTOX. The exposure frequency for ingestion exposures is dependent on the scenario being considered for the site. For example, in a residential scenario the exposure frequency could be assumed to be 350 days per year. The values for exposure duration and averaging time depend upon whether the calculated intake value will be used to determine carcinogenic risk or systemic health hazard of the chemical of concern.

a. Ingestion of Tap Water

As modified in the CalTOX model, the RAGS/HHEM equation (U.S. EPA 1989b, pg 6-35) for ingestion of a chemical in drinking water is:

$$Intake_{dwi} = C_{drink} \; x \left[\frac{IR_{drink}}{BW} \right] x \; FI \; x \; \frac{EF x ED}{AT} \qquad [5]$$

The RAGS/HHEM equation is modified by the inclusion of FI, the fraction ingested from the contaminated source, and the rearrangment of terms.

Where:

$Intake_{dwi}$ = Intake of chemical by the exposed individual via ingestion of contaminated drinking water (mg chemical/kg body weight per day)

C_{drink} = chemical concentration in drinking water (mg/L),

IR_{drink} = ingestion rate of fluids (L/day),

BW = body weight (kg),

FI = fraction of drinking water ingested from contaminated source, assumed to be 1 (unitless),

EF = exposure frequency (days/year),

ED = exposure duration (year),

AT = averaging time (days).

Since the CalTOX model assumes a correlation of contact rate with body weight, the value representing the ratio of IR_{drink} to BW (IR_{drink}/BW) is depicted in Table II, "Parameter

Values and Ranges for CalTOX".

C_{drink} can be a mixture of C_w, the chemical concentration in the environmental compartment of surface water, and C_q, the chemical concentration in the environmental compartment of ground water. With the CalTOX exposure model, when there is a mix of ground and surface water being used, the inter-media transfer factors for surface water to drinking water and for ground water to drinking water may be considered mathematically as follows:

$TF(w \rightarrow drink) = (1 - f^w_q)$

$TF(q \rightarrow drink) = f^w_q$

where:

f^w_q = fraction of water needs provided by ground water (Table III, "Parameter Values and Ranges for CalTOX")

The following equation is then used to calculate C_{drink}:

$$C_{drink} = f^w_q \, x \, C_q + (1 - f^w_q) \, x \, C_w \qquad [6]$$

where:

C_{drink} = chemical concentration in drinking water

f^w_q = fraction of water needs provided by ground water (Table III, "Parameter Values and Ranges for CalTOX")

C_q = chemical concentration in ground water

C_w = chemical concentration in surface water

CW_{drink} is then input into the drinking water intake equation (equation 5).

b. Ingestion of Soil

The RAGS/HHEM equation (U.S. EPA 1989b, pg. 6-40) for the incidental ingestion of soil contaminated with a chemical may be written as follows:

$$Intake_{soil} = C_g x \left[\frac{IR_{soil}}{BW} \right] xFIx \frac{EFxED}{AT} xCF$$

[7]

where:

$Intake_{soil}$ = intake of chemical of concern by an exposed individual via ingestion of contaminated soil (mg chemical/kg body weight per day)

C_g = concentration in surface soil of chemical of concern (mg of chemical/kg soil)

IR_{soil} = ingestion rate (mg soil/day),

BW = body weight (kg),

FI = fraction of soil ingested from contaminated source, assumed to be 1 (unitless),

EF = exposure frequency (days/year),

ED = exposure duration (years),

AT = averaging time (days),

CF = conversion factor (10^{-6} kg/mg).

As for equation 5, since the CalTOX model assumes a correlation of contact rate with body weight, the value representing the ratio of IR_{soil} to BW (IR_{soil}/BW) is depicted in Table III, "Parameter Values and Ranges for CalTOX".

For this intake, it is not necessary to use an inter-media TF to estimate the concentration in the exposure medium, since, the environmental compartment of surface soil is the exposure medium. In the CalTOX exposure model, the concentration of a chemical in household soil is equal to the concentration of that chemical in the environmental compartment of surface soil, on the assumption that household dust results from soil blown or carried into the house from outside. Because the CalTOX model considers exposure as contact of the chemical with the outer boundary of a human, such as the mouth (in keeping with the definition given by the U.S. EPA (U.S. EPA 1992b)), the CalTOX model does not consider bioavailability of the chemical from the ingested soil matrix in the intake equation.

c. Ingestion of Contaminated Homegrown Fruits, Vegetables, or Grains

There are sites and facilities where the ingestion of contaminated homegrown foodstuffs is an exposure pathway that should be considered. The RAGS/HHEM equation (U.S. EPA 1989b, pg. 6-46) for calculating the ingestion of contaminated fruits and vegetables may be written as follows:

$$Intake_{fvg} = C_{fvg} x \left[\frac{IR_{fvg}}{BW} \right] xFIx \frac{EFxED}{AT}$$

[8]

where:

Intake$_{fvg}$ = Intake of chemical by an exposed individual via ingestion of contaminated fruit, vegetables, grain (mg chemical/kg body weight per day)

C$_{fvg}$ = concentration of chemical in the foods of vegetable, fruit, or grain (mg/kg produce),

IR$_{fvg}$ = ingestion rate (kg produce/day),

BW = body weight (kg),

FI = fraction ingested from contaminated source (unitless),

EF = exposure frequency (days/year),

ED = exposure duration (years), and

AT = averaging time (days).

In this equation, IR$_{fvg}$/BW is a generic term which is represented by IR$_{fv}$/BW (ingestion rate per body weight of fruits and vegetables) or IR$_{g}$/BW (ingestion rate per body weight of grains) in Table II, "Parameter Values and Ranges for CalTOX".

In section 6.5.7 of RAGS/HHEM (U.S. EPA 1989b), there is a general discussion of the approaches that may be considered in calculating the chemical concentrations in foods, but little specific guidance is provided. The CalTOX exposure pathway model fills this gap by explicitly calculating the contamination of the exposure media of fruits, vegetables, and grains by the chemical present in the environmental compartments of contaminated air (both the gas phase and particles), water, surface soil, and root-zone soil. Fruits and vegetables are divided into two groups: exposed produce representing above-ground edible plant parts and protected produce representing root crops and produce protected from the environmental compartment of ambient air, such as citrus fruits. Grains are considered exposed produce. In order to determine C_{fvg}, the concentration of the chemical in the exposure medium, TFs must first be calculated for the contamination of the two exposure media of exposed produce, C^{abg}_{fvg}, and protected produce, C^{protp}_{fv}, by each relevant environmental compartment. Using these TFs, chemical concentrations are calculated for each of the following secondary pathways:

1) from chemical vapors in ambient air to exposed produce to ingestion,
2) from chemical in the dust phase of ambient air to exposed produce to ingestion,
3) from surface water to exposed produce to ingestion,
4) from ground water to exposed produce to ingestion,
5) from surface water to protected produce to ingestion,
6) from ground water to protected produce to ingestion,
7) from surface soil to exposed produce to ingestion,
8) from root-zone soil to exposed produce to ingestion,
9) from root-zone soil to protected produce to ingestion.

These concentrations are then summed to get the C_{fvg} parameter in equation 8. The calculations are given below.

i. Contamination by Airborne Chemicals

The ingestion intake of fruits, vegetables, and grains contaminated by chemicals from the air involves the transfer of chemicals from air through deposition/resuspension of particle-bound chemicals or through foliar uptake of gas-phase chemicals. The concentration of a chemical on fruits, vegetables and grains from the transfer of that chemical in ambient outdoor air to edible plant parts is given by the equation:

$$C^{abga}_{fvg} = K^{gs}_{pa} \, x \, C_{a} + K^{pt}_{pa} \, x \, C_{ap}$$

[9]

where:

C^{abga}_{fvg} = concentration of the chemical on fruits, vegetables and grains exposed to the chemical in ambient air (mg chemical/kg plant fresh mass)

K^{gs}_{pa} = the TF(a $\rightarrow$ plant), the ratio of chemical concentration in fresh produce, mg/kg (fresh mass), to chemical concentration in the gas phase of the ambient outdoor air (mg/m^3) (Table V, "Parameter Values and Ranges for CalTOX")

C_a = the concentration of the chemical in the gas phase of ambient outdoor air (mg/m^3)

K^{pt}_{pa} = the TF(ap $\rightarrow$ plant), the ratio of chemical concentration in fresh produce, mg/kg (fresh mass), to chemical concentration in the particle (or dust) phase of the ambient outdoor air (mg/m^3) (Table V, "Parameter Values and Ranges for CalTOX")

C_{ap} = the concentration of the chemical in the dust phase of the ambient outdoor air (mg/m^3)

ii. Contamination by Irrigation Water

The ingestion intake of fruits, vegetables, and grains contaminated by chemicals from irrigation water involves the transfer of chemicals from: 1) surface water to exposed produce, 2) ground water to exposed produce, 3) surface water to protected produce, and 4) ground water to protected produce.

For exposed produce (above ground plant parts), inter-media TFs are based on rainsplash and on partition transfers from soil to above ground plant parts. The inter-media transfer factor for exposed produce to ground water (TF(q $\rightarrow$ expp)) is calculated as follows:

$$TF(q \rightarrow expp) = f_q^w \; x \left(K_{ps}^{rain} + K_{ps}\right) x \; K_D \; x \; f_{ir}$$

[10]

where:

$TF(q \rightarrow expp)$ = the ratio of chemical concentration of exposed produce to the chemical concentration in ground water;

f^w_q = the fraction of water irrigation needs provided by ground water (unitless) (Table III, "Parameter Values and Ranges for CalTOX")

K^{rain}_{ps} = plant-soil partition coefficient for surface soil due to rainsplash (kg soil / kg plant fresh mass) (Table V, "Parameter Values and Ranges for CalTOX"),

K_{ps} = plant-soil partition coefficient from root-zone soil to above-ground plant parts due to uptake through roots (kg soil / kg plant fresh mass) (Table V, "Parameter Values and Ranges for CalTOX")

K_D = soil/soil-water partition coefficient (kg water / kg soil solids) (Table V, "Parameter Values and Ranges for CalTOX")

f_{ir} = fraction of the chemical concentration in irrigation water retained in soil water (unitless) (Table IV, "Parameter Values and Ranges for CalTOX")

The inter-media TF for exposed produce to surface water ($TF(w \rightarrow expp)$) is calculated as follows:

$$TF(w \rightarrow expp) = \left(1 - f_q^w\right) x \left(K_{ps}^{rain} + K_{ps}\right) x \; K_D \; x \; f_{ir}$$

[11]

where:

$TF(w \rightarrow expp)$ = the ratio of chemical concentration of exposed produce to the chemical concentration in surface water;

$1-f^w_q$ = the fraction of water irrigation needs provided by surface water (unitless) (Table III, "Parameter Values and Ranges for CalTOX")

Then, the equation for the concentration of a chemical in exposed fruits, vegetables, and grains from the transfer of the chemical in surface and ground water is:

$$C_{fvg}^{abgw} = TF(w \rightarrow expp)\ x\ C_w + TF(q \rightarrow expp)\ x\ C_q$$

[12]

where:

C^{abgw}_{fvg} = concentration of the chemical in above ground fruits, vegetables, and grains exposed to the chemical in irrigation water (mg chemical/kg plant fresh mass)

C_w = chemical concentration in surface water (mg/L)

C_q = chemical concentration in ground water (mg/L)

TF(w $\rightarrow$ expp) = see equation 11

TF(q $\rightarrow$ expp) = see equation 10

The inter-media transfer factor for protected produce and root crops to ground water (TF(q $\rightarrow$ protp)) is calculated as follows:

$$TF(q \rightarrow protp) = f_q^w\ x\ K_{ps}(roots)\ x\ K_D\ x\ f_{ir}$$

[13]

where:

TF(q $\rightarrow$ protp) = the ratio of chemical concentration of protected or root crops to the chemical concentration in ground water.

f^w_q = fraction of water needs provided by ground water (unitless) (Table III, "Parameter Values and Ranges for CalTOX")

K_{ps}(roots) = the plant-soil partition coefficient from root-zone soil to roots (kg soil / kg plant fresh mass) (Table V, "Parameter Values and Ranges for CalTOX")

K_D = soil/soil-water partition coefficient (kg water / kg soil solids) (Table V, "Parameter Values and Ranges for CalTOX")

f_{ir} = fraction of the chemical concentration in irrigation water retained in soil water (unitless) (Table IV, "Parameter Values and Ranges for CalTOX")

The inter-media transfer factor for surface water to protected produce and root crops (TF(w $\rightarrow$ protp)) is calculated as follows:

$$TF(w \rightarrow protp) = \left(1 - f_q^w\right) x\ K_{ps}(roots)\ x\ K_D\ x\ f_{ir} \tag{14}$$

where:

TF(w $\rightarrow$ protp) = the ratio of chemical concentration of protected produce or root crops to the chemical concentration in surface water

$1-f^w_q$ = fraction of water needs provided by surface water (unitless)

iii. Contamination by Surface Soil

The ingestion of chemicals in fruits, vegetables, and grains contaminated by surface soil involves the transfer of chemicals from soil to plants. The inter-media transfer factor, TF(g $\rightarrow$ expp), is the ratio of the chemical concentration in exposed produce (in mg/kg fresh mass) to chemical concentration in surface soil (in mg/kg soil). TF(g $\rightarrow$ expp) is equal to the rainsplash partition coefficient, K^{rain}_{ps} (see Table V). The grains contaminated from that chemical in surface soil is given by multiplying K^{rain}_{ps} times the concentration of the chemical in surface soil (C_s).

iv. Contamination by Root-Zone Soil

The ingestion intake of chemicals in fruits, vegetables, and grains contaminated by root-zone soil. Root-zone soil is defined in the CalTOX model as soil below the surface layer, from 1 cm to approximately 1 m in depth (or 0.4 to 39 inches). Contamination by root-zone soil involves the transfer of chemicals from that soil layer to both exposed and protected produce.

For exposed produce, the inter-media TF(s $\rightarrow$ expp) is equal to K_{ps} (Table V, "Parameter Values and Ranges for CalTOX"). Thus, the concentration of chemical on exposed produce from contaminated root-zone soil is given by multiplying K_{ps} by the concentration of the chemical in root-zone soil (C_s).

For protected produce, the inter-media TF(s $\rightarrow$ protp) is equal to K_{ps}(roots) (Table V, "Parameter Values and Ranges for CalTOX") and the concentration of chemical in protected produce from contaminated root-zone soil is given by multiplying K_{ps}(roots) by the concentration of the chemical in root-zone soil (C_s).

v. Calculating the Concentration of Chemical in Exposed and Protected Produce

The equation for the concentration of chemical in exposed produce resulting from contamination by air, irrigation water, and soil may now be depicted as follows:

$$C_{fvg}^{abg} = K_{pa}^{gs} \; x \; C_a + K_{pa}^{pt} \; x \; C_{ap} + TF(w \rightarrow expp) \; x \; C_w + TF(q \rightarrow expp) \; x \; C_q + K_{ps}^{rain} \; x \; C_g + K_{ps} \; x \; C_s \quad [15]$$

where:

C^{abg}_{fvg} = concentration of the chemical on fruits, vegetables and grains exposed to the chemical in ambient air, irrigation water, and soil (mg chemical/kg plant fresh mass)

K^{gs}_{pa} = the TF(a $\rightarrow$ plant), the ratio of chemical concentration in fresh produce, mg/kg (fresh mass), to chemical concentration in the gas phase of the ambient outdoor air (mg/m^3) (see Table V, "Parameter Values and Ranges for CalTOX" and equation 9)

C_a = the concentration of the chemical in the gas phase of ambient outdoor air (mg/m^3)

K^{pt}_{pa} = the TF(ap $\rightarrow$ plant), the ratio of chemical concentration in fresh produce, mg/kg (fresh mass), to chemical concentration in the particle (or dust) phase of the ambient outdoor air (mg/m^3) (see Table V, "Parameter Values and Ranges for CalTOX" and equation 9)

C_{ap} = the concentration of the chemical in the dust phase of the ambient outdoor air (mg/m^3)

$TF(w \rightarrow expp)$ = the ratio of chemical concentration of exposed produce to the chemical concentration in surface water (equation 11)

C_w = chemical concentration in surface water (mg/L)

$TF(q \rightarrow expp)$ = the ratio of chemical concentration of exposed produce to the chemical concentration in ground water (equation 10)

C_q = chemical concentration in ground water (mg/L)

K^{rain}_{ps} = $TF(g \rightarrow expp)$, the ratio of chemical concentration in exposed produce to chemical concentration in surface soil (Table V, "Parameter Values and Ranges for CalTOX")

C_g = concentration of the chemical in surface soil (mg chemical/kg soil)

K_{ps} = $TF(s \rightarrow expp)$, the ratio of chemical concentration in exposed produce to chemical concentration in root-zone soil (Table V, "Parameter Values and Ranges for CalTOX")

C_s = chemical concentration in root-zone soil (mg chemical/kg soil)

The comparable equation for the concentration of chemical in protected produce (equation 16) has terms for ground water, surface water, and root-zone soil. Unlike the equation for the concentration of chemical in exposed produce (equation 15), there are no terms for air or surface soil.

$$C_{fv}^{protp} = TF(q \rightarrow protp) \; x \; C_q + TF(w \rightarrow protp) \; x \; C_w + K_{ps}(roots) \; x \; C_s \qquad [16]$$

where:

C^{protp}_{fv} = chemical concentration of protected produce contaminated by water and root-zone soil (mg chemical/ kg plant fresh mass)

$TF(q \rightarrow protp)$ = the ratio of chemical concentration of protected or root crops to the chemical concentration in ground water (equation 13)

C_q = chemical concentration in ground water (mg/L)

$TF(w \rightarrow protp)$ = the ratio of chemical concentration of protected produce or root crops to the chemical concentration in surface water (equation 14)

C_w = chemical concentration in surface water (mg/L)

K_{ps}(roots) = TF (s $\rightarrow$ protp), the ratio of chemical concentration of protected produce or root crops to the chemical concentration in root-zone soil (Table V, "Parameter Values and Ranges for CalTOX")

C_s = chemical concentration in root-zone soil (mg chemical/kg soil)

vi. Calculating the Intake of Chemical by Ingestion of Contaminated Fruits, Vegetables, Grains

The intake of exposed produce is calculated by using specific parameters in equation 8:

$$I_{fvg}^{abg} = C_{fvg}^{abg} \; x \left[\left(\frac{IR_{fv}}{BW} \; x \; f_{fv}^{abg} \; x \; f_{local}^{v} \right) + \left(\frac{IR_{g}}{BW} \; x \; f_{local}^{g} \right) \right] x \; \frac{EF \; x \; ED}{AT}$$

[17]

where:

I^{abg}_{fvg} = the intake of a chemical from above ground or exposed fruits, vegetables and grains contaminated by the presence of that chemical in the environmental media of air, water and soil (mg chemical/kg body weight/day)

IR_{fv} = ingestion rate of fruits and vegetables (kg food/day)

IR_g = ingestion rate of grains (kg grains/day)

The values for the ratios, IR_{fv}/BW and IR_g/BW, are given in Table II, "Parameter Values and Ranges for CalTOX".

For this intake, the FI, or fraction ingested from the contaminated source, is designated as:

f^{abg}_{fv} = fraction of fruits and vegetables consumed that are exposed produce (unitless) (Table III, "Parameter Values and Ranges for CalTOX")

f^{v}_{local} = fraction of fruits and vegetables consumed that are locally grown (unitless) (Table III, "Parameter Values and Ranges for CalTOX"), and

f^{g}_{local} = fraction of grains consumed that are locally grown (unitless) (Table III, "Parameter Values and Ranges for CalTOX").

The intake of a chemical from protected produce is similarly calculated, using equation 8:

$$I_{fv}^{protp} = C_{fv}^{protp}\ x \left(\frac{IR_{fv}}{BW}\ x\ f_{local}^{v}\ x\,(\,1 - f_{fv}^{abg}\ ) \right) x \frac{EF\ x\ ED}{AT}$$

[18]

where:

I^{protp}_{fv} = the intake of a chemical from the ingestion of protected produce contaminated with that chemical through water or root-zone soil (mg chemical/kg body weight/day)

For this intake, the FI, or fraction ingested from the contaminated source, is designated as:

f^{v}_{local} = fraction of fruits and vegetables locally grown (unitless) (Table III, "Parameter Values and Ranges for CalTOX")

$1-f^{abg}_{fv}$ = fraction of fruits and vegetables consumed that are protected produce (unitless) (Table III, "Parameter Values and Ranges for CalTOX")

By summing these two calculated intakes (equations 17 and 18), the ingestion intake for all contaminated fruits, vegetables, and grains is obtained ($Intake_{fvg}$):

$$Intake_{fvg} = I_{fvg}^{abg} + I_{fv}^{protp}$$

[19]

d. Ingestion of Contaminated Fish

The equation for ingestion of fish and shellfish contaminated with a chemical of concern is given in RAGS/HHEM (U.S. EPA 1989b) on page 6-45, and may be written as:

$$Intake_{fish} = C_{fish}\ x \left[\frac{IR_{fish}}{BW} \right] x\ FI\ x \frac{EF\ x\ ED}{AT}$$

[20]

where:

$Intake_{fish}$ = Intake of chemical of concern by an exposed individual via ingestion of contaminated fish or shellfish (mg chemical/kg body weight per day)

C_{fish} = concentration of chemical of concern in fish or shellfish (mg/kg fish)

IR_{fish} = ingestion rate (kg fish/day)

BW = body weight (kg),

FI = fraction ingested from contaminated source (unitless) (Table III, "Parameter Values and Ranges for CalTOX"),

EF = exposure frequency (days/year),

ED = exposure duration (years), and

AT = averaging time (days).

The value for the ratio, IR_{fish}/BW, is given in Table II, "Parameter Values and Ranges for CalTOX". In calculating the ingestion intake of locally caught fish, the CalTOX exposure model assumes that the contamination of fish by a chemical of concern is due to the transfer of that chemical from the environmental compartment of surface water to the fish. The inter-media TF between fish and surface water is the bioconcentration factor (BCF, see Table V, "Parameter Values and Ranges for CalTOX"), defined as the organism/water partition coefficient by RAGS/HHEM (U.S. EPA 1989b, Section 6.5.7). In the CalTOX exposure model, the BCF is multiplied by the concentration of the chemical in surface water (C_w) to get the tissue concentration in the fish (C_{fish}, the contact medium, see equation 4). This method is the same as that described in RAGS/HHEM (U.S. EPA 1989b, Section 6.5.7) for circumstances where no fish tissue measurements have been made. The fraction ingested from the contaminated source, FI, is given by f^{fsh}_{local}, the fraction of an individual's intake of fish that comes from local surface water contaminated with the chemical in question (Table III, "Parameter Values and Ranges for CalTOX").

e. Ingestion of Contaminated Meat, Milk, and Eggs

The RAGS/HHEM equation for the ingestion of contaminated meat, milk, and eggs (U.S. EPA 1989b, pg. 6-48) may be written as follows:

$$Intake_{mke} = C_{mke} \ x \left[\frac{IR_{mke}}{BW}\right] x \ FI \ x \ \frac{EFxED}{AT}$$

[21]

where:

$Intake_{mke}$ = Intake of chemical of concern by an exposed individual via ingestion of contaminated meat, milk and eggs (mg chemical/kg BW per day)

C_{mke} = concentration of chemical of concern in meat, milk products, or eggs (mg/kg food),

IR_{mke} = ingestion rate (kg meat, milk, eggs/day),

BW = body weight (kg),

FI = fraction ingested from contaminated source,

EF = exposure frequency (days/year),

ED = exposure duration (years), and

AT = averaging time (days).

Section 6.5.7 of RAGS/HHEM (U.S. EPA 1989b) recommends the use of transfer coefficients and provides references in the literature to estimate the extent of human exposure to chemicals in the terrestrial food chain when there are no tissue monitoring data. A default method is given in the CalTOX exposure model which incorporates transfer coefficients for calculating the concentration of the chemical in meat, milk and dairy products, and eggs (C_{mke}) from the concentration of the chemical in the environmental compartments of contaminated air (gas phase and particles), water (ground and surface), and soil (surface and root-zone). First, the TFs are derived for the contamination of the exposure media by each relevant environmental compartment. Then, chemical concentrations for the exposure media are calculated from each of the following secondary pathways using these TFs:

1) inhalation of chemical vapors in air and ingestion of feed contaminated with such vapors by meat and dairy-producing animals, and egg-laying poultry with subsequent contamination of meat, dairy products and eggs,
2) inhalation of the chemical in the dust phase of air and ingestion of feed contaminated with such particles by meat and dairy-producing animals, and egg-laying poultry with subsequent contamination of meat, dairy products and eggs,
3) ingestion of the chemical in ground water and in feed contaminated by irrigation

water containing the chemical by meat and dairy-producing animals, and egg-laying poultry with subsequent contamination of these foods,

4) ingestion of the chemical in surface water and in feed contaminated by irrigation water containing the chemical by meat and dairy-producing animals, and egg-laying poultry with subsequent contamination of these foods,

5) ingestion of the chemical in surface soil and feed contaminated from surface soil by meat and dairy-producing animals, and egg-laying poultry with subsequent contamination of these foods,

6) ingestion of the chemical in root-zone soil and feed contaminated with the chemical from root-zone soil by meat and dairy-producing animals, and egg-laying poultry with subsequent contamination of these foods.

These concentrations are then summed to get the C_{mke} parameter in equation 21. The calculations are given below.

i. Inter-Media Transfer Factors - Ambient Air to Animal Products

The ingestion intake of meat, milk products, and eggs contaminated by chemicals from the air involves the transfer of chemicals via inhalation by meat and dairy-producing animals and egg-laying poultry and via ingestion of feed that have taken up those chemicals from air. The inter-media TFs for the gas phase of ambient air are calculated as follows:

for meat:

$$TF(a \rightarrow meat) = [\, Inh_c + K_{pa}^{gs} \, x \, I_{vbc} \,] \, x \, B_t \qquad [22]$$

for milk products:

$$TF(a \rightarrow milk) = [\, Inh_c + K_{pa}^{gs} \, x \, I_{vdc} \,] \, x \, B_k \qquad [23]$$

for eggs:

$$TF(a \rightarrow eggs) = [\, Inh_h + K^{gs}_{pa} \times I_{vh} \,] \times B_e \qquad [24]$$

where:

TF(a → meat) = the ratio of chemical concentration in meat to chemical concentration in the gas phase of the ambient outdoor air

Inh_c = the daily inhalation rate of cattle (m^3/day) (Table IV, "Parameter Values and Ranges for CalTOX")

K^{gs}_{pa} = the TF(a → plant), the ratio of chemical concentration in fresh produce, mg/kg (fresh mass), to chemical concentration in the gas phase of the ambient outdoor air (mg/m^3) (Table V, "Parameter Values and Ranges for CalTOX")

I_{vbc} = the daily intake of feed (pasture) by beef cattle (kg fresh mass/day) (Table IV, "Parameter Values and Ranges for CalTOX")

B_t = biotransfer factor, the ratio of chemical concentration in meat to the intake of that chemical by beef cattle (day/kg meat) (Table V, "Parameter Values and Ranges for CalTOX")

TF(a → milk) = the ratio of the chemical concentration in milk to the chemical concentration in the gas phase of ambient outdoor air

I_{vdc} = the daily intake of feed (pasture) by dairy cattle (kg fresh mass/day) (Table IV, "Parameter Values and Ranges for CalTOX")

B_k = biotransfer factor, the ratio of chemical concentration in milk to the intake of that chemical by dairy cattle (day/kg milk) (Table V, "Parameter Values and Ranges for CalTOX")

TF(a → eggs) = the ratio of the chemical concentration in eggs to the chemical concentration in the gas phase of ambient outdoor air

Inh_h = the daily inhalation rate of egg-laying hens (m^3/day) (Table IV, "Parameter Values and Ranges for CalTOX")

I_{vh} = the daily intake of feed by egg-laying hens (kg fresh mass/day)

(Table IV, "Parameter Values and Ranges for CalTOX")

B_e = biotransfer factor, the ratio of the chemical concentration in eggs to the intake of that chemical by egg-laying hens (day/kg eggs) (Table V, "Parameter Values and Ranges for CalTOX")

The inter-media TFs for the dust or particulate phase of ambient air are calculated as follows:

for meat:

$$TF(ap \rightarrow meat) = [\,Inh_c + K^{pt}_{pa} \; x \; I_{vbc}\,] \; x \; B_t$$

[25]

for milk:

$$TF(ap \rightarrow milk) = [\,Inh_c + K^{pt}_{pa} \; x \; I_{vdc}\,] \; x \; B_k$$

[26]

for eggs:

$$TF(ap \rightarrow eggs) = [\,Inh_h + K^{pa}_{pt} \; x \; I_{vh}\,] \; x \; B_e$$

[27]

where:

$TF(ap \rightarrow meat)$ = the ratio of chemical concentration in meat to chemical concentration in the particulate phase of the ambient outdoor air

Inh_c = the daily inhalation rate of cattle (m^3/day) (Table IV, "Parameter Values and Ranges for CalTOX")

K^{pt}_{pa} = the TF($ap \rightarrow plant$), the ratio of chemical concentration in fresh pasture, mg/kg fresh mass, to chemical concentration in the particulate phase of the ambient outdoor air (mg/m^3) (Table V, "Parameter Values and Ranges for CalTOX")

I_{vbc} = the daily intake of feed (pasture) by beef cattle (kg fresh mass/day) (Table IV, "Parameter Values and Ranges for CalTOX")

B_t = biotransfer factor, the ratio of chemical concentration in meat to the intake of that chemical by beef cattle (day/kg meat) (Table V, "Parameter Values and Ranges for CalTOX")

$TF(ap \rightarrow milk)$ = the ratio of the chemical concentration in milk to the chemical concentration in the particulate phase of ambient outdoor air

I_{vdc} = the daily intake of feed (pasture) by dairy cattle (kg fresh mass/day) (Table IV, "Parameter Values and Ranges for CalTOX")

B_k = biotransfer factor, the ratio of chemical concentration in milk to the intake of that chemical by dairy cattle (day/kg milk) (Table V,"Parameter Values and Ranges for CalTOX")

$TF(ap \rightarrow eggs)$ = the ratio of the chemical concentration in eggs to the chemical concentration in the particulate phase of ambient outdoor air

Inh_h = the daily inhalation rate of egg-laying hens (m^3/day) (Table IV, "Parameter Values and Ranges for CalTOX")

I_{vh} = the daily intake of feed by egg-laying hens (kg fresh mass/day) (Table IV, "Parameter Values and Ranges for CalTOX")

B_e = biotransfer factor, the ratio of the chemical concentration in eggs to the intake of that chemical by egg-laying hens (day/kg eggs) (Table V, "Parameter Values and Ranges for CalTOX")

ii. Inter-Media Transfer Factors - Water to Animal Products

The ingestion intake of meat, milk products, and eggs contaminated by chemicals from surface and ground water involves the transfer of chemicals from water by ingestion of water by meat and dairy-producing animals and egg-laying poultry and by ingestion of feed that have taken up those chemicals from water. The inter-media TFs for surface water to animal products are calculated as follows:

for meat:

$$TF(w \rightarrow meat) = \left[(1 - f_q^w)\ x\ I_{wbc} + (I_{vbc}\ x\ TF(w \rightarrow \exp)\right] x\ B_t$$

[28]

for milk:

$$TF(w \rightarrow milk) = \left[(1 - f_q^w) \; x \; I_{wdc} + (I_{vdc} \; x \; TF(w \rightarrow expp)\right] x \; B_k$$

[29]

for eggs:

$$TF(w \rightarrow eggs) = \left[(1 - f_q^w) \; x \; I_{wh} + (I_{vh} \; x \; TF(w \rightarrow expp)\right] x \; B_e$$

[30]

where:

$TF(w \rightarrow meat)$ = the ratio of chemical concentration in meat to chemical concentration in surface water

$1 - f^w_q$ = the fraction of water needs provided by surface water (unitless) (Table III, "Parameter Values and Ranges for CalTOX")

I_{wbc} = ingestion of water by beef cattle (L/day) (Table IV, "Parameter Values and Ranges for CalTOX")

I_{vbc} = the daily intake of feed (pasture) by beef cattle (kg fresh mass/day) (Table IV, "Parameter Values and Ranges for CalTOX")

$TF(w \rightarrow expp)$ = the ratio of chemical concentration of exposed produce to the chemical concentration in surface water (equation 11)

B_t = biotransfer factor, the ratio of chemical concentration in meat to the intake of that chemical by beef cattle (day/kg meat) (Table V, "Parameter Values and Ranges for CalTOX")

$TF(w \rightarrow milk)$ = the ratio of chemical concentration in milk to the chemical concentration in surface water

I_{wdc} = ingestion of water by dairy cattle (L/day) (Table IV, "Parameter Values and Ranges for CalTOX")

I_{vdc} = the daily intake of feed (pasture) by dairy cattle (kg fresh mass/day)

(Table IV, "Parameter Values and Ranges for CalTOX")

B_k = biotransfer factor, the ratio of chemical concentration in milk to the intake of that chemical by dairy cattle (day/kg milk) (Table V, "Parameter Values and Ranges for CalTOX")

TF(w $\rightarrow$ eggs) = the ratio of chemical concentration in eggs to the chemical concentration in surface water

I_{wh} = ingestion of water by hens (L/day) (Table IV, "Parameter Values and Ranges for CalTOX")

I_{vh} = the daily intake of feed by egg-laying hens (kg fresh mass/day) (Table IV, "Parameter Values and Ranges for CalTOX")

B_e = biotransfer factor, the ratio of the chemical concentration in eggs to the intake of that chemical by egg-laying hens (day/kg eggs) (Table V, "Parameter Values and Ranges for CalTOX")

The inter-media TFs for ground water to animal products are calculated as follows:

for meat:

$$TF(q \rightarrow meat) = \left[f_{gw}^{w} \; x \; I_{wbc} + (I_{vbc} \; x \; TF(q \rightarrow expp) \right] x \; B_t \qquad [31]$$

for milk:

$$TF(q \rightarrow milk) = \left[f_{gw}^{w} \; x \; I_{wdc} + (I_{vdc} \; x \; TF(q \rightarrow expp) \right] x \; B_k \qquad [32]$$

for eggs:

$$TF(q \rightarrow eggs) = \left[f_{gw}^{w} \; x \; I_{wh} + (I_{vh} \; x \; TF(q \rightarrow expp) \right] x \; B_e \qquad [33]$$

where:

TF(q $\rightarrow$ meat) = the ratio of chemical concentration in meat to chemical concentration in ground water

f^{w}_{q} = the fraction of water needs provided by ground water (unitless) (Table III, "Parameter Values and Ranges for CalTOX")

I_{wbc} = ingestion of water by beef cattle (L/day) (Table IV, "Parameter Values and Ranges for CalTOX")

I_{vbc} = the daily intake of feed (pasture) by beef cattle (kg fresh mass/day) (Table IV, "Parameter Values and Ranges for CalTOX")

$TF(q \rightarrow expp)$ = the ratio of chemical concentration of exposed produce to the chemical concentration in ground water (equation 10)

B_t = biotransfer factor, the ratio of chemical concentration in meat to the intake of that chemical by beef cattle (day/kg meat) (Table V, "Parameter Values and Ranges for CalTOX")

$TF(q \rightarrow milk)$ = the ratio of chemical concentration in milk to the chemical concentration in ground water

I_{wdc} = ingestion of water by dairy cattle (L/day) (Table IV, "Parameter Values and Ranges for CalTOX")

I_{vdc} = the daily intake of feed (pasture) by dairy cattle (kg fresh mass/day) (Table IV, "Parameter Values and Ranges for CalTOX")

B_k = biotransfer factor, the ratio of chemical concentration in milk to the intake of that chemical by dairy cattle (day/kg milk) (Table V, "Parameter Values and Ranges for CalTOX")

$TF(q \rightarrow eggs)$ = the ratio of chemical concentration in eggs to the chemical concentration in ground water

I_{wh} = ingestion of water by hens (L/day) (Table IV, "Parameter Values and Ranges for CalTOX")

I_{vh} = the daily intake of feed by egg-laying hens (kg fresh mass/day) (Table IV, "Parameter Values and Ranges for CalTOX")

B_e = biotransfer factor, the ratio of the chemical concentration in eggs to the intake of that chemical by egg-laying hens (day/kg eggs) (Table V, "Parameter Values and Ranges for CalTOX")

iii. Inter-Media Transfer Factors - Soil to Animal Products

The ingestion intake of meat, milk products, and eggs contaminated by chemicals from surface and root-zone soil involves the transfer of chemicals from soil by ingestion of soil by meat and dairy-producing animals and egg-laying poultry and by ingestion of feed that have taken up those chemicals from soil. The inter-media TFs for surface soil to animal products are calculated as follows:

for meat:

$$TF(g \rightarrow meat) = [\, I_{sc} + (\, I_{vbc} \ x \ K_{ps}^{rain} \,)] \ x \ B_t \qquad [34]$$

for milk:

$$TF(g \rightarrow milk) = [\, I_{sc} + (\, K_{ps}^{rain} \ x \ I_{vdc} \,)] \ x \ B_k \qquad [35]$$

for eggs:

$$TF(g \rightarrow eggs) = [\, I_{sh} + (\, K_{ps}^{rain} \ x \ I_{vh} \,)] \ x \ B_e \qquad [36]$$

where:

$TF(g \rightarrow meat)$ = the ratio of chemical concentration in meat to chemical concentration in surface soil

I_{sc} = ingestion of soil by cattle (kg/day) (Table IV, "Parameter Values and Ranges for CalTOX")

I_{vbc} = the daily intake of feed (pasture) by beef cattle (kg fresh mass/day) (Table IV, "Parameter Values and Ranges for CalTOX")

K^{rain}_{ps} = the plant-soil partition coefficient for surface soil due to rainsplash; equivalent to the ratio of chemical concentration in pasture vegetation (exposed produce) to the chemical concentration in surface soil (kg soil/ kg plant fresh mass) (Table V, "Parameter Values and Ranges for CalTOX")

B_t = biotransfer factor, the ratio of chemical concentration in meat to the intake of that chemical by beef cattle (day/kg meat) (Table V, "Parameter Values and Ranges for CalTOX")

$TF(g \rightarrow milk)$ = the ratio of chemical concentration in milk to the chemical concentration in surface soil

I_{vdc} = the daily intake of feed (pasture) by dairy cattle (kg fresh mass/day) (Table IV, "Parameter Values and Ranges for CalTOX")

B_k = biotransfer factor, the ratio of chemical concentration in milk to the intake of that chemical by dairy cattle (day/kg milk) (Table V, "Parameter Values and Ranges for CalTOX")

$TF(g \rightarrow eggs)$ = the ratio of chemical concentration in eggs to the chemical concentration in surface soil

I_{sh} = ingestion of soil by hens (kg/day) (Table IV, "Parameter Values and Ranges for CalTOX")

I_{vh} = the daily intake of feed by egg-laying hens (kg fresh mass/day) (Table IV, "Parameter Values and Ranges for CalTOX")

B_e = biotransfer factor, the ratio of the chemical concentration in eggs to the intake of that chemical by egg-laying hens (day/kg eggs) (Table V, "Parameter Values and Ranges for CalTOX")

The inter-media TFs for root-zone soil to animal products are calculated as follows:

for meat:

$$TF(s \rightarrow meat) = (I_{vbc} \times K_{ps}) \times B_t \qquad [37]$$

for milk:

$$TF(s \rightarrow milk) = (K_{ps} \times I_{vdc}) \times B_k$$

[38]

for eggs:

$$TF(s \rightarrow eggs) = (K_{ps} \; x \; I_{vh}) \; x \; B_e$$

[39]

where:

TF(s $\rightarrow$ meat) =	the ratio of chemical concentration in meat to chemical concentration in root-zone soil
K_{ps} =	plant-soil partition coefficient from root-zone soil to above-ground plant parts; equivalent to the ratio of the chemical concentration in feed to the chemical concentration in root-zone soil (kg soil / kg plant fresh mass) (Table V, "Parameter Values and Ranges for CalTOX")
I_{vbc} =	the daily intake of feed (pasture) by beef cattle (kg fresh mass/day) (Table IV, "Parameter Values and Ranges for CalTOX")
B_t =	biotransfer factor, the ratio of chemical concentration in meat to the intake of that chemical by beef cattle (day/kg meat) (Table V, "Parameter Values and Ranges for CalTOX")
I_{vdc} =	the daily intake of feed (pasture) by dairy cattle (kg fresh mass/day) (Table IV, "Parameter Values and Ranges for CalTOX")
B_k =	biotransfer factor, the ratio of chemical concentration in milk to the intake of that chemical by dairy cattle (day/kg milk) (Table V, "Parameter Values and Ranges for CalTOX")
I_{vh} =	the daily intake of feed by egg-laying hens (kg fresh mass/day) (Table IV, "Parameter Values and Ranges for CalTOX")
B_e =	biotransfer factor, the ratio of the chemical concentration in eggs to the intake of that chemical by egg-laying hens (day/kg eggs) (Table V, "Parameter Values and Ranges for CalTOX")

iv. Calculating the Concentration of Chemical in Meat, Eggs, and Dairy Products

The concentration of a chemical in the exposure medium of meat due to the transfer of that chemical from the environmental compartments of ambient air, surface and ground water, and surface and root-zone soils is given by the equation:

$$C_{meat} = TF(a \rightarrow meat)\, x\, C_a + TF(ap \rightarrow meat)\, x\, C_{ap} + TF(w \rightarrow meat)\, x\, C_w$$
$$+ TF(q \rightarrow meat)\, x\, C_q + TF(g \rightarrow meat)\, x\, C_g + TF(s \rightarrow meat)\, x\, C_s$$

[40]

where:

C_{meat} = the concentration of chemical of concern in meat (mg/kg meat)

$TF(a \rightarrow meat)$ = the ratio of chemical concentration in meat to the chemical concentration in the gas phase of ambient air (equation 22)

C_a = the concentration of the chemical in the gas phase of ambient outdoor air (mg/m^3)

$TF(ap \rightarrow meat)$= the ratio of chemical concentration in meat (mg/kg meat) to chemical concentration in the particle (or dust) phase of the ambient outdoor air (mg/m^3) (equation 25)

C_{ap} = the concentration of the chemical in the dust phase of the ambient outdoor air (mg/m^3)

$TF(w \rightarrow meat)$ = the ratio of chemical concentration in meat (mg/kg meat) to the chemical concentration in surface water (mg/L) (equation 28)

C_w = chemical concentration in surface water (mg/L)

$TF(q \rightarrow meat)$ = the ratio of chemical concentration in meat to the chemical concentration in ground water (equation 31)

C_q = chemical concentration in ground water (mg/L)

$TF(g \rightarrow meat)$ = the ratio of chemical concentration in meat to chemical concentration in surface soil (equation 34)

C_g = concentration of the chemical in surface soil (mg chemical/kg soil)

TF(s $\rightarrow$ meat) = the ratio of chemical concentration in meat to chemical concentration in root-zone soil (equation 37)

C_s = chemical concentration in root-zone soil (mg chemical/kg soil)

The concentration of a chemical in milk and dairy products from the transfer of that chemical from ambient air, surface and ground water, and surface and root-zone soils is given by the equation:

$$C_{milk} = TF(a \rightarrow milk)\ x\ C_a + TF(ap \rightarrow milk)\ x\ C_{ap} + TF(w \rightarrow milk)\ x\ C_w$$
$$+ TF(q \rightarrow milk)\ x\ C_q + TF(g \rightarrow milk)\ x\ C_g + TF(s \rightarrow milk)\ x\ C_s$$

[41]

where:

C_{milk} = concentration of chemical of concern in milk and dairy products (mg/kg milk)

TF(a $\rightarrow$ milk) = the ratio of chemical concentration in milk to the chemical concentration in the gas phase of ambient air (equation 23)

C_a = the concentration of the chemical in the gas phase of ambient outdoor air (mg/m^3)

TF(ap $\rightarrow$ milk)= the ratio of chemical concentration in milk to chemical concentration in the particle (or dust) phase of the ambient outdoor air (equation 26)

C_{ap} = the concentration of the chemical in the dust phase of the ambient outdoor air (mg/m^3)

TF(w $\rightarrow$ milk) = the ratio of chemical concentration in milk to the chemical concentration in surface water (equation 29)

C_w = chemical concentration in surface water (mg/L)

TF(q $\rightarrow$ milk) = the ratio of chemical concentration in milk to the chemical concentration in ground water (equation 32)

C_q = chemical concentration in ground water (mg/L)

TF(g $\rightarrow$ milk) = the ratio of chemical concentration in milk to chemical concentration in surface soil (equation 35)

C_g = concentration of the chemical in surface soil (mg chemical/kg soil)

TF(s $\rightarrow$ milk) = the ratio of chemical concentration in milk to chemical concentration in root-zone soil (equation 38)

C_s = chemical concentration in root-zone soil (mg chemical/kg soil)

The concentration of a chemical in eggs from the transfer of that chemical from ambient air, surface and ground water, and surface and root-zone soils is given by the equation:

$$C_{eggs} = TF(a \rightarrow eggs)\ x\ C_a + TF(ap \rightarrow eggs)\ x\ C_{ap} + TF(w \rightarrow eggs)\ x\ C_w + TF(q \rightarrow eggs)\ x\ C_q + TF(g \rightarrow eggs)\ x\ C_g + TF(s \rightarrow eggs)\ x\ C_s \quad [42]$$

where:

C_{eggs} = concentration of chemical of concern in eggs (mg/kg eggs)

TF(a $\rightarrow$ eggs) = the ratio of chemical concentration in eggs to the chemical concentration in the gas phase of ambient air (equation 24)

C_a = the concentration of the chemical in the gas phase of ambient outdoor air (mg/m^3)

TF(ap $\rightarrow$ eggs)= the ratio of chemical concentration in eggs to chemical concentration in the particle (or dust) phase of the ambient outdoor air (equation 27)

C_{ap} = the concentration of the chemical in the dust phase of the ambient outdoor air (mg/m^3)

TF(w $\rightarrow$ eggs) = the ratio of chemical concentration in eggs to the chemical concentration in surface water (equation 30)

C_w = chemical concentration in surface water (mg/L)

TF(q $\rightarrow$ eggs) = the ratio of chemical concentration in eggs to the chemical concentration in ground water (equation 33)

C_q = chemical concentration in ground water (mg/L)

TF(g $\rightarrow$ eggs) = the ratio of chemical concentration in eggs to chemical concentration in surface soil (equation 36)

C_g = concentration of the chemical in surface soil (mg chemical/kg soil)

TF(s $\rightarrow$ eggs) = the ratio of chemical concentration in eggs to chemical concentration in root-zone soil (equation 39)

C_s = chemical concentration in root-zone soil (mg chemical/kg soil)

v. Calculating the Intake of Chemical by Ingestion of Contaminated Meat, Eggs, and Dairy Products

The intake of contaminated meat is calculated by using specific parameters for meat only in equation 21:

$$Intake_{meat} = C_{meat}\ x \left[\frac{IR_{meat}}{BW}\right] x\ f^{mt}_{local}\ x\ \frac{EFxED}{AT}$$

[43]

where:

$Intake_{meat}$ = Intake of chemical of concern by an exposed individual via ingestion of contaminated meat (mg chemical/kg body weight per day)

C_{meat} = concentration of chemical of concern in meat, given by equation 40 (mg/kg meat),

IR_{meat} = meat ingestion rate (kg meat/day),

BW = body weight (kg),

f^{mt}_{local} = or FI, fraction of meat ingested from homegrown or local source (Table III, "Parameter Values and Ranges for CalTOX"),

EF = exposure frequency (days/year),

ED = exposure duration (years), and

AT = averaging time (days).

The value for the ratio, IR_{meat}/Bw, is given in Table II, "Parameter Values and Ranges for

CalTOX". Section 6.6.4 of RAGS/HHEM gives a value for the fraction of homegrown beef ingested by rural residents (FI) which is the same as that given in Table III, "Parameter Values and Ranges for CalTOX".

The intake of contaminated milk and dairy products is calculated by using specific parameters for milk products only in equation 21:

$$Intake_{milk} = C_{milk}\ x \left[\frac{IR_{milk}}{BW}\right] x\ f^{mk}_{local}\ x\ \frac{EFxED}{AT}$$

[44]

where:

Intake$_{milk}$ = Intake of chemical of concern by an exposed individual via ingestion of contaminated milk (mg chemical/kg body weight per day)

C$_{milk}$ = concentration of chemical of concern in milk, given by equation 41 (mg/kg milk),

IR$_{milk}$ = milk/dairy ingestion rate (kg milk/day),

BW = body weight (kg),

f^{mk}_{local} = or FI, fraction of milk ingested from homegrown or local source (unitless) (Table III, "Parameter Values and Ranges for CalTOX"),

EF = exposure frequency (days/year),

ED = exposure duration (years), and

AT = averaging time (days).

The value for the ratio, IR$_{milk}$/BW, is given in Table II, "Parameter Values and Ranges for CalTOX". Section 6.6.4 of RAGS/HHEM gives a value for the fraction of dairy products ingested by rural residents (FI) which is the same as that given in Table III, "Parameter Values and Ranges for CalTOX".

The intake of contaminated eggs is calculated by using specific parameters for eggs only in equation 21:

$$Intake_{eggs} = C_{eggs}\ x \left[\frac{IR_{eggs}}{BW}\right] x\ f^{egg}_{local}\ x\ \frac{EFxED}{AT}$$

[45]

where:

$Intake_{eggs}$ = Intake of chemical of concern by an exposed individual via ingestion of contaminated eggs (mg chemical/kg body weight per day)

C_{eggs} = concentration of chemical of concern in eggs, given by equation 42 (mg/kg eggs),

IR_{eggs} = egg ingestion rate (kg eggs/day),

BW = body weight (kg),

f^{egg}_{local} = or FI, fraction of eggs ingested from homegrown or local source (unitless) (Table III, "Parameter Values and Ranges for CalTOX"),

EF = exposure frequency (days/year),

ED = exposure duration (years), and

AT = averaging time (days).

The value for the ratio, IR_{eggs}/BW, is given in Table II, "Parameter Values and Ranges for CalTOX". By summing the meat, milk/dairy product and egg intakes given above, the ingestion intake for contaminated meat, milk and eggs is obtained (designated as $Intake_{mke}$ in equation 21):

$$Intake_{mke} = Intake_{meat} + Intake_{milk} + Intake_{eggs}$$

[46]

f. Ingestion of Water While Swimming

The RAGS/HHEM equation for the incidental ingestion of a chemical while swimming in a contaminated surface water body (U.S. EPA 1989b, pg. 6-36) may be written as follows:

$$Intake_{swim} = C_w \; x \left[\frac{IR_{swim}}{BW} \right] x \; ET_{sw} \; x \; \frac{EF_{sw} \; x ED}{AT}$$

[47]

where:

$Intake_{swim}$ = Intake of chemical of concern by an exposed individual via ingestion of surface water while swimming (mg chemical/kg body weight per day),

C_w = concentration of chemical of concern in surface water (mg/L),

IR_{swim} = ingestion rate (L/hour),

BW = body weight (kg),

ET_{sw} = exposure time (hours in contaminated water/day) (Table III, "Parameter Values and Ranges for CalTOX"),

EF_{sw} = exposure frequency (days/year) (Table III, "Parameter Values and Ranges for CalTOX"),

ED = exposure duration (years), and

AT = averaging time (days).

The value of the ratio, IR_{swim}/BW, is given in Table III, "Parameter Values and Ranges for CalTOX". No inter-media TF is necessary for the estimation of the chemical concentration in the exposure medium, since, for this intake, the environmental compartment of surface water is the exposure medium. This CalTOX equation is essentially identical to the RAGS/HHEM equation and includes the pathway specific factors, ET_{sw}, expressed as hours/day swimming, and EF_{sw}, expressed as days/year swimming.

g. Ingestion of Mother's Milk

There is no equation in RAGS/HHEM for the ingestion of mother's milk by nursing infants. However, lactating women can transfer to breast milk their intake of chemicals from all routes (ingestion, inhalation, and dermal contact). All routes to the mother must be considered in determining the chemical concentration in breast milk, including those routes yet to be discussed (inhalation and dermal routes). One hundred percent of the ingestion intake of infants may be breast milk ingestion. Thus, the population of nursing infants may be at risk. The intake equation is:

$$Intake_{milk} = C_{bmilk} \; x \left[\frac{IR_{bm}}{BW} \right] x \; \frac{EFxED}{AT}$$

[48]

where:

Intake$_{milk}$ = Intake of chemical of concern by a nursing infant via ingestion of contaminated mothers milk (mg chemical/(kg body weight per day)

C_{bmilk} = concentration in breast milk of chemical of concern (mg/L),

IR_{bm} = ingestion rate of breast milk (L/day),

BW = body weight (kg),

EF = exposure frequency (days/year),

ED = exposure duration (set to one year), and

AT = averaging time (days).

The value for the ratio, IR_{bm}/BW, is given in Table III, "Parameter Values and Ranges for CalTOX". For this intake the inter-media TF is the ratio of the concentration of the chemical in the contact or exposure medium of breast milk to the concentration of the chemical in the "environmental compartment" of the mother due to the exposure of the mother to the chemical in each of the environmental compartments of ambient air, water and soil. The inter-media TF in this circumstance is the partition factor, B_{bmk}, the ratio of chemical concentration in mother's milk to the intake of that chemical by the mother (see Table V, "Parameter Values and Ranges for CalTOX"). The concentration of the chemical in breast milk may be estimated using the following equation:

$$C_{bmilk} = I_{mo} \; x \; BW_{mo} \; x \; B_{bmk}$$

[49]

where:

C_{bmilk} = concentration of chemical in breast milk due to the intake of that chemical by the mother from a specific environmental compartment (mg/kg milk)

I = the sum of all intakes of the chemical from a specific environmental compartment by the mother (mg/kg body weight per day)

BW_{mo} = the body weight of the mother (kg) (Table II, "Parameter Values and Ranges for CalTOX")

B_{bmk} = the ratio of chemical concentration in mother's milk to the intake of that chemical by the mother (days/kg milk) (Table V, "Parameter Values and Ranges for CalTOX")

After calculating the chemical concentration in breast milk resulting from each pathway to which the mother has been potentially exposed, the total chemical concentration in breast milk is given by summing the results from each pathway. This summed value is input as C_{bmilk} in equation 48. All the exposure pathways considered in this section (section D; ingestion, inhalation, dermal routes) are assumed to contribute to the chemical concentration in the mother.

2. THE INHALATION ROUTE

The methods provided in this section fill a gap that exists in the RAGS/HHEM (U.S. EPA 1989b) method for estimating the intake of chemicals of concern by inhalation. Section 6.5.4 of RAGS/HHEM discusses the monitoring and modeling approaches that may be used to estimate exposure concentrations in air. However, this section of RAGS largely references other guidance documents which are collections of methods and specific guidance is not given. RAGS/HHEM (U.S. EPA 1989b, section 6.6.3) also gives a brief general discussion on the calculation of air intakes but does not provide recommendations for specific exposure scenarios. The CalTOX model provides detailed methods for estimating air intakes for a number of potential exposure pathways.

First, the structure of the CalTOX inhalation equations explicitly defines three locations in which potentially exposed people could inhale air contaminated by chemicals originating in soil at a site. These three locations are outdoors, indoors, and in the bathroom. Outdoor air is the air directly above the site. Indoor air is the air in an on-site building excluding the bathroom.

Bathroom air is the air in the bathroom in an on-site building. The bathroom is separated because water-use during bathing/showering can greatly increase the concentration of volatile chemicals in the bathroom. By defining indoor air and bathroom air CalTOX extends the RAGS guidance.

A second extension of the RAGS guidance results from the multiple pathways by which the air in these three locations can become contaminated. CalTOX provides explicit guidance for relating the air concentration in the three exposure locations to the measured or modeled concentrations in various environmental compartments. There are six environmental compartments which may give rise to chemicals in air inhaled by people. Concentrations levels in these compartments are denoted by a capital C followed by a lower case letter(s)indicating the compartment. The environmental compartments are the particulate phase of ambient air outdoors (ap), the vapor phase of ambient air outdoors (a), the ground-surface soil (g), the root-zone soil (s), volatile chemicals dissolved in groundwater (q), and volatile chemical dissolved in surface water (w).

Outdoor air has chemicals bound to particulate phase (Cap) and in the vapor phase (Ca) as described in the HHEM. Chemical contaminants in indoor air can originate from the following sources:

1) outdoor air vapors (Ca),
2) outdoor airborne particles (Cap),
3) indoor airborne particles from soil brought in from surface soil (Cg),
4) indoor air vapors which migrate from root-zone soil through basements, slabs, crawl spaces (Cs)
5) indoor air vapors which volatilize from ground water used as tap water in the kitchen and laundry room (Cq),
6) indoor air vapors which volatilize from surface water used as tap water the kitchen and laundry room (Cw).

Bathroom air may have concentrations of volatile waterborne chemicals due to showering and/or bathing greater than elsewhere in the home. Therefore, inhalation exposure in the bathroom is treated independently from inhalation exposure in the rest of the home. These volatiles may come from either the ground water (Cq) or the surface water (Cw) depending on the origin of the tap water.

The RAGS/HHEM recommends using the equation for inhalation of vapor-phase chemicals (U.S. EPA 1989b, page 6-44) appropriately modified for calculating intake via inhalation of dusts. This equation is:

$$Intake_{air} = C_{air}\ x \left[\frac{IR_{air}}{BW}\right] x\ \frac{EF\ x\ ED}{AT}$$

[50]

where:

Intake$_{air}$ = Intake of a chemical of concern by an exposed individual via inhalation of contaminated air (mg/kg body weight per day)

C_{air} = concentration of chemical of concern in air(mg/m^3 air)

IR_{air} = inhalation rate (m^3 air/day)

BW = body weight (kg)

EF = exposure frequency (days/year)

ED = exposure duration (years)

AT = averaging time (days)

For the purposes of this chapter we will consider the above equation to consist of three parts. The third part, (EF x ED)/AT, is the timing consideration which is independent of the pathway of inhalation and relates to whether the chemical is a carcinogen. Therefore, the subsequent discussion on the inhalation pathways will ignore these timing factors and focus the other two parts: the average daily inhalation rate, IR_{air}/BW, and the concentration in inhaled air,

C_{air}.

The average daily inhalation rate and the concentration in inhaled air are both dependent on the location in which the air is inhaled. The remainder of the inhalation portion of this document will be divided into three section: outdoor exposures, indoor exposures, and bathroom exposure. The average daily inhalation rate in m^3 air/day will differ for each of the three locations. The equation used to compute average daily inhalation rate is presented at the begining of each section. Then each section is divided into a different number of subsections to describe the intermedia transfer factors. The intermedia transfer factors (TF) relate the chemical concentration in the six environmental compartments to the air concentration in the outdoor air, indoor air and bathroom air. TFs are ratios of the concentrations the inhaled air to the environmental compartment concentrations. The number of subsections depends on the number of pathways by which chemicals can reach the air in the exposure location from the environmental media.

a. Inhalation of Outdoor Air

The equation for inhalation intake, equation 50, requires an estimate of the average daily inhalation rate (IR/BW) to estimate the intake due to inhalation for air. The equation for computing the outdoor daily intake rate IR_{outair}/BW is as follows:

$$\frac{IR_{outair}}{BW} = (\,ET_{out}\ x\ f_{out,l}\ x\ BR_l\,) + [\,ET_{out}\ x(1 - f_{out,l}\,)\ x\ BR_h\,] \qquad [51]$$

where:

IR_{outair}/BW = outdoor inhalation rate per kg body weight (m^3 air/kg per day)

ET_{out} = the total hours per day spent outdoors at the contaminated site (hours/day)

$f_{out,l}$ = fraction of total hours spent outdoors spent with a breathing rate associated with light activity. The remaining time is assumed to be spent with a breathing rate associated with high activity (unitless)

BR_l = light activity breathing rate per kg body weight (m^3/kg per hour)

BR_h = high activity breathing rate per kg body weight (m^3/kg per hour)

This equation provides the method by which the average daily outdoor inhalation rate can be estimated. It allows for two different breathing rates depending on the level of physical exertion. This is the second part of equation 50.

The first part of equation 50 is concentration in the inhaled outdoor air, C_{air}. Intermedia transfer factors (TF) are used to relate the concentration in the exposure medium, inhaled air, to the environmental compartment media. The following subsection show the equations used to derive the TFs for the outdoor vapor and particulate phase compartments

i. Outdoor Air Dusts/Particles

The CalTOX exposure model assumes that the relationship between the chemical concentration in the inhaled outdoor dust/particulate phase is equal to the product of the environmental air particulate phase compartment (C_{ap}) and an intermedia transfer factor (TF). This TF is defined in the following equation:

$$TF(ap \rightarrow outair) = 1$$

[52]

The TF is equal to 1 because the inhaled dust outdoors is equal to the particulate phase measured or modeled in the outdoor air. This TF may seem unnecessary, but the assumption of the exposure air equalling the environmental air should be explicitly stated.

ii. Outdoor Vapor Phase of a Chemical

The CalTOX exposure model assumes that the chemical concentration of inhaled outdoor vapor is equal to the product of the environmental air particulate phase compartment (C_a) and an intermedia transfer factor (TF). This TF is defined in the following equation:

$$TF(a \rightarrow outair) = 1$$

[53]

The TF is equal to 1 because the inhaled vapor outdoors is equal to the vapor concentration measured or modeled in the outdoor air.

b. Inhalation of Indoor Air, Excluding Bathroom Air

This section describes the equations which estimate that portion of the average daily inhalation intake which takes place indoors, excluding the potentially higher exposures which can occur in the bathroom. The equation for inhalation intake, equation 50, requires an estimate of the average daily inhalation rate (IR/BW) to estimate the intake due to inhalation for air. The equation for computing the indoor daily intake rate IR_{inair}/BW is as follows:

$$\frac{IR_{inair}}{BW} = [(ET_{ind} - ET_{sb}) \times f_{ind,l} \times BR_l] + [(ET_{ind} - ET_{sb}) x(1 - f_{ind,l}) \times BR_s]$$

[54]

where:

IR_{inair}/BW = average indoor inhalation rate per kg body weight (m^3 air/kg per day)

ET_{ind} = the total hours per day spent indoors including the bathroom at the contaminated site (hours/day)

ET_{sb} = the total hours per day spent in the bathroom at the contaminated site (hours/day)

$f_{ind,l}$ = fraction of total hour spent indoors spent with a breathing rate associated with light activity. The remaining time is assumed to be spent with a breathing rate associated with sleeping. (unitless)

BR_l = light activity breathing rate per kg body weight (m^3/kg per hour)

BR_s = sleeping breathing rate per kg body weight (m^3/kg per hour)

All six environmental compartments can theoretically contribute to indoor air. Therefore, six intermedia transfer factors for indoor air are provided below.

i. Indoor Particulate Phase from Outdoor Airborne Particulate

This intermedia transfer factor (TF) relates the indoor air and outdoor air particulate phase concentrations. This TF is defined in the following equation:

$$TF(ap \rightarrow inair) = 1$$

[55]

This TF is equal to 1 because all of the particulate phase bound chemical measured or modeled in the outdoor air is assumed to be transported indoors.

ii. Indoor Air Vapor Phase from Outdoor Air Vapors

The CalTOX exposure model assumes that the chemical concentration in the inhaled indoor vapor is equal to the product of the environmental air vapor compartment (C_a) and an intermedia transfer factor (TF). This TF is defined in the following equation:

$$TF(a \rightarrow inair) = 1$$

[56]

The TF is equal to 1 because all of the vapor phase chemical measured or modeled in the outdoor air is assumed to be transported indoors.

iii. Inhalation Indoors of Dusts/Particulate Phase Tracked in from Outdoor Ground Surface Soil

In this scenario the structure under consideration is proximate to contaminated soil. The CalTOX exposure model assumes that contaminated surface soil enters the structure, becomes part of the indoor dust burden, and is inhaled. The CalTOX exposure models the relationship between the chemical concentration in the inhaled indoor dust as equal to the product of the surface soil concentration (C_g) and an intermedia transfer factor (TF). This TF is defined in the following equation:

$$TF(g \rightarrow inair) = \frac{Dust_{ind} \, x \, C_g}{C_g}$$

[57]

where:

Dust$_{ind}$ = indoor dust load attributable to tracked in soil (kg soil/m^3)

C$_q$ = concentration in ground surface soil (mg chemical/kg soil)

The concentration of airborne particles indoors includes airborne particles from outdoor air and resuspended dust form tracked in soil.

iv. Indoor Chemical Vapors Transferred from Root-Zone Soil

The building is assumed to be on contaminated soil with the foundation within one meter of contaminated root-zone soil, so vapor migration of volatile chemicals into the structure may occur. The inter-media TF is the ratio of the chemical concentration in the gas phase of personal air attributable to soil gas migration to the chemical concentration in root-zone soil, C_s. The TF is defined as follows.

$$TF(s \rightarrow inair) = \frac{K_d \, xH}{RT} \, x \, \alpha_{inair}$$

[58]

where:

TF(s ® inair) = the ratio of chemical concentration in indoor air to the chemical concentration in root zone soil (mg/m^3 air)/(mg/kg soil)

K_d = root-zone soil/water partition coefficient

(m^3 soil/m^3 water)

H = Henry's law constant (Pa-m^3/mole)

R = Universal gas constant (Pa-L/mol-K)

T = Temperature in degrees Kelvin

α_{inair} = the ratio of soil gas concentration (mg/m^3) to indoor air concentration (mg/m^3).

The ratio of soil gas concentration to indoor air concentration is based directly on the work of Johnson and Ettinger (1991). This ratio includes the permeability of the soil, the diffusion distance and the size of the cracks in the foundation. It has been reduced to a single input parameter, α_{inair}. This is a ratio of soil gas concentration, not soil particle concentration, to house air. Therefore, the soil gas concentration must be estimated from the concentration of chemical in the root-zone soil. This is accomplished assuming that the soil gas is in chemical equalibrium with the soil particle concentration.

v. Chemicals Transferred from Ground Water to Indoor Air Outside the Bathroom

Chemicals may volatilize from ground water to indoor air in residential homes from either the laundry and kitchen. The inter-media transfer factor (TF) for transfer of chemicals via this route is given by the equation shown below:

$$TF(q \rightarrow inair) = f_q^w \; x \; \frac{W_{house} \; x \; f_x(house)}{VR_{house}}$$

[59]

where:

TF(q ® inair) = the ratio of chemical concentration in indoor air outside the bathroom from household water use to the chemical concentration in ground water

f^w_q = the fraction of water needs provided by ground water (unitless)

W_{house} = water use rate for all household activities (L/hour)

VR_{house} = average house ventilation rate (m^3/hour)

$f_x(house)$ = the mass transfer efficiency of a chemical from water to air in the house (unitless)

This equation is taken from McKone and Bogen (1992). W_{house} and VR_{house} are both house specific parameters. W_{house}, water flow in the house, is the rate at which water enters the house. VR_{house}, ventilation rate, is the rate at which air leaves the house. The mass transfer efficiency, $f_x(house)$, indicates how readily the chemical becomes airborne from the running water. This chemical related parameter may be computed as follows:

$$f\,(house) = 0.7x\,\frac{3x\,10^{6}\,(\,m^{2}\,/s\,)^{-2/3}}{\left[\dfrac{2.5}{D_l^{2/3}} + \dfrac{RT}{Hx\,D_a^{2/3}}\right]}$$

[60]

where:

D_l = contaminant diffusion coefficient in water(m^2/s)

D_a = contaminant diffusion coefficient in air(m^2/s)

R = universal gas constant(Pa-L/mol-k)

T = temperature (degrees Kelvins)

H = Henry's law constant(Pa-L/mol).

The $f_x(house)$ factor is computed according the McKone (1987).

vi. Chemicals Transferred from Surface Water to Indoor Air Outside the Bathroom

Chemicals may volatilize from surface water to indoor air in residential homes from either the laundry and kitchen. The inter-media transfer factor (TF) for this transfer of chemicals via this route is given by the equation shown below:

$$TF(w \rightarrow inair) = (1 - f_q^w)\ x\ \frac{W_{house}\ x\ f_x(house)}{VR_{house}}$$

[61]

where:

$TF(w \rightarrow inair)$ = the ratio of chemical concentration in indoor air from household water use to the chemical concentration in surface water

$1 - f^w_q$ = the fraction of water needs provided by surface water (unitless)

W_{house} = water use rate for all household activities (L/hour)

VR_{house} = average house ventilation rate (m^3/hour)

$f_x(house)$ = the mass transfer efficiency of a chemical from water to air in the house (unitless)

The parameters W_{house}, VR_{house} and ϕ_x (house) were discussed above.

c. Inhalation of Bathroom Air

This section describes the equation which estimates that portion of the total inhalation intake from the bathroom air. The equation for average inhalation intake, equation 50, requires an estimate of the daily inhalation rate (IR/BW). The equation for computing the average daily inhalation rate in the bathroom ($IR_{bathair}$/BW) is as follows:

$$\frac{IR_{bathair}}{BW} = ET_{sb} \times BR_{l} \qquad [62]$$

where:

$IR_{bathair}/BW$ = inhalation rate per kg body weight (m^3 air/kg per day)

ET_{sb} = the total hours per day spent in the bathroom at the contaminated site (hours/day)

BR_l = light activity breathing rate per kg body weight (m^3/kg per hour)

This daily inhalation rate will be used for estimating exposures while showering or bathing in contaminated tap water. Tap water may be derived from either ground water or surface water. The equations describing the intermedia transfer of chemicals from ground water and surface water to bathroom air are shown in the two subsequent subsection.

i. Chemicals Transferred from Ground Water to Bathroom Air

Chemicals may volatilize from ground water to bath air during showering or bathing. The inter-media transfer factor (TF) for this transfer of chemicals is given by the equation shown below:

$$TF(q \rightarrow bathair) = f_q \; x \; \frac{W_{bath} \; x \; f_x(bath)}{VR_{bath}}$$

[63]

where:

$TF(q \rightarrow bathair)$ = the ratio of chemical concentration in indoor air in the bathroom from bathroom water use to the chemical concentration in ground water

f_q = the fraction of tap water provided by ground water (unitless)

W_{bath} = water use rate for showering/bathing (L/hour)

VR_{bath} = average bathroom ventilation rate (m^3/hour)

$f_x(bath)$ = the mass transfer efficiency of a chemical from water to air in the bathroom (unitless)

Equation 63 is taken from McKone and Bogen (1992). W_{bath} and VR_{bath} are both bathroom specific parameters. W_{bath}, water flow in the shower is the rate at which water enters the shower. VR_{bath}, ventilation rate, is the rate at which air leaves the bathroom. The mass transfer efficiency $f_x(bath)$, indicates how readily the chemical becomes airborn from the running water. This chemical related parameter may be computed as follows:

$$f(bath) = 0.6x \frac{3x\,10^{6}\,(m^{2}/s)^{-2/3}}{\left[\frac{2.5}{D_l^{2/3}} + \frac{RT}{Hx\,D_a^{2/3}}\right]}$$

[64]

where:

D_l = contaminant diffusion coefficient in water(m^2/s)

D_a = contaminant diffusion coefficient in air(m^2/s)

R = universal gas constant(Pa-L/mol-k)

T = temperature (degrees Kelvins)

H = Henry's law constant(Pa-L/mol).

The $\phi_x(bath)$ factor is computed according the McKone (1987).

ii. Chemicals Transferred from Surface Water to Bathroom Air

Chemicals may volatilize from surface water to bath air during showering or bathing. The intermedia transfer factor (TF) for this transfer of chemicals is given by the equation shown below:

$$TF(w \rightarrow bathair) = (1 - f_q^w)\ x\ \frac{W_{bath}\ x\ f_x(bath)}{VR_{bath}}$$

[65]

where:

TF(w ® bathair) = the ratio of chemical concentration in indoor air from bathroom water use to the chemical concentration in surface water

$1 - f_q$ = the fraction of water needs provided by surface water (unitless)

W_{bath} = water use for all bathhold activities (L/hour)

VR_{bath} = average bath ventilation rate (m^3/hour)

$f_x(bath)$ = the mass transfer efficiency of a chemical from water to air in the bath (unitless)

The parameters W_{bath}, VR_{bath} and $f_x(bath)$ were discussed above.

3. THE DERMAL ROUTE

In the multiple pathway approach of the CalTOX exposure model, a chemical in contaminated surface soil, ground water, and surface water may be transferred to the outer skin layer, the stratum corneum, via the exposure media of household soil, tap water, or swimming water. This transfer cannot be treated simply as contact with the skin, nor is there sufficient scientific knowledge for most chemicals to model transfer through the skin and into the blood. Instead, the CalTOX exposure model addresses the uptake of the chemical of concern from an exposure medium and into the skin as a basis for estimating potential dose. Thus, dermal exposure is treated differently than ingestion and inhalation exposures in both RAGS/HHEM and the CalTOX model. The RAGS/HHEM equations for dermal exposure are called calculations of "absorbed dose" (U.S. EPA 1989b, page 6-37, 6-41), whereas, the CalTOX model dermal equations are calculations of "uptake". We use the term "uptake" in the CalTOX model as the best description of the equation (see Appendix A: Terminology).

For the following dermal exposure equations, inter-media transfer factors (TFs) are not needed to calculate the concentration of the chemical in exposure media, since the concentrations of the chemical in the exposure media of household soil, tap water, or swimming water may be considered equivalent to the concentrations in the environmental compartments of surface soil, ground water, and surface water.

The values for exposure duration and averaging time to be used in the following equations depend upon whether the calculated uptake value will be used to determine carcinogenic risk or chronic systemic health hazard of the chemical of concern.

a. Dermal Uptake of a Chemical While Bathing or Swimming with Contaminated Water

The RAGS/HHEM equation for dermal uptake of chemicals while bathing or swimming with contaminated water (U.S. EPA 1989b, page 6-37) may be written as follows:

$$Uptake_{bathsw} = C_w \; x \; \frac{PC \; x \; SA}{BW} \; x \; ET \; x \; \frac{EFxED}{AT} \; x \; CF$$

[67]

where:

$Uptake_{bathsw}$ = Uptake of chemical of concern by an exposed individual via dermal contact with contaminated bathing or swimming water (mg chemical/kg body weight per day)

C_w = concentration of chemical of concern in surface water; may also be C_{drink}, concentration of chemical of concern in drinking water (mg/L),

PC = dermal permeability constant (cm/hour),

SA = skin surface area available for contact (m^2),

BW = body weight (kg),

ET = exposure time (hour/day),

EF = exposure frequency (days/year),

ED = exposure duration (years),

AT = averaging time (days),

CF = conversion factor (10 L/(cm times m^2)).

In this equation, the contact rate per body weight (CR/BW) term has been replaced by parameters for dermal permeability of the chemical and skin surface area available for contact. Values for the ratio, SA/BW, are provided in Table II, "Parameter Values and Ranges for CalTOX". A conversion factor (CF) has also been added.

RAGS/HHEM recommends using chemical-specific permeability constants. However, these values are often not available in the scientific literature. The CalTOX dermal exposure model provides a series of equations to calculate:

1) K^w_p, the steady-state permeability coefficient for the chemical from water into the stratum corneum, calculated from the molecular weight and octanol-water partition coefficient, K_{ow}, of the chemical, and
2) AR_{water}, the ratio of uptake of the chemical by skin to the concentration of the chemical in water, based on the skin-water partition coefficient, K_m (see Table V, "Parameter Values and Ranges for CalTOX"), skin thickness, and exposure time per exposure event.

These calculations are used to specify the dermal permeability constant parameter for the exposure time and are discussed in depth in McKone and Howd (1992).

i. Calculating the Chemical-Specific Permeability Coefficient

The equation for calculating the steady-state permeability coefficient for a chemical from water into the stratum corneum when the molecular weight of the chemical is less than or equal to 280 g/mole is:

$$K_p^w = MW^{-0.6}\ x \left[\frac{2.4\ x\ 10^{-6} + 3.0\ x\ 10^{-5} (K_{ow})^{0.8}}{d_{skin}} \right]$$

[68]

where:

K_p^w = chemical-specific steady-state permeability coefficient from water into the stratum corneum (cm/hour)

MW = molecular weight of the chemical (g/mole)

K_{ow} = octanol-water partition coefficient of the chemical (kg water/kg octanol)

δ_{skin} = skin thickness (cm)

For chemicals with a molecular weight greater than 280, the equation is (U.S. EPA 1992a, equation 5.8):

$$K_p^w = 0.0019\ x\ (K_{ow})^{0.71}\ x\ 10^{(-0.0061\ x\ MW)}$$

[69]

If either equation 68 or 69 predicts a value higher than one cm/hour, 1 cm/hour is used as the default, since no value higher than this has been measured experimentally. The calculated K_p^w value is used in the following equations to determine the AR_{water} value.

ii. Calculating the Ratio of the Uptake of the Chemical by Skin to Concentration of the Chemical in Water

The ratio of the uptake of a chemical by skin from dermal contact with contaminated water to the chemical concentration in water is dependent on the lag time and exposure time. The lag time is defined as the time it takes the outer skin layer (stratum corneum) to reach chemical equilibrium with the medium applied to it (such as, water) and is given as:

$$LT = \frac{0.0017 + 0.00067(K_{ow})^{0.8}}{6\ K_p^w}$$

[70]

where:

LT = lag time (hour)

K_{ow} = octanol-water partition coefficient of the chemical (kg water/kg octanol)

K^w_p = chemical-specific steady-state permeability coefficient from water into the stratum corneum (cm/hour), from equation 68 or 69

The exposure time for swimming is given in hours/day (ET_{sw}, Table III, "Parameter Values and Ranges for CalTOX"). The exposure time in the shower or bath is the hours/day spent in the bathroom divided by 2 (ET_{sb}/2, see Table III, "Parameter Values and Ranges for CalTOX"), because the assumption is made that one-half the time in the bathroom is spent in the shower or bath. When the exposure time is less than and within a factor of five of the lag time, the absorption ratio is:

$$AR_{water} = \frac{d_{skin} K_m}{2}$$

[71]

where:

AR_{water} = absorption ratio of dermal uptake of a chemical to concentration of the chemical in water (mg/cm^2 skin per mg/cm^3 water)

δ_{skin} = skin thickness (cm)

K_m = skin-water partition coefficient (cm^3 water per cm^3 skin) (Table V, "Parameter Values and Ranges for CalTOX")

When the exposure time is much less than the lag time (greater than a factor of five), the AR_{water} ratio is adjusted to avoid overestimation:

$$AR_{water} = \frac{d_{skin} K_m}{2}\ x\ \frac{5\ x\ ET}{LT}$$

[72]

where:

ET = exposure time (hours/day); either exposure time in shower or bath (ET_{sb} divided by 2, Table III, "Parameter Values and Ranges for CalTOX") or exposure time swimming (ET_{sw}, Table III, "Parameter Values and Ranges for CalTOX")

LT = lag time (hours)

When the exposure time is greater than the lag time, the equation for the ratio is:

$$AR_{water} = \frac{d_{skin} K_m}{2} + (ET - LT) \; x \; K_p^w$$

[73]

where:

K^w_p = chemical-specific steady-state permeability coefficient from water into the stratum corneum (cm/hour); from equation 68 or 69

iii. Calculating the Dermal Uptake of a Chemical from Swimming in Contaminated Surface Water

The dermal uptake of a chemical from swimming in contaminated surface water is calculated using the specific parameter value for AR_{water}, calculated in equation 71, 72, or 73, for the product of permeability constant times exposure time, PC times ET. Other specific parameter values are the body surface area corrected for the fraction in contact with the water, and the appropriate exposure frequency value for swimming (EF_{sw}). With these specific parameters the uptake equation is:

$$Uptake_{swim} = C_w \; x \; AR_{water} \; x \left(f_{dc} \; x \; \frac{SA}{BW} \right) x \frac{EF_{sw} \; x \; ED}{AT} \; xCF$$

[74]

where:

$Uptake_{swim}$ = Uptake of chemical of concern by an exposed individual via dermal contact with surface water while swimming (mg chemical/ kg body weight per day)

C_w = concentration of chemical in surface water (mg/L)

AR_{water} = absorption ratio of dermal uptake of a chemical to concentration of the chemical in water (mg/cm^2 skin per mg/cm^3 water) (from equation 71, 72, or 73)

f_{dc} = fraction of body surface area assumed to be in contact with water during swimming, equivalent to one (unitless)

SA/BW = body surface area per kg body weight (m^2/kg body weight) (Table II, "Parameter Values and Ranges for CalTOX")

EF_{sw} = exposure frequency for swimming (episodes/year),

ED = exposure duration (years),

AT = averaging time (days),

CF = conversion factor (10 L/(cm times m^2).

In this equation, it is assumed that EF_{sw}, the exposure frequency for swimming, given in Table III, "Parameter Values and Ranges for CalTOX", in days/year, is equal to episodes/year.

iv. Calculating the Dermal Uptake of a Chemical from Bathing or Showering in Contaminated Tap Water

In calculating the dermal uptake of a chemical from bathing in contaminated tap water, the concentration of the chemical in tap water (C_{drink}) must be appropriately corrected if tap water is a mixture of surface water and ground water (see Section C.1.a. Ingestion of Tap Water). The following equation is used to calculate the concentration of the chemical in tap water:

$$C_{drink} = f_q^w \, x \, C_q + (1 - f_q^w) \, x \, C_w \quad [75]$$

where:

C_{drink} = chemical concentration in drinking water

f^w_q = fraction of water needs provided by ground water (Table III, "Parameter Values and Ranges for CalTOX")

C_q = chemical concentration in ground water

C_w = chemical concentration in surface water

With the specific parameters for bathing or showering in contaminated tap water, the uptake equation is:

$$Uptake_{bath} = C_{drink} \; x \; AR_{water} \; x \; \frac{SA}{BW} \; x \; \frac{EF_{sb} \; x \; ED}{AT} \; x \; CF$$

[76]

where:

$Uptake_{bath}$ = Uptake of chemical of concern by an exposed individual via dermal contact with drinking water while showering or bathing (mg chemical/ kg body weight per day)

C_{drink} = concentration of chemical in drinking water (mg/L)

AR_{water} = absorption ratio of dermal uptake of a chemical to concentration of the chemical in water (mg/cm^2 skin per mg/cm^3 water)

SA/BW = body surface area per kg body weight (m^2/kg body weight) (Table II, "Parameter Values and Ranges for CalTOX")

EF_{sb} = exposure frequency for bathing or showering (episodes/year),

ED = exposure duration (years),

AT = averaging time (days),

CF = conversion factor (10 L/(cm times m^2).

The combined uptake of chemical from dermal contact with contaminated water while bathing or swimming is given by:

$$Uptake_{bathsw} = Uptake_{swim} + Uptake_{bath}$$

[77]

b. Dermal Uptake from Contaminated Soil

The RAGS/HHEM equation for dermal contact with chemicals in soil (U.S. EPA 1989b, page 6-41) may be written as follows:

$$Uptake_{soil} = C_g \; x \; \frac{AF \; x \; ABS \; x \; SA}{BW} \; x \; FC \; x \; \frac{EFxED}{AT} \; x \; CF$$

[78]

where:

Uptake$_{soil}$ = Uptake of chemical of concern by an exposed individual via dermal contact with contaminated soil (mg chemical/kg body weight per day)

C_g = concentration in surface soil of chemical of concern (mg/kg),

AF = soil to skin adherence factor (mg/cm^2),

ABS = dermal absorption factor (unitless),

SA = skin surface area available for contact (m^2),

BW = body weight (kg),

FC = fraction of soil on skin which is contaminated soil (unitless),

EF = exposure frequency (events/year),

ED = exposure duration (years),

AT = averaging time (days), and

CF = conversion factor (10^{-6} kg/mg)

In this equation, the contact rate per body weight (CR/BW) term has been replaced by parameters for soil adherence, absorption of chemical by the skin, and skin surface area available for contact. Values for the ratio, SA/BW, are found in Table II, "Parameter Values and Ranges for CalTOX". The CalTOX equation includes a fraction contacted (FC) parameter as a modification to the RAGS/HHEM equation.

RAGS/HHEM recommends using chemical-specific values for absorption of the chemical from soil to skin and soil-type specific adherence factors. These values are often not available in the scientific literature. Therefore, the CalTOX dermal exposure model provides a series of equations to calculate:

1) K^s_p, the permeability (or absorption) of the chemical from soil into the stratum corneum from the octanol-water partition coefficient, K_{ow}, of the chemical, and

2) AR_{soil}, the ratio of uptake of the chemical by skin to the soil concentration, based on soil adherence, exposure time per exposure event, and K^s_p (soil-to-skin permeability).

These calculations are used to specify the ABS and AF parameters of equation 78 and are discussed in depth in McKone and Howd (1992).

i. Calculating Soil-to-Skin Permeability

The equation for soil-to-skin permeability is:

$$K_p^s = \frac{K_m^{soil}}{K_m} \; x \; K_p^w \; x \; 1.7$$

[79]

where:

K^s_p = chemical-specific soil to skin permeability coefficient (cm/hour)

K^{soil}_m = skin-soil partition coefficient, the ratio of concentration of the chemical in stratum corneum to the concentration of the chemical in soil (cm^3 soil/cm^3 skin) (Table V, "Parameter Values and Ranges for CalTOX")

K_m = skin-water partition coefficient, the ratio of concentration of the chemical in stratum corneum to the concentration of the chemical in water (cm^3 water/cm^3 skin) (Table V, "Parameter Values and Ranges for CalTOX")

K^w_p = chemical-specific steady-state permeability coefficient from water into the stratum corneum (cm/hour) (equation 68 or 69)

1.7 = conversion factor to adjust for skin thickness differences in different media (fully hydrated skin in water vs less hydrated skin in contact with soil) (cm^3 water/ cm^3 soil)

This calculated K^s_p value is input into the AR_{soil} equation below.

ii. Calculating the Ratio of the Uptake of the Chemical by Skin to Concentration of the Chemical in Soil

The ratio of the uptake of a chemical by skin from dermal contact with contaminated soil to the chemical concentration in soil is dependent on the thickness of the soil layer on the skin, the soil-skin permeability, and the exposure time. The equation is:

$$AR_{soil} = d_{soil}\ x \left[1 - \exp\left(- \frac{K_p^s\ x\ ET_{sl}}{d_{soil}} \right) \right]$$

[80]

where:

AR_{soil} = the ratio of the dermal uptake of the chemical during the exposure time, ET_{sl}, to the concentration of the chemical in soil (mg/cm^2 skin per mg/cm^3 soil)

δ_{soil} = the thickness of the soil layer on skin (cm)

K^s_p = soil to skin permeability (cm/hour)

ET_{sl} = exposure time per exposure event (hour/day)

The equation for AR_{soil} differs from that found in McKone and Howd (1992). The correction factor for volatilization into the air has been eliminated. The soil available for contact with the skin would be the ground surface soil. Therefore, all of the chemical that would volatilize would have already volatilized. Therefore, the measured or modeled concentration in that soil would have already accounted for that process.

iii. Calculating the Dermal Uptake of a Chemical from Contact with Contaminated Soil

The dermal uptake of a chemical from contact with contaminated soil is calculated using the specific parameter value for AR_{soil}, given in equation 80, for the soil to skin adherence factor (AF) and the dermal absorption factor (ABS). Other specific parameter values are the body surface area corrected for the fraction in contact with soil, and the appropriate exposure frequency value for soil contact (EF_{sl}). With these specific parameters the uptake equation is:

$$Uptake_{soil} = C_g \; x \; AR_{soil} \; x \left(f_{soil} \; x \frac{SA}{BW} \right) x \frac{EF \; x \; ED}{AT} \; x \; CF$$

[81]

where:

$Uptake_{soil}$ = Uptake of chemical of concern by an exposed individual via dermal contact with contaminated soil (mg chemical/kg body weight per day)

C_g = concentration in surface soil of chemical of concern (mg/kg),

AR_{soil} = the ratio of the dermal uptake of the chemical during the exposure time, ET_{sl}, to the concentration of the chemical in soil (mg/cm^2 skin per mg/cm^3 soil) (equation 80),

f_{soil} = fraction of skin surface area in contact with contaminated soil (unitless),

SA = skin surface area available for contact (m^2),

BW = body weight (kg),

FC = fraction of soil on skin which is contaminated soil (unitless),

EF = exposure frequency (days/year),

ED = exposure duration (years),

AT = averaging time (days), and

CF = conversion factor (15 kg/cm per m^2), based on a soil density of 1500 kg/m^3.

Values for the ratio, SA/BW, are found in Table II, "Parameter Values and Ranges for CalTOX".

4. TOTAL EXPOSURE INTAKE

In the CalTOX exposure model, intakes calculated for each exposure pathway considered are summed by route (ingestion intake, inhalation intake, dermal uptake) to get route specific intake values (see Section B.3 and Table I, "Parameter Values and Ranges for CalTOX").

The exposure pathways by which the chemical in each environmental compartment can contribute to ingestion, inhalation, and dermal uptakes are tabulated below:

Air (gases and particles):

1) inhalation of gases and particles in outdoor and indoor air
2) ingestion of produce contaminated by chemicals transferred from air (either as vapor or particles)
3) ingestion of meat, dairy products, and eggs contaminated by inhalation of chemicals in air (either as vapor or particles) by meat, dairy, and egg-producing animals or by ingestion by these animals of feed contaminated by chemicals transferred from air

Surface and Root-Zone Soil:

1) inhalation of surface soil resuspended in air as dust
2) inhalation of vapors from root-zone soil
3) ingestion of produce contaminated by chemicals transferred from surface or root-zone soil
4) ingestion of meat, dairy products, and eggs contaminated by chemicals in surface or root-zone soil by direct ingestion of soil by these animals and by ingestion of feed contaminated by chemicals transferred from soil
5) incidental ingestion of surface soil
6) dermal contact with surface soil

Ground and Surface Water:

1) inhalation indoors of chemicals volatilizing from ground water or from surface water used for bathing, showering, washing dishes, etc.
2) ingestion of ground water or surface water as drinking water
3) ingestion of produce contaminated by chemicals transferred from irrigation water
4) ingestion of meat, dairy products, and eggs contaminated by ingestion of chemicals in ground or surface water by meat, dairy and egg-producing animals
5) ingestion of fish and seafood contaminated by chemicals in surface water

6) ingestion of surface water during swimming and other water recreation

7) dermal contact with ground or surface water while bathing, showering or swimming

In the CalTOX exposure model, intakes calculated for the inhalation, ingestion and dermal uptake routes are summed by environmental compartment to get the potential intake for each compartment (air, surface soil, root-zone soil, ground water, surface water).

D. RISK CHARACTERIZATION

1. CONVERTING PATHWAY SPECIFIC INTAKES TO RISKS AND HAZARDS

In RAGS/HHEM (U.S. EPA 1989b, Section 8.2.1) equations are provided for quantifying carcinogenic and noncarcinogenic effects. Carcinogenic effects are expressed as the incremental probability (or risk) of an individual developing cancer over a lifetime as a result of exposure to a potential carcinogen. The equation is:

$$Risk = Chronic\ \ Daily\ \ Intake\ x\ \ Slope\ \ Factor$$

[82]

where:

Risk = the probability of an individual developing cancer (unitless)

Chronic Daily Intake = the intake averaged over an averaging time (AT) of 70 years (mg chemical/kg body weight per day)

Slope Factor = a constant which converts intake averaged over a lifetime to an incremental risk of developing cancer ((mg chemical/kg body weight per day)$^{-1}$)

The chronic daily intake is given by the intake equations provided in Section C above when 70 years (or a lifetime) is the parameter value used for the averaging time (AT). A cancer-causing chemical (carcinogen) may have a different slope factor for different routes of exposure; that is, the inhalation slope factor for a chemical may be different from the ingestion slope factor for the same chemical. Therefore, the CalTOX exposure model first calculates the chronic daily intake for each exposure route by summing the intakes for all pathways involving that route. Second, inhalation, ingestion, and dermal slope factors are chosen and entered into the CalTOX model as three separate slope factors. Then, the route-specific slope factor is multiplied by the calculated route-specific intake to get the risk for that route (inhalation, ingestion, dermal contact). Cancer slope factors for specific chemicals have been calculated and listed by the California Environmental Protection Agency (Cal/EPA 1992), the Integrated Risk Information System (IRIS) of the U.S. Environmental Protection Agency (U.S. EPA 1992c), and the Health Effects Assessment Summary Tables (HEAST) of the U.S. Environmental Protection Agency (U.S. EPA 1992d). Most of these slope factors have been calculated from administered or applied doses and, thus, are based on intakes reasonably equivalent to the intakes calculated from the equations given in the RAGS/HHEM (U.S. EPA 1989b) and in this manual.

Noncarcinogenic effects are not expressed in the probabilistic terms of risk but are expressed as a direct comparison of the exposure intake value to a chemical-specific reference dose. When the intake value used is for a specific chemical in a specific exposure pathway, the ratio is called a hazard quotient and is expressed as follows:

$$\textit{Noncancer Hazard Quotient} = \frac{\textit{Intake}}{\textit{Reference Dose}} \qquad [83]$$

where:

Noncancer Hazard Quotient =	ratio of the exposure intake value to a reference dose or concentration (unitless)
Intake =	the intake over a specific exposure duration (mg chemical/kg body weight per day)
Reference dose =	a level of exposure at or below which adverse health effects are unlikely to occur (mg chemical/kg body weight per day)

In this ratio, the intake and reference dose values must be in the same units, must reflect the same route of exposure (inhalation, ingestion, or dermal), and must represent the same exposure duration (chronic, sub-chronic, short-term). In the CalTOX exposure model this equation is used to calculate only chronic noncarcinogenic hazards (exposure duration of approximately seven years). Reference doses for chronic exposures via the inhalation or oral routes are available from the Integrated Risk Information System (IRIS) of the U.S. Environmental Protection Agency (U.S. EPA 1992c) and the Health Effects Assessment Summary Tables (HEAST) of the U.S. Environmental Protection Agency (U.S. EPA 1992d). The input parameter for the reference dose into the CalTOX model is in mg chemical/kg body weight per day. Therefore, if the desired reference dose is given in terms of a reference concentration, such as, mg chemical per volume of air, that reference concentration must be converted to mg chemical/ kg body weight per day for entry into the CalTOX model. The CalTOX exposure model does not segregate hazard quotients by mechanism of action or toxic endpoint.

The CalTOX multiple pathway exposure model uses these equations to calculate the carcinogenic risk and noncarcinogenic hazards associated with exposure to a chemical and in the concentrations predicted for the various environmental media at the site. The intake values used are calculated from the intake equations described in Section C, and the chemical-specific toxicity values (cancer slope factors, reference doses, or reference concentrations) are obtained from the state of California or the U.S. EPA.

The CalTOX model does not consider absorption in calculating either ingestion or inhalation intakes. Therefore, for those circumstances where a slope factor or reference dose is based on an absorbed dose, the intakes calculated by the model must be corrected for absorption outside the model. The corrected intakes are compared to criteria values based on absorbed doses outside the model.

2. SUMMING THE RISKS AND HAZARDS

In RAGS/HHEM (U.S. EPA 1989b, Sections 8.2.2 and 8.3) instructions are provided for assessing multiple chemicals at a site and for combining risks and hazards across exposure pathways. In RAGS/HHEM, the risks and hazards for each chemical are calculated for each exposure pathway; these are summed to obtain a pathway-specific risk or hazard; and, the pathway-specific risks or hazards are again summed to obtain the total cancer risk or noncarcinogenic hazard from exposure to multiple chemicals.

The CalTOX exposure model provides a chemical-specific exposure assessment, considering all pathways by which exposure occurs. For each chemical, the pathway-specific intakes are first summed by route of exposure (inhalation, ingestion, or dermal contact). For carcinogens, the route-specific risk is then calculated by multiplying the intake by the chemical- and route-specific slope factor (equation 82). For noncarcinogens, the route-specific hazard quotient is calculated by dividing the intake by the chemical- and route-specific reference dose (equation 83). Finally, the risk or hazard for each route is summed to get the total cancer risk or the total chronic hazard index posed by exposure to the chemical present at the site. To determine the total risk or hazard of exposure to multiple chemicals, the chemical-specific risks or hazards are summed outside the model.

E. SOIL REMEDIATION LEVELS

In this manual, a soil remediation level refers to a target level of a chemical of concern in the soil which is considered to be protective of human health and which is derived from risk assessment or risk-based calculations. This term is synonymous with the concept of preliminary remediation goals described in the U.S. EPA Risk Assessment Guidelines for Superfund, Human Health Evaluation Manual (RAGS/HHEM), Part B (U.S. EPA 1991), except for the following. A different mathematical model is used to relate soil concentration to the daily dose of a chemical, as described below; and multiple exposure pathways are considered in calculating preliminary soil remediation levels in the CalTOX model, whereas, the goals described in Part B RAGS/HHEM are based on a limited number of pathways.

1. CALCULATION OF PRELIMINARY REMEDIATION GOALS IN THE RISK ASSESSMENT FOR SUPERFUND/HUMAN HEALTH EVALUATION MANUAL (PART B)

In the Risk Assessment Guidance for Superfund: Volume I - Human Health Evaluation Manual (RAGS/HHEM), Part B, Development of Risk-Based Preliminary Remediation Goals, instructions are provided for calculating risk-based preliminary remediation goals (Chapter 3).

For carcinogenic effects, the total risk for a specific chemical in a specific environmental compartment is calculated by summing the risks from all pathways which involve that environmental compartment (such as the ingestion of ground water and the inhalation of vapors from ground water). As shown in equation 82, the risk is equal to the cancer slope factor multiplied by the chronic daily intake. The risk equation is expanded to include the intake equation, which, in turn, includes the concentration of the chemical and the exposure parameters. Therefore, the total risk equation may be rearranged to solve for the concentration of the chemical in the environmental compartment which would correspond to a target risk.

For noncarcinogenic effects, a hazard index for a chemical in a specific environmental compartment is calculated by summing the hazard quotients of that chemical for all exposure pathways involving the environmental compartment (see equation 83). Since the hazard quotient includes intake, the hazard index equation is expanded to include chemical concentration and exposure parameters. Then, the hazard index equation is rearranged to solve for the concentration of chemical in the environmental compartment which would correspond to a target hazard index level. By using the appropriate exposure parameter values, these total risk and hazard index equations calculate the risk-based remediation goals for soil (the environmental compartment of concern at most hazardous waste sites) for the land use scenarios of interest (residential, industrial, commercial, etc.).

2. CALCULATION OF SOIL REMEDIATION LEVELS IN THE CALTOX EXPOSURE MODEL

The CalTOX exposure model simplifies the calculations summarized above and provided in Part B of RAGS/HHEM. A major assumption of the CalTOX model in Part II, transport and transformation, is that the environmental compartment of soil serves as the primary reservoir of contamination at most hazardous waste sites. From soil, chemicals of concern can move to other environmental compartments (air, ground and surface water), and to other exposure media (personal air, drinking water). Since all exposure intakes calculated in the CalTOX exposure model are ultimately connected to or based upon the present soil concentration, the equation for determining the target soil remediation levels for a chemical at a site may be derived from the following ratio:

$$\frac{TargetSoilConcentration}{TargetRisk} = \frac{PresentSoilConcentration}{CalculatedRisk}$$

[84]

Therefore:

$$TargetSoilConcentration = \frac{PresentSoilConcentration}{CalculatedRisk} \ x \ TargetRisk$$

[85]

where:

Target Soil Concentration = the soil remediation level of the chemical of concern (mg/kg soil)

Target Risk = the risk considered to be protective of the health of the population on the site (unitless)

Present Soil Concentration = the measured or estimated concentration of chemical in soil at the site (mg/kg soil)

Calculated Risk = the risk associated with the present soil concentration of the chemical of concern (unitless)

For noncarcinogenic effects, the equations are:

$$\frac{TargetSoilConcentration}{TargetHI} = \frac{PresentSoilConcentration}{CalculatedHI}$$

[86]

and, therefore:

$$TargetSoilConcentration = \frac{PresentSoilConcentration}{CalculatedHI} \ x \ TargetHI$$

[87]

where:

Target soil concentration = the soil remediation level of the chemical of concern (mg/kg soil)

Target HI = the hazard index considered to be protective of the health of the population on the site (unitless)

Present Soil Concentration = the measured or estimated concentration of chemical in soil at the site (mg/kg soil)

Calculated HI = the hazard index associated with the present soil concentration of the chemical of concern (unitless)

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APPENDIX A: TERMINOLOGY

Terms used in this manual are defined below. These definitions are based primarily on RAGS/HHEM (U.S. EPA 1989b) and EPA Guidelines for Exposure Assessment (U.S. EPA 1992b).

Absorbed Dose. The amount of chemical penetrating the exchange boundaries of an organism after contact. Also referred to as the internal dose. Absorbed dose is calculated from the intake and absorption efficiency. It is usually expressed as the mass of chemical absorbed into the body per unit body weight per unit time such as mg/kg/day. For inhalation exposure, absorbed dose is the amount of chemical that is retained in the body after inhalation exposure. For ingestion exposure, absorbed dose is the rate of chemical that passes from the gastrointestinal tract across the gut wall and into the blood stream. For dermal exposure, absorbed dose is the rate of chemical that passes through the stratum corneum into the living cells of the epidermis and then into the blood stream (U.S. EPA 1989b).

Applied Dose. The rate of a chemical in mg/kg/day that comes in contact with the living tissue of an individual by entering into the lungs, by entering the gastrointestinal tract, and/or by contacting the skin (U.S. EPA 1992b). Identical to administered dose as defined in RAGS/HHEM (U.S. EPA 1989b).

Contact Rate. Amount of an environmental medium (air, water, soil, food) contacted by the body per unit time or per event, such as liters of water ingested per day (U.S. EPA 1989b).

Environmental Compartment (or medium). Air, surface soil, root-zone soil, surface water, or ground water.

Environmental Compartment Chemical Concentration. The measured or estimated concentration of chemical in the environment. These concentrations are distinct from the exposure media concentrations. The following are the abbreviations used in this manual for this term:

$C_{environm}$ = generic abbreviation for concentration of a chemical in an environmental compartment

C_a in mg/m^3 = the chemical concentration in ambient air gases;

C_{ap} in mg/m^3 = the concentration of chemical bound to all air particles (dust);

C_g in mg/kg = chemical concentration in surface soil (to a depth of 1 cm or 0.4 inches);

C_s in mg/kg = chemical concentration in root-zone soil below the surface layer (1 cm to approximately 1 m in depth or 0.4 inches to 39 inches);

C_q in mg/L = chemical concentration in ground water;

C_w in mg/L = chemical concentration in surface water.

Exposed Produce. Above ground edible plant parts including leafy vegetables and grains. Examples include cabbage, cauliflower, brocooli, celery, lettuce, spinach, apples, pears, berries, cucumber, grapes, peaches, tomatoes. These produce can potentially intercept chemicals from the air, as well as from soil and water (McKone, 1992).

Exposure. Contact of a chemical with the outer boundary of a human (skin, nose, mouth, skin punctures, and lesions) (U.S. EPA 1992b).

Exposure Factor. A parameter, such as body weight, breathing rate, or a time/activity factor, that may be needed to calculate human exposure to a contaminant.

Exposure (or Contact) Medium. The medium with which a human population has contact, such as, personal air, tap water, foods, household dusts, soils.

Exposure Medium Chemical Concentration. The concentration of chemical in the medium with which a human population has contact. The following are the abbreviations used in this manual to define this term:

$C_{exposure}$ = generic abbreviation for concentration of a chemical in an eexposure medium

C_{drink} = the chemical concentration in tap (or drinking) water (mg/L)

C_{fvg} = the chemical concentration in fruits, vegetables, and grains (mg/kg plant fresh mass)

C^{abga}_{fvg} = the chemical concentration on fruits, vegetables and grains exposed to the chemical in ambient air (mg chemical/kg plant fresh mass)

C^{abgw}_{fvg} = concentration of the chemical in above ground fruits, vegetables, and grains exposed to the chemical in irrigation water (mg chemical/kg plant fresh mass)

C^{abg}_{fvg} = concentration of the chemical on fruits, vegetables and grains exposed to the chemical in ambient air, irrigation water, and soil (mg chemical/kg plant fresh mass)

C^{protp}_{fv} = chemical concentration of protected produce contaminated by water and root-zone soil (mg chemical/ kg plant fresh mass)

C_{fish} = concentration of chemical of concern in fish or shellfish (mg/kg fish)

C_{mke} = concentration of chemical of concern in meat, milk products, or eggs (mg/kg food),

C_{meat} = the concentration of chemical of concern in meat (mg/kg meat)

C_{milk} = the concentration of chemical of concern in milk and dairy products (mg/kg milk)

C_{eggs} = concentration of chemical of concern in eggs (mg/kg eggs)

C_{bmilk} =concentration of chemical of concern in breast milk (mg/L)

C_{dust} = concentration in personal air of chemical of concern adhered to airborne particulate phase (mg/m^3 air); equivalent to C_{ap}

C_{vapor} = concentration in personal air of chemical of concern in vapor phase (mg/m^3 air); equivalent to C_a

C^{indoor}_{dust} = concentration in personal air of chemical of concern adhered to airborne particulate phase (mg/m^3 air)

C^{indoor}_{vapor} = concentration in personal air of chemical of concern in vapor phase (mg/m^3

air)

C_{pairsb} = concentration in personal air of chemical of concern in vapor phase in the shower or bathroom (mg/m^3 air)

C_{pairh} = concentration in personal air of chemical of concern in vapor phase resulting from general household water use (mg/m^3 air)

Exposure Pathway. The course a chemical or physical agent takes from a source to an exposed organism. An exposure pathway describes a unique mechanism by which an individual or population is exposed to chemicals or physical agents at or originating from a site. Each exposure pathway includes a source or release from a source, an exposure point, and an exposure route. If the exposure point differs from the source, the transport/exposure medium (such as air) or media (in cases of intermedia transport, such as water to air) are also included (U.S. EPA 1989b).

Exposure Point. A geographical location of potential contact between an organism and a chemical or physical agent (U.S. EPA 1989b).

Exposure Route. The way a chemical or physical agent comes in contact with an organism, i.e., inhalation, ingestion, dermal contact (U.S. EPA 1989b).

Intake. A measure of exposure expressed as the mass of a substance that crosses an outer boundary (mouth, nose, intact or broken skin) of the body per unit body weight per unit time, that is, mg chemical/kg/day. This definition differs slightly from the definition given in RAGS/HHEM (U.S. EPA 1989b), where intake is defined as the mass of a substance in contact with the exchange boundary (gastrointestinal tract, lungs, skin). In this manual, "intake" should be considered equivalent to the following terms common in other EPA documents: normalized exposure rate, administered dose, average daily dose, and applied dose.

Inter-media Transfer Factor. The ratio of the chemical concentration in the exposure medium to the chemical concentration in the environmental compartment for which there is a measurement.

Usually represented by an appropriate chemical-specific partition coefficient (a K value, see Table V for examples) or calculated from compartment models.

Population at Risk. The people who do or plausibly could inhabit, visit, work, or trespass on the location that is in the vicinity of the source of contamination.

Protected Produce. Root crops and produce protected from the environmental compartment of ambient air (but exposed to soil and water). Examples include carrots, beets, turnips, potatoes, legumes, melons (McKone, 1992).

Soil Remediation Level. A target level of a chemical of concern in the soil which is considered to be protective of human health and which is derived from risk assessment or risk-based calculations.

Uptake. The absorption of a chemical into the skin or other exposed tissue. Although the chemical is often contained in a carrier medium, the medium itself is typically not absorbed at the same rate as the chemical. In this manual, dermal exposure is calculated as dermal uptake and does not represent absorption from the skin into the blood stream.

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