CAirTOX: A Compartment Model for Assessing the Fate of and Human Exposure to Toxic- Chemical Emissions to Air

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Prepared for:

The California Air Resources Board

and

The Office of Environmental Health Hazard Assessment

California Environmental Protection Agency

October 1993

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FORWARD AND ACKNOWLEDGEMENTS

As part of an effort to improve the Health Risk Assessment (HRA) computer program developed by the State of California Air Resources Board (ARB), the objectives of this report are to improve the current mathematical model used to estimate the relationship of chemical concentrations in air to concentrations in the air, soil, water, and food with which human populations have contact. The report describes research performed at the University of California, Lawrence Livermore National Laboratory (LLNL) to support this objective. This work was performed under the auspices of the U.S. Department of Energy (DOE) through LLNL as part of the Risk Sciences Program under Contract W-7405-Eng-48 with funding provided by the ARB through Contract Agreement A147-111.

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INTRODUCTION

Risk assessment is a quantitative evaluation of information on potential health hazards of environmental contaminants and the extent of human exposure to these contaminants. As applied to toxic chemical emissions to air, risk assessment involves four interrelated steps. These are (1) determination of source concentrations or emissions characteristics, (2) exposure assessment, (3) toxicity assessment, and (4) risk characterization. These steps can be carried out with assistance from analytical models in order to estimate the potential risk associated with existing and future releases.

CAirTOX has been developed as a spreadsheet model to assist in making these types of calculations. CAirTOX follows an approach that has been incorporated into the CalTOX model, which was developed for the California Department of Toxic Substances Control (McKone, 1993a, 1993b, 1993c). With CAirTOX, we can address how contaminants released to an air basin can lead to contamination of soil, food, surface water, and sediments. The modeling effort includes a multimedia transport and transformation model, exposure scenario models, and efforts to quantify uncertainty in multimedia, multiple-pathway exposure assessments. This overall process is illustrated in Figure 1.

The multimedia transport and transformation model is a steady-state, but non-equilibrium model that can be used to assess concentrations of contaminants released continuously to air. This model assists the user in examining how chemical and landscape properties impact both the ultimate route and quantity of human contact. Using this model, we view the environment as a series of interacting compartments. The model allows the user to determine whether a substance will (a) remain or accumulate within the compartment of its origin, (b) be physically, chemically, or biologically transformed within the compartment of its origin (i.e., by hydrolysis, oxidation, etc.), or (c) be transported to another compartment by cross-media transfer that involves dispersion or advection (i.e., volatilization, precipitation, etc.).

Multimedia, multiple-pathway exposure models are used in CAirTOX to estimate average daily doses within a human population in a region having toxic chemicals released to its air. The exposure assessment process consists of relating contaminant concentrations in the multimedia compartments of the model to contaminant concentrations in the media with which a human population has

Figure 1. The relationship between source-medium concentration (e.g., air), subsequent concentrations in other environmental media, toxicology, and exposure pathways.

contact (personal air, tap water, foods, household dusts, soils, etc.). The average daily dose is the product of the exposure concentrations in these contact media and an intake or uptake factor that relates the concentrations to the distributions of potential dose within the population.

The remainder of this report is divided into five parts. In Part I, we describe the multimedia transport and transformation model used to determine the fate of air emissions. In Part II, we describe inputs and data needs for CAirTOX and the development of a set of landscape factors, which can be used to represent regional air basin/water-shed systems in California. In Part III, we describe the multiple-pathway exposure scenarios and exposure algorithms. In Part IV, we compare the HRA approach and results and the CAirTOX exposure equations. We provide a summary table for the exposure scenarios in CAirTOX and compare these to the exposure scenarios in HRA. In Part V, we consider model sensitivity and uncertainty to determine how variability and uncertainty in model inputs affects the precision, accuracy, and credibility of the model output.

PART I. THE TRANSPORT AND TRANSFORMATION MODEL

The multimedia-compartment model consists of seven compartments for assessing the fate of air emissions in a regional air basin. These compartments are air, surface soil, root-zone soil, plant leaves, plant roots, surface water, and sediments. This compartment model provides an algorithm for calculating contaminant concentrations in air, water, and biota based on a defined steady-state concentration in air or a continuous input to air. The steady-state solution is based on a constant contaminant concentration in the air compartment. It is important to note that, in contrast to other models used for assessing environmental fate, this model imposes conservation of mass on the air-basin/water-shed systems. In addition, the model accounts systematically for gains and losses in each compartment and for the whole system in concert. This type of approach avoids many of the errors and omissions that exist in many multimedia models. The resulting model is tractable and credible.

Efforts to assess human exposure from multiple media date back to the 1950's when the need to assess human exposure to global fallout led rapidly to a framework that included transport both through and among air, soil, surface water, vegetation, and food chains (Whicker and Kirchner, 1987). Efforts to apply such a

framework to nonradioactive organic and inorganic toxic chemicals have been more recent and have not as yet achieved the level of sophistication extant in the radioecology field. In an early book on multimedia transport, Thibodeaux (1979) proposed the term "chemodynamics" to describe a set of integrated methods for assessing the cross-media transfers of organic chemicals. The first widely used multimedia compartment models for organic chemicals were the "fugacity" models proposed by Mackay (1979, 1991) and Mackay and Paterson (1981, 1982). Cohen and his co-workers introduced the concept of the multimedia compartment model, MCM, (Cohen and Ryan, 1985) as a screening tool and more recently introduced the spatial multimedia compartment model (SMCM) model (Cohen et al., 1990), which allows for nonuniformity in some compartments. However, neither of these models explicitly addresses human exposure. Another multimedia screening model, called GEOTOX (McKone and Layton, 1986; McKone, et al., 1987), was one of the earliest multimedia models to explicitly address human exposure.

Model Structure

Three dynamic processes must be balanced in a multimedia model—sources, transport, and transformation. Knowledge of source-term characteristics is an important first step in the multimedia analysis. Pertinent information includes the physical and chemical properties of the substance(s) released and attributes of the source (e.g., emission rates). Sources can be categorized in terms of space (e.g., area source vs. point source), time (e.g., transient vs. chronic release), and mode of formation.

CAirTOX is a seven-compartment-, regional-, dynamic- and multimedia-fugacity model. The fugacity approach is best suited to nonionic organic chemicals for which partitioning is related strongly to chemical properties, such as vapor pressure, solubility, and the octanol-water partition coefficient. However, CAirTOX has been designed to also handle ionic organic contaminants, inorganic contaminants, radionuclides, and metals, with a modified fugacity-type approach. For all species, fugacity and fugacity capacities are used to represent mass potential and mass storage within compartments.

The seven-compartment structure used in CAirTOX is illustrated in Figure 2. The seven CAirTOX compartments are (1) air, (2) ground-surface soil, (3) root-zone

Figure 2. Mass-exchange processes modeled in a seven-compartment environmental transport model.

soil, (4) plant leaves, (5) plant roots (6) surface water, and (7) sediments. It is important to restate here that, in contrast to many models used for assessing environmental fate, CAirTOX imposes conservation of mass on the contaminated landscape unit. In addition, the model accounts systematically for gains and losses in each compartment and for the whole system in concert.

Fugacity Models

Fugacity models have been used extensively for modeling the transport and transformation of nonionic organic chemicals in complex environmental systems (see Mackay, 1991). Modified fugacity and fugacity-type models have also been used for ionic-organic and inorganic species, including metals. Fugacity is a way of representing chemical activity at low concentrations. Fugacity has units of pressure [pascal (Pa)] and can be regarded physically as the partial pressure or escaping potential exerted by a chemical in one physical phase or compartment on another (Mackay, 1979, 1991; Mackay and Paterson, 1981, 1982). When two or more media are in equilibrium, the escaping tendency (the fugacity) of a chemical is the same in all phases. This characteristic of fugacity-based modeling often simplifies the mathematics involved in calculating partitioning. Fugacity models can also be used to represent a dynamic system in which the fugacities in two adjacent media are

changing in time due to an imbalance of sources and losses, or a dynamic system that has achieved steady state by balancing gains and losses even though fugacities are not equal.

At low concentrations, like those typical of environmental interest, fugacity, f (Pa), is linearly related to concentration C (mol/m³) through the fugacity capacity, Z (mol/m³-Pa),

$$C = fZ . \quad (1)$$

Z depends on the physical and chemical properties of the chemical and on various characteristics of phase, such as temperature and density. The property that fugacities are equal at equilibrium allows for simple determination of Z values from partition coefficients. For example for two phases in equilibrium (phases 1 and 2),

$$C_1/C_2 = fZ_1/fZ_2 = Z_1/Z_2 = K_{12} , \quad (2)$$

where C_1 and C_2 are the concentrations in each phase, Z_1 and Z_2 are the fugacity capacities of each phase, and K_{12} is a dimensionless partition coefficient, such as K_{ow} , the octanol-water partition coefficient. One of the major advantages of fugacity models is the ease with which they represent diffusive and advective intermedia-transport processes. In a fugacity model, the net diffusive flux, in mol/m²-d, across an interface is given by

$$flux = Y_{12} (f_1 - f_2) , \quad [3]$$

where Y_{12} is the fugacity mass-transfer coefficient across the boundary between medium 1 and medium 2 with units mol/(m²-Pa-d) and f_1 and f_2 are the fugacities of medium 1 and medium 2. Equation [3] is analogous to the flow of electrons in a circuit, in which $(f_1 - f_2)$ acts as a voltage difference, Y_{12} acts as a conductance, and the mass flux serves as the equivalent of electrical current. The fugacity mass-transfer coefficient depends only on the mass transfer coefficient on either side of the interface.

$$Y_{12} = \left(\frac{1}{Z_1 U_1} + \frac{1}{Z_2 U_2} \right)^{-1} , \quad [4]$$

where U_1 and U_2 are the mass-transfer coefficients (m/d) in the boundary layers in medium 1 and medium 2 and Z_1 and Z_2 are the fugacity capacities of medium 1 and medium 2. The net advective flux between medium 1 and medium 2 is given by

$$flux = Z_{water} [F_{12}^W f_1 - F_{21}^W f_2] + Z_{1p} F_{12}^P f_1 - Z_{2p} F_{21}^P f_2 \quad [5]$$

where Z_{water} is the fugacity capacity of water, mol/m³-Pa; F_{12}^W is the flux of water from medium 1 to 2, m³/m²-d; F_{21}^W is the flux of water from medium 2 to 1, m³/m²-d; Z_{1p} and Z_{2p} are, respectively, the fugacity capacities of the solid phases of media 1 and 2, mol/m³-Pa; F_{12}^P is the flux of solids from medium 1 to 2, m³/m²-d; and F_{21}^P is the flux of solids from medium 2 to 1, m³/m²-d.

Intermedia Transfer Factors (ITFs)

Multimedia models also require that we measure or estimate solid/liquid phase partition coefficients between soil and soil water and between surface water and sediments; air/liquid partition coefficients; and the diffusion coefficients of substances in air and water. A companion report to this one (McKone et al., 1993) describes methods for estimating the intermedia transfer factors needed for the CAirTOX model.

The exchange of contaminants at the boundary between two environmental compartments that are made up in part of fluids in motion (i.e., air or water) involves advection (e.g., deposition, washout, etc.) and two modes of diffusion—molecular diffusion within a thin boundary layer and turbulent diffusion within the bulk of the compartment. In a compartment such as the atmosphere, in which turbulent mixing is rapid and continuous, molecular diffusion will only be significant at boundaries with other less turbulent compartments, such as soil and surface water. At these boundaries the air makes a transition from a well-mixed turbulent fluid to an essentially zero velocity boundary. In a multimedia model, it is assumed that turbulent diffusion within a compartment, such as the lower atmosphere, is so efficient that the bulk concentration is simply the compartment inventory divided by the compartment volume. However, at the boundary between two compartments, modeling of diffusive mass transfer must include both turbulent and molecular processes that can not be lumped or assumed away at these transition zones.

The Seven CAirTOX Compartments

In this section, we describe the seven CAirTOX compartments in terms of their mass, volume, and the characteristics that influence advection and diffusion at the boundaries of each compartment. We put particular emphasis on those factors that determine whether a substance will (a) remain or accumulate within the compartment, (b) be physically, chemically, or biologically transformed within the compartment, or (c) be transported to another compartment by cross-media transfer that involves dispersion or advection. In the remaining sections of this report, we often refer to these compartments using a single letter representations as follows: air (a), ground-surface soil (g), root-zone soil (s), plant leaves (l), plant roots (r), surface water (w), and sediments (d).

The Lower-Atmosphere or Air Compartment (a)

Substances in outdoor (or ambient) air are dispersed by atmospheric advection and diffusion. The volume and mass of the air compartment is defined by the area of the contaminated landscape and the mixing height of the lower atmosphere. Meteorological parameters have an overwhelming influence on the behavior of contaminants in the lower atmosphere. Among them, wind parameters (direction, velocity, and turbulence) and thermal properties (stability) are the most important. A simple approach to the dispersion of substances in the atmosphere is based on the application of a mass balance to a volume element, such as a parcel or box of air. This gives rise to the "box" models for atmospheric dispersion. In this approach, the region to be studied is divided into cells or boxes. The concentration in each box is assumed to be uniform and is a function of the box volume, the rate at which material is being imported, emission rates within the box, and the rate at which material is exported from the box. Gifford and Hanna (1973) have shown that in a simple box model, the yearly average concentration of contaminant within the box is proportional to the source strength in mass per unit area divided by the wind speed. Based on data from U.S. cities, they have developed for both gases and particles proportionality coefficients that can be used to estimate long-term contaminant concentrations. The air-compartment model in CAirTOX is based on the box-model approach.

The Ground-Surface-Soil Compartment (g).

Soil, the thin outer zone of the earth's crust that supports rooted plants, is the product of climate and living organisms acting on rock. A true soil is a mixture of air, water, mineral, and organic components. The relative mix of these components determines to a large extent how a chemical will be transported and/or transformed within the soil. The movement of water and contaminants in soil is typically vertical as compared to horizontal transport in the ground-water (i.e., saturated) zone. A chemical in soil partitions among soil water, soil solids (mineral and organic phases), and soil air. For example, the rate of volatilization of an organic compound from soil depends on the partitioning of the compound into the soil air and on the porosity and permeability of the soil. Soils are characteristically heterogeneous. A trench dug into the soil zone reveals typically several horizontal layers having different colors and textures. These multiple layers are often divided into three major horizons: the A horizon, which encompasses the root zone and contains a high concentration of organic matter; the B horizon, which is unsaturated, is below the roots of most plants, and contains a much lower organic carbon content; and the C horizon, which is the unsaturated zone of weathered parent rock consisting of bedrock, alluvial material, glacial material, and/or soil of an earlier geological period (Bowen, 1979).

Studies of radioactive fallout in agricultural land-management units reveal that, in the absence of tilling, particles deposited from the atmosphere accumulate in and are resuspended from a thin ground-surface-soil layer with a thickness in the range 0.1 to 1 cm (Whicker and Kirchner, 1987). The ground-surface-soil layer is at the top of the A soil horizon. The ground-surface-soil layer has a lower water content and higher gas content than underlying layers. Contaminants in this surface-soil layer are transported horizontally by mechanical runoff and soil-solution runoff to nearby surface waters. Surface-soil contaminants are susceptible to wind erosion, volatilization, photolysis, biodegradation, and transfer to plant surfaces by rainsplash. These contaminants are transferred to and from the root-zone soil by diffusion and leaching.

The Root-Zone-Soil Compartment. (s)

Contaminants in the A horizon below the surface layer, that is, in the root-zone soil, are transported upward by diffusion, volatilization, root uptake, and capillary motion of water; transported downward by diffusion and leaching; and transformed chemically primarily by biodegradation or hydrolysis. Soil-water

content in the root zone is somewhat higher than that in surface soils, because the presence of clay in this layer serves to retain water. The roots of most plants are confined within the first meter of soil depth. In agricultural lands, the depth of plowing is 15 to 25 cm. In addition, the diffusion depth, which is the depth below which a contaminant is unlikely to escape by diffusion, is on the order of a meter or less for all but the most volatile contaminants (Jury et al., 1990).

The Plant-Leaves Compartment (l)

The dominant component of the terrestrial biota compartment is land plants. Plants generally have contact with two environmental media—air and soil. Plant interactions with these media are not understood well enough to define an accurate method of predicting chemical uptake. The translocation of chemicals from soils appears to be a relatively minor pathway for the accumulation of these compounds in plants (Fiedler *et al.*, 1991). In the absence of experimental studies, there has been a reliance on simple bioconcentration factors (BCFs) that relate either a soil or air concentration to a plant concentration. The earliest use of vegetation BCFs was for assessing the effects of global fallout by relating concentrations of radionuclides in plants to concentrations in soil (Ng, 1982). More recently, vegetation BCFs have been proposed for organic chemicals (Travis and Arms, 1988). What is meant by the “concentration in a plant” is difficult to define in large plants where roots, stems, and leaves each may have different chemical concentrations. In the CAirTOX model, plant leaves are modeled as a single biota compartment consisting of air, water, and plant lipids. The fugacity capacity of this compartment is based on a simplified version of the model proposed by Paterson and Mackay (1989).

The Plant-Roots Compartment (r)

Plant roots have contact with roughly the top meter of the soil column. The plant-root hairs penetrate the pore spaces of soil in order to bring water and nutrients into the plant. Typically, only chemical species available in the soil water are capable of entering the plant from the root. Contaminants bound to the organic phase of soil cannot be transferred directly into the plant. Once contaminants have entered the root compartment, they can be transferred to the plant leaves by translocation in the xylem solution. In the CAirTOX model, plant roots are modeled as a single biota compartment consisting of air, water, and plant lipids. The fugacity capacity of this compartment is based on a simplified version of the model proposed by Paterson and Mackay (1989).

The Surface-Water Compartment (w)

The behavior of chemicals in surface waters is determined by two factors—the rate of physical transport in the water system and chemical reactivity. Physical transport processes are dependent to a large extent on the type of water body under consideration—oceans, seas, estuaries, lakes, rivers, or wetlands. Schnoor (1981) and Schnoor and MacAvoy (1981) have summarized important issues relating to surface-water transport. Fugacity models have been developed by Mackay et al. (1983a) for lakes and also by Mackay et al. (1983b) for rivers.

At low concentration, contaminants in natural waters exist in both a dissolved and a sorbed phase. In slow-moving surface waters, both advection and dispersion are important. In rapidly moving water systems, advection controls mass transport and dissolved substances move at essentially the same velocity as the bulk water in the water system. Contaminants that are sorbed to colloidal material and fine suspended solids can also be entrained in water currents, but they may undergo additional transport processes that alter their effective residence time in surface waters. Such processes include sedimentation and deposition and scouring and resuspension. Thus, determining the transport of contaminants in surface waters requires that we follow both water movement and deposition and resuspension from sediment.

A water balance is the first step in assessing surface-water transport. A water balance is established by equating gains and losses in a water system with storage. Water can be stored within estuaries, lakes, rivers, and wetlands by a change in elevation or stage. Water gains include inflows (both runoff and stream input) and direct precipitation. Water losses include outflows and evaporation.

In CAirTOX the surface-water compartment is composed of two phases, pure water and suspended sediment material that contains the sorbed contaminants. Surface waters are assumed to be well-mixed systems. The surface-water velocity relative to area, depth, and volume determines the residence time of the pure-water phase. The effective residence time of suspended sediments is determined by both the residence time of the water phase and the deposition and resuspension rates of the sediments. Contaminants in surface water are transported into this compartment by deposition from air, by runoff from soil, and by diffusion and resuspension from the sediment layer. Contaminants in surface water are transported out of this compartment by advection in both the liquid and sediment

phases, by diffusion to air at the upper surface of the water body and by diffusion and deposition to sediments.

Contaminants in surface water are also taken up by aquatic organisms and this can also impact the distribution of these contaminants. In CAirTOX, the modeling of contaminant transport in surface water is based on the assumption that essentially all the contaminant mass is in either liquid or suspended-solid phases. This assumption implies that a very small fraction of the total compartment inventory is distributed among aquatic species. However, this does not imply that there are low concentrations in these organisms. Quite the contrary is often the case.

The Sediment-Zone Compartment (d)

This compartment represents the porous, active layer of water and solid material that forms at the bottom of the surface-water compartment primarily as a result of sediment and organic-matter deposition from the surface water above. Reuber et al. (1991) note that the bottom sediments of surface-water bodies have at least two distinct layers—an active layer characterized by a high degree of chemical and biological activity and a deeper, inactive layer in which chemicals are essentially isolated from the water column.

Deposition, resuspension, burial, diffusion, oxidation, and biotransformation are continuous processes that impact the inventory of contaminants in bottom sediments. Deposition of mineral matter and organic matter from surface water to sediments is a continuous process in any water body and an important mechanism for transferring particle-bound contaminants to the sediment layer. In any water system, some of the deposited material is resuspended by water currents, which depend on the hydrology of the system. In lakes, deposition is typically greater than resuspension and, in rivers, resuspension can equal or exceed deposition. Burial refers to the rate at which contaminants move from the active to the inactive layer. The pore water of the sediment layer together with the colloidal organic matter in this pore water provide vehicles for diffusion. Contaminants dissolved in the pore water or sorbed to the colloids can diffuse or migrate from sediments up to the water column or down to deeper sediment layers.

Physical Composition of Model Compartments and Fugacity Capacities

For each model compartment, we determine the fugacity capacity of the total compartment from the sum of the volume-fraction-weighted fugacity capacities of the constituent phases—air, water, particles, and lipids.

Fugacity Capacities in Pure Air, Pure Water, and Particles

The fugacity capacity in units of mol/m³-Pa for a nonionic organic chemical in pure air, Z_{air} , is given by

$$Z_{\text{air}} = 1/RT , \quad [6]$$

where R is the universal gas constant, 8.314 Pa-m³/mol-K, and T is temperature in kelvins (K).

The fugacity capacity in units of mol/m³-Pa for a nonionic organic chemical in pure water, Z_{water} , is given by

$$Z_{\text{water}} = 1/H , \quad [7]$$

where H is the Henry's law constant, Pa-m³/mol, which expresses the ratio of equilibrium activities of a chemical in air (expressed as vapor pressure, Pa) and in water (mol/m³) when the two phases are well mixed.

A chemical in the solid or particle phase of soils, sediments, and surface waters has a fugacity capacity given by

$$Z_{ip} = K_{di} \times \rho_{si} \times Z_{\text{water}} \times \frac{1 \text{ m}^3 \text{ water}}{1000 \text{ L water}} , \quad [8]$$

where Z_{ip} is the fugacity capacity of the pure solid phase, mol/m³-Pa; i refers to the compartment name (i.e., a , g , b , s , etc.); K_{di} represents, for compartment i , the sorption coefficient, which is the ratio at equilibrium of chemical concentration attached to particles (mol/kg) to chemical concentration in the solution, mol/L; and ρ_{si} is the density of the actual particles in kg/m³ (not the bulk density of the particles when mixed in solution).

In the air compartment contaminants bound to aerosol particles achieve equilibrium with gas-phase contaminants. The derivation here of the fugacity capacity of aerosol particles is based on a model originally developed by Junge (1977)

but used frequently by others (for example, Cohen and Ryan, 1985; Mackay et al., 1986; Pankow, 1987; Ryan and Cohen, 1986). In this model the fraction of contaminant bound to aerosol particles, ϕ , is given by

$$\phi = \frac{c\theta}{(VP + c\theta)} \quad [9]$$

where, θ is the total suspended particle surface area concentration in m^2/m^3 , VP is the vapor pressure of the pure contaminant in Pa, and c is an approximate constant that Junge (1977) sets equal to 0.173 m-Pa. Whitby (1978) reports values for θ ranging from $4.2 \times 10^{-5} \text{ m}^2/\text{m}^3$ for a clean continental site to $1.1 \times 10^{-3} \text{ m}^2/\text{m}^3$ for urban sites. Following the recommendation of Mackay et al. (1986), we use the sub-cooled liquid vapor pressure to estimate the fugacity capacity of air particles. The fugacity capacity for air particles, Z_{ap} in $\text{mol}/\text{m}^3\text{-Pa}$, is derived from equation [9] by noting that

$$f_{\text{vap}} \times Z_{ap} / Z_{\text{air}} = \frac{c\theta}{VP} \quad [10]$$

where f_{vap} is the volume fraction of the air that is occupied by air particles. Under the assumption that the particle load in the air is $100 \mu\text{g}/\text{m}^3$ and that particle density is $1500 \text{ kg}/\text{m}^3$, this fraction is 6.7×10^{-11} . Substituting this value into equation [10] with θ equal to $1.1 \times 10^{-3} \text{ m}^2/\text{m}^3$, c equal to 0.173 m-Pa, and Z_{air} equal to $1/RT$ gives

$$Z_{ap} = \frac{3 \times 10^6}{VP \times RT} \quad [11]$$

This expression is similar to one derived by Mackay et al. (1986) using a somewhat different approach. For contaminants that exist as solids at ambient temperatures, it is not clear whether the vapor pressure, VP is that of the sub-cooled liquid, or the vapor pressure of the solid, should be used (Mackay et al. 1986; Mackay, 1991; Taylor, 1992). Following the recommendation of Mackay et al. (1986) for solids we use the vapor pressure of the subcooled liquid, which is equal to the vapor pressure of the solid times $\exp [6.79 (T_m/T - 1)]$, where T_m is the melting point of the compound and T is the ambient temperature.

Fugacity Capacity of the Air Compartment

In the air compartment, the total fugacity capacity, Z_a in mol/m³-Pa, is composed of the volume-weighted average of the fugacity capacities of its two constituent phases, air and air particles,

$$Z_a = Z_{\text{air}} + (f_{\text{vap}} \times Z_{\text{ap}}) , \quad [12]$$

where f_{vap} is the volume fraction of particles in air. The volume fraction of the gas phase is essentially unity.

Fugacity Capacity of Plants Leaves

Riederer (1990) has shown that, for foliar uptake of gas-phase organic contaminants, the most general form of a steady-state plant-air partition model is

$$K_{\text{pa}} = f_{\text{pa}} + (f_{\text{pw}} + f_{\text{pl}} \times K_{\text{ow}}) \times \frac{RT}{H} , \quad [13]$$

where K_{pa} is the ratio of contaminant concentration in plant tissue to that in air, mol/m³ per mol/m³; f_{pa} is the volume fraction of plant tissue that is air; f_{pw} is the volume fraction of plant tissue that is water; f_{pl} is the volume fraction of the plant tissue that is lipid; R is the universal gas constant, 8.31 Pa-m³/mol-K; T is the temperature in kelvins (293 K); and H is the Henry's law constant of the contaminant in Pa-m³/mol. Based on azalea-leaf experiments with five chemicals, Bacci et al. (1990) have developed a correlation of leaf-air bioconcentration factors with air-water and octanol-water partition coefficients and have shown that f_{pl} is on the order of 0.01. Paterson and Mackay (1989) have estimated that f_{pa} is 0.5. This implies that the remainder of the plant volume fraction, 0.49, is either water or non-lipid solids. Based on our assumption that 80% of total plant mass is water, we set f_{pw} equal to 0.4. These assumptions together with the recognition that K_{pa} is the ratio of plant fugacity capacity to air fugacity capacity—that is, Z_l/Z_{air} or $Z_l \times RT$ —leads to the following expression to estimate the plant fugacity capacity Z_l for organic chemicals in plant tissue relative to air,

$$Z_l = \frac{0.5}{RT} + (0.4 + 0.01 \times K_{\text{ow}}) \times Z_{\text{water}} . \quad [14]$$

Fugacity Capacity of Plants Roots

The fugacity capacity of plant-root tissues relative to soil can be related to the plant-soil partition coefficient, K_{ps} , which expresses the ratio of contaminant concentration, mol/kg, in the fresh mass of vegetation to the contaminant concentration in the root-zone soil, mol/kg. This means K_{ps} is equal to $(Z_p \rho_{bs}) / (Z_s \rho_p)$, where ρ_{bs} is the soil bulk density in kg/m³ and ρ_p is the plant density, assumed to be 1000 kg/m³. For nonionic organic chemicals, there are methods for estimating K_{ps} or Z_p from chemical solubility in the absence of measured data. Briggs et al. (1982, 1983) have developed an equation to estimate uptake of contaminants by roots from soil solution. They refer to this partition coefficient as the root concentration factor, RCF. It represents the ratio of contaminant concentration in root tissue, mol/kg(fresh mass), to contaminant concentration in soil solution, mol/kg, and it takes the form

$$RCF = 0.82 + (0.03 K_{ow}^{0.77}) . \quad [15]$$

We note that RCF is the ratio of plant-root fugacity capacity to soil-solution fugacity capacity, that is, Z_r / Z_{water} (or $Z_r \times H$). This means that equation [15] leads to the following expression for estimating the plant-root fugacity capacity Z_r ,

$$Z_r = (0.82 + 0.03 \times K_{ow}^{0.77}) \times Z_{water} . \quad [16]$$

It is of interest that, based on experiments that measured chemical uptake from air to leaves and experiments that measured chemical uptake from soil solution to roots, the implied fugacity capacity of plants in both cases as expressed by, respectively, equations [14] and [16], are quite similar.

For inorganic species and ionic organic compounds, we estimated Z_l and Z_r as

$$Z_l = Z_r = K_{ps} \times Z_{soil} / \rho_{bs} . \quad [17]$$

As a rule, for inorganic species and ionizing organic compounds, K_{ps} should be obtained from measured data. In the absence of measured data, we obtain K_{ps} by assuming that the contaminant concentration in plant water is equal to that in soil water so that K_{ps} is equal to $(1 - bio_{dm}) / K_{ds}$, where bio_{dm} is the dry-mass fraction of plants and $(1 - bio_{dm})$ is the water-mass fraction of the plants.

Fugacity Capacity of the Soil Compartment

For the soil compartments, which have air, water, and solid components all at the same fugacity, the total compartment fugacity capacities are the volume-weighted average of the fugacity capacities of three component phases. For ground-surface and root-zone soil; these compartment fugacities are, respectively, Z_g , and Z_s , in mol/m³-Pa. As an example, for the root-zone soil compartment (s), the equation describing the overall fugacity capacity of this compartment is

$$Z_s = \alpha_s Z_{\text{air}} + \beta_s Z_{\text{water}} + (1 - \phi_s) Z_{\text{sp}} , \quad [18]$$

where α_s is the volume fraction of air in the soil compartment, β_s is the volume fraction of water in the compartment, $(1 - \phi_s)$ is the volume fraction of solid in the compartment, $\phi_s (= \alpha_s + \beta_s)$ is the total void fraction in soil, and Z_{sp} is the fugacity capacity of the soil particles, mol/m³-Pa.

Fugacity Capacity of Surface Water

In the surface-water compartment the total fugacity capacity, Z_w in mol/m³-Pa, is composed of the volume-weighted average of the fugacity capacities of its two constituent phases, water and suspended particles,

$$Z_w = Z_{\text{water}} + (\rho b_w / \rho_{\text{sw}}) \times Z_{\text{wp}} \quad [19]$$

where ρb_w is the suspended particle load in surface water, kg/m³, ρ_{sw} is density of the suspended-particle material, kg/m³, and Z_{wp} is the fugacity capacity of the particles and given by

$$Z_{\text{wp}} = K_{\text{dw}} \times \rho_{\text{sw}} \times Z_{\text{water}} \times \frac{1 \text{ m}^3 \text{ water}}{1000 \text{ L water}} , \quad [20]$$

in which K_{dw} represents the sorption coefficient of suspended particles, L/kg. The volume fraction of suspended particles in water is assumed to be so small that the volume fraction of the water phase is essentially unity.

Fugacity Capacity of Sediment

In the sediment compartment the total fugacity capacity, Z_d in mol/m³-Pa, is composed of the volume-weighted average of the fugacity capacities of its two constituent phases, sediment particles and water,

$$Z_d = \beta_d \times Z_{\text{water}} + (1-\beta_d) \times Z_{dp} , \quad [21]$$

where β_d is the void fraction of the sediment compartment, $1-\beta_d$ is the volume fraction of sediment particles in the sediment compartment, and Z_{dp} is the fugacity capacity of the sediment layer particles and given by

$$Z_{dp} = K_{dd} \times \rho_{sd} \times \frac{1 \text{ m}^3 \text{ water}}{1000 \text{ L water}} , \quad [22]$$

in which K_{dd} represents the sorption coefficient of sediment layer particles, L/kg.

Modifications to Fugacity Capacities for Inorganic and Ionic-Organic Chemicals

The traditional fugacity approach was developed for nonionic organic chemicals. The modifications described here make possible the treatment of inorganic species (including radionuclides), metals, and fully ionized organic species. In order to make these adjustments, it should be recognized that the basic premise of the fugacity approach is that the mass potential of any compartment can be scaled to a single phase through a series of partition coefficients. In the traditional fugacity approach this scaling is $1/RT$. However, for chemicals that have extremely low vapor pressure and relatively high water solubility this leads to the problem of having extremely large fugacity capacities in water. To avoid this problem for chemicals with very low vapor pressure, such as inorganic chemicals and speciated or ionized organic chemicals, we assume that these chemicals can be described by zero fugacity in air, that is, $Z_{\text{air}} = 0$. We then set the fugacity capacity of water, Z_{water} , equal to 1 mol/m³-Pa. This approach has been used by Mackay and Diamond (1989) and Diamond et al. (1992) for inorganic species in lakes. They refer to this modification as "equivalence." This leads to a scaling of other phases and compartment fugacity capacities based on the fugacity capacity of the water phase. Thus, as above, the fugacity capacity of the particles of compartments ($i=g, s, w, d$) is of the form

$$Z_{ip} = K_{di} \times \rho s_i \times Z_{water} \times \frac{1 \text{ m}^3 \text{ water}}{1000 \text{ L water}} , \quad [23]$$

and, since Z_{air} is now assumed equal to zero, the fugacity capacity of air particles becomes the same as that of the ground-surface-soil particles,

$$Z_{ap} = Z_{gp} = K_{dg} \times \rho s_g \times Z_{water} \times \frac{1 \text{ m}^3 \text{ water}}{1000 \text{ L water}} . \quad [24]$$

Transport Processes in the CAirTOX Model

In a multimedia model, major components of the environment are lumped into homogeneous subsystems or compartments that can exchange mass with other adjacent compartments. Mass flows among compartments include solid-phase flows, such as dust suspension or deposition, and liquid-phase flows, such as surface runoff and ground-water recharge. In the previous section, we considered the use of fugacity to describe how each chemical species is partitioned among the phases within a single compartment. The nature of this partitioning in combination with mass flows at compartment boundaries defines the overall rate of cross-media transfer of contaminants between any two adjacent compartments. The transport of individual chemical species among compartments occurs by diffusion and advection at the compartment boundaries. The modeling of these two processes is described in this section.

As was noted earlier in this report, one of the major advantages of fugacity models is their ability to more easily represent diffusive transfer. In a fugacity model, the net diffusive flux, in mol/m²-d, across the interface described above is

$$\text{net flux at the surface} = Y_{aw} (f_a - f_w) , \quad [25]$$

where Y_{aw} is the fugacity mass-transfer coefficient across the boundary between air and water with units mol/(m²-Pa-d) and f_a and f_w are the fugacities of air and water. Y_{aw} acts as a conductance, and the difference in fugacities is the mass potential driving mass transfer across this boundary. The overall fugacity mass-transfer coefficient depends only on the mass-transfer coefficient on either side of the interface.

$$Y_{aw} = [1/(Z_a U_a) + 1/(Z_w U_w)]^{-1} . \quad [26]$$

It should be noted that the overall fugacity mass-transfer coefficient, Y_{aw} , is related to the air-side fugacity mass-transfer coefficient for this interface, Y_{aw}^a , and the water-side fugacity mass-transfer coefficient for this interface, Y_{aw}^w . These mass-transfer coefficients have units of $\text{mol}/(\text{m}^2\text{-Pa-d})$ and are given by

$$Y_{aw}^a = Z_a U_a = Z_a \frac{D_{air}}{\delta_{aw}} \quad [27]$$

and

$$Y_{aw}^w = Z_w U_w = Z_w \frac{D_w}{\delta_{wa}}, \quad [28]$$

where D_{air} is the diffusivity in the air compartment, m^2/d ; δ_{aw} is the boundary-layer thickness in the air above water, m ; where D_w is the effective diffusivity in the water compartment, m^2/d ; and δ_{wa} is the boundary-layer thickness in the water below the air, m . The relationships derived in this section for mass transfer at the air-water interface can be generalized to mass transfer at air-soil, soil-soil, and water-sediment interfaces.

Diffusive Mass Transfer at the Air and Surface-Water Interface

The exchange by diffusion of organic chemicals between the lower atmosphere and surface-water bodies is an important component of the overall rate constant defining transport between air and water. The exchange of chemicals between air and water bodies depends on both the physicochemical properties of the contaminant and the physical properties of the air and water compartments involved. Important physicochemical properties include solubility, molecular weight, vapor pressure, and diffusion coefficients in air and water. The important landscape properties include temperatures of air and water, wind speed, water-flow velocity, water depth, and water turbulence.

The air-side fugacity mass transfer coefficient, Y_{aw}^a , and the water-side fugacity mass-transfer coefficient, Y_{aw}^w , for the air-water interface are given by equations [27] and [28]. These mass-transfer coefficients have units of $\text{mol}/(\text{m}^2\text{-Pa-d})$. Lyman et al. (1982) have reviewed several methods for estimating water-side and gas-side mass transfer coefficients for atmosphere-surface water exchange of organic chemicals. In CAirTOX, the estimation of the water-side boundary mass-transfer

coefficient, $D_{\text{water}}/\delta_{\text{wa}}$, is based on methods developed by Southworth (1979) from laboratory data for chemicals with H in the range 1 to 100 Pa-m³/mol. When the surface-water current, current_w in m/s, is less than 0.04 times the wind velocity, v_w in m/s, to the 0.67 power, then $D_{\text{water}}/\delta_{\text{wa}}$ is 0.24 m/d. For larger surface-water currents and for land units in which the yearly average wind velocity, v_w , is less than 1.9 m/s,

$$D_{\text{water}}/\delta_{\text{wa}} = 5.64 \left(\frac{\text{current}_w^{0.969}}{d_w^{0.673}} \right) \sqrt{\frac{32}{MW_x}} \text{ m/d} , \quad [29]$$

where d_w is the average depth of the surface-water body in m and MW is the molecular weight of the contaminant. For land units in which the yearly average wind velocity, v_w , is larger than 1.9 m/s,

$$D_{\text{water}}/\delta_{\text{wa}} = 5.64 \left(\frac{\text{current}_w^{0.969}}{d_w^{0.673}} \right) \sqrt{\frac{32}{MW_x}} e^{0.526 (v_w - 1.9)} \text{ m/d} . \quad [30]$$

For estimating the air-side mass-transfer coefficient, $D_{\text{air}}/\delta_{\text{aw}}$, we also used methods developed by Southworth (1979), based on laboratory data for chemicals with H in the range from 1 to 100 Pa-m³/mol. In this case the mass-transfer coefficient, D_a/δ_{aw} , in m/d, is given by

$$D_{\text{air}}/\delta_{\text{aw}} = 273 (v_w + \text{current}_w) \sqrt{\frac{18}{MW_x}} \text{ m/d} , \quad [31]$$

when the sum, $v_{\text{wind}} + \text{current}_w$, is greater than 0.5 m/s, and by

$$D_{\text{air}}/\delta_{\text{aw}} = 140 \sqrt{\frac{18}{MW_x}} \text{ m/d} , \quad [32]$$

when the sum, $v_{\text{wind}} + \text{current}_w$, is less than 0.5 m/s.

Diffusive Mass Transfer in Air at the Air and Ground-Surface Soil Interface

Diffusive mass transfer at the soil-air interface accounts for both net volatilization of contaminants from soil and deposition of gas-phase contaminants to the ground-surface-soil layer. Once again, net mass transfer depends on mass

transfer through both the air-side and ground-soil-side boundary layers. The fugacity mass transfer coefficient on the air side of the air-ground-soil interface is given by

$$Y_{ag}^a = Z_a \frac{D_{air}}{\delta_{ag}}, \quad [33]$$

where, δ_{ag} is the boundary layer thickness in the air above the ground-soil layer. This thickness is assumed to be on the order of 0.005 m. On smooth surfaces the boundary layer thickness varies from about 1 cm in still air to 1 mm when the air moves over the surface at 1 m/s.

Diffusive Mass Transfer in the Ground-Surface and Root-Zone Soil Layers

Because soil is not a well-mixed compartment such as air or surface water, the boundary-layer approach described above is not readily applicable to soil. The concentration gradient of contaminants may not level off for several meters. In well-mixed air and water compartments, the boundary layer thickness is on the order of centimeters. Cohen et al. (1990) have noted that the soil compartment in a multimedia model should include a spatial-diffusion model. Jury et al. (1990) have shown that the "limiting soil-cover depth" varies from 0.001 m (for chrysene) to 160 m (for dichlorodifluoromethane) in sandy soil and from <0.001 to 61 m for the same compounds in clay soil. The limiting soil depth is the thickness of soil that is required to limit volatilization loss over an infinite time to less than 1% of the initial concentration. This is the depth at which volatilization at the surface has essentially no impact on concentration. Above this depth, there is a gradient of concentration that will be controlled by the rate of evaporation at the surface of the soil.

There have been several approaches to the problem of devising a simple but accurate model of soil transport. In one of the more simple approaches, Mackay and Paterson (1991) use a diffusion-path length that is half the depth of the soil compartment as the boundary-layer thickness in their regional fugacity model. This value is independent of chemical species.

In CAirTOX we deal with the problem of nonuniform concentration in soils by using two soil layers to represent the region between the soil surface and the bottom of the "limiting soil layer depth". An approach developed by McKone (1993b) was used to determine an effective soil diffusion coefficients to estimate

boundary layer thicknesses in each of these two soil layers by an optimized fit against the more exact soil transport model of Jury et al. (1983). The optimization goal was to minimize the estimation error in the surface flux and compartment inventories predicted for the surface and root-zone soil layers relative to values obtained from the Jury et al. (1983) analytical solution. In effect, this procedure allows us to mimic the Jury et al (1983) model with a more simple regression model based on effective diffusivity. The price we pay for this increased simplicity is less precision. However, we can calculate this loss of precision and note that so long as it is comparable to the variability or uncertainty in characterizing the initial soil concentrations, it should not lead to significant degradation of the model reliability relative to the Jury et al. (1983) model from which it is derived. The following expressions were used to estimate the boundary layer thickness or diffusion length in CAirTOX,

$$\delta_g = 0.108 \times D_g^{0.229} \quad \text{and} \quad [34]$$

$$\delta_s = 318 \times D_s^{0.683} \quad [35]$$

In these expressions, δ_g and δ_s are the diffusion lengths (in m) in the ground-surface and root-zone-soil compartments and D_g and D_s are the effective diffusivities in these compartments (in m^2/d) as obtained from

$$D_i = \frac{Z_{\text{air}}}{Z_i} (\alpha_i^{10/3} / \phi_i^2) D_{\text{air}} + \frac{Z_{\text{water}}}{Z_i} (\beta_i^{10/3} / \phi_i^2) D_{\text{water}} \quad [36]$$

where i is replaced by g for ground-surface soil and by s for root soil; D_i is the effective tortuous, mixed-phase diffusion coefficient in soil zone i , the Z 's are the fugacity capacities derived previously, and other parameters are as defined previously.

Diffusive Mass Transfer at the Surface-Water and Sediment Interface

Diffusive mass transfer at the sediment-water interface accounts for the net volatilization of contaminants from sediment and deposition of dissolved contaminants to the sediment layer. In each case, total mass transfer depends on both the water-side and sediment-side boundary layers. The fugacity mass-transfer coefficient on the water side is given by

$$Y_{wd}^w = Z_w \frac{D_{\text{water}}}{\delta_{wd}} , \quad [37]$$

where Z_w is the fugacity capacity in the surface-water compartment, D_{water} is the effective diffusivity in the surface-water compartment, and δ_{wd} is the boundary-layer thickness in the water above the sediment layer. The fugacity mass-transfer coefficient on the sediment side is given by

$$Y_{wd}^d = Z_d \frac{D_d}{\delta_{dw}} , \quad [38]$$

where Z_d is the fugacity capacity in the sediment compartment, D_d is the effective diffusivity in the sediment compartment, and δ_{dw} is the boundary-layer thickness in the sediment layer below water. Formica et al. (1988) have described a method for calculating for the sediment layer effective diffusivity based on corrections for the solids content of sediment. This approach is similar to that used by Jury et al. (1983) as described in equation [36] with the volume fraction of the gas phase set to zero. We use fluxes of radon from the Hudson river estuary measured by Hammond et al. (1975) to estimate the water-side boundary-layer thickness. The reported flux is 200 atoms/m²-s above sediments with a concentration of radon in water of 2.6×10^9 atoms per m³ with a diffusion coefficient of 1.4×10^{-9} m²/s. This implies a boundary-layer thickness of 0.02 m, which is what we use in CAirTOX for the water-side boundary-layer thickness above sediments. For the boundary-layer thickness in sediments below the water column, we use equation [36] with d substituted for i .

Mass Transfer by Advection in Water and Solids

In CAirTOX, the cross-media transfer of contaminants by advection is treated as an advection flux. This flux is modeled as the product of the velocity of the moving phase times the contaminant concentration in that phase. This flux has units of mol/m²-d, the velocity of the moving phase is in m/d, and the concentration in the moving phase is the product of the contaminant fugacity in that phase, Pa, and the fugacity capacity of that phase in mol/m³-Pa,

$$\text{advection flux} = \text{velocity} \times Z_{ik} f_i , \quad [39]$$

where Z_{ik} and f_i represent the fugacity capacity of the moving phase and the fugacity, respectively, in compartment i . As an example, the flux of contaminant from air to surface soil through particle deposition is the product of deposition velocity, v_d ; the fugacity capacity of air particles, Z_{ap} ; and the total fugacity of the air compartment, f_a :

$$\text{flux (air to ground-surface soil)} = v_d \times Z_{ap} \times f_a \quad [40]$$

Advection processes used in the CAirTOX model include deposition of aerosol particles, resuspension of particles from soil, water-borne erosion of soil, rainfall, evaporation, runoff of precipitation, infiltration of water through soil, deposition of sediment particles in surface water, resuspension of sediment particles from the sediment layer, and surface water flows. The advective or nondiffusive flux terms used in the CAirTOX model are summarized in Table I.

Transformation Processes in the CAirTOX Model

The transformation of contaminants in the environment can have a profound effect on their potential for persistence. Chemical transformations, which may occur as a result of biotic or abiotic processes, can significantly reduce the concentration of a substance. For organic chemicals, knowledge of a compound's half-life for any given transformation process provides a very useful index of persistence in environmental media. Because these processes determine the persistence and form of a chemical in the environment, they also determine the amount and type of substance that is available for the exposure of species of interest. Experimental methods (Howard et al., 1978) and estimation methods (Lyman et al., 1982) are available for defining these fate processes in a variety of media. Specific information on the rates and pathways of transformation for individual chemicals of concern must be obtained directly from experimental determinations or derived indirectly from information on chemicals that are structurally similar. In CAirTOX, all removal reactions are modeled using a first-order rate constant with units of day^{-1} .

Table I. Advective or non-diffusive flux terms used for intermedia transfers in the CAirTOX model.

Intermedia Transfer	Description of the non-diffusive process	Formula
Air to ground-surface soil	Rain scavenging of gaseous contaminants from air to ground	$flux = rain \times Z_{water} \times f_a$
Air to plant leaves ^a	Wet and dry deposition of particle-bound species	$flux = F_v \times v_d \times Z_{ap} \times f_a$
Air to ground-surface soil ^a	Wet and dry deposition of particle-bound species	$flux = (1 - F_v) \times v_d \times Z_{ap} \times f_a$
Air to surface water	Rain scavenging of gaseous contaminants from air to ground	$flux = rain \times Z_{water} \times f_a$
Air to surface water	Wet and dry deposition of particle-bound contaminants	$flux = v_d \times Z_{ap} \times f_a$
From air compartment out of the system	Wind induced movement of the air mass out of the landscape boundary	$flux = Z_a \frac{0.23 \times v_w \times d_a}{\sqrt{Area}}$
Ground-surface soil to air	Resuspension of soil particles	$flux = v_d \times Z_{gp} \times f_g$
Ground-surface soil to root-zone soil	Leaching due to ground-water recharge	$flux = recharge \times Z_{water} \times f_g$
Ground-surface soil to surface water	Soil-solution runoff	$flux = runoff \times Z_{water} \times f_g$
Ground-surface soil to surface water	Erosion (mineral runoff) to surface water	$flux = erosion \times Z_{gp} \times f_g$
Root-zone soil to vadose-zone soil	Leaching due to ground-water recharge	$flux = recharge \times Z_{water} \times f_s$
Surface water to sediment	Sediment deposition	$flux = deposit \times Z_{wp} \times f_w$
From surface water out of the landscape	Surface-water outflow	$flux = outflow \times Z_w \times f_w$
Sediment to surface water	Sediment resuspension	$flux = resuspend \times Z_{dp} \times f_d$

^a F_v is the fraction of deposited material intercepted by vegetation and given by $1 - \exp(-2.8 \times bio_{inv}/2)$, where $bio_{inv}/2$ is the dry-mass inventory of above-ground biomass in kg/m^2 .

Transfer-Rate, Loss-Rate, and the Gain-Loss Equations

The steady-state equations describing gains and losses in each of the seven compartments are used to solve for the steady-state inventory in each compartment. Table II lists the gains and losses considered for each compartment. The following equations express losses and gains for each of the seven CAirTOX compartments.

$$S_a + T_{la} N_l + T_{ga} N_g + T_{wa} N_w = L_a N_a \quad (\text{air}) \quad [41]$$

$$T_{al} N_a + T_{gl} N_g + T_{rl} N_r = L_l N_l \quad (\text{plant leaves}) \quad [42]$$

$$T_{ag} N_a + T_{lg} N_l + T_{sg} N_s = L_g N_g \quad (\text{ground-surface soil}) \quad [43]$$

$$T_{gs} N_g = L_s N_s \quad (\text{root-zone soil}) \quad [44]$$

$$T_{sr} N_s = L_r N_r \quad (\text{plant root}) \quad [45]$$

$$T_{aw} N_a + T_{gw} N_g + T_{dw} N_d = L_w N_w \quad \text{and} \quad (\text{surface water}) \quad [46]$$

$$T_{wd} N_w = L_d N_d \quad (\text{sediments}) \quad [47]$$

In the equations above the N 's represent compartment inventories and the T_{ij} ($i, j = a, l, g, s, r, w$, or d) are transfer rate constants, with units of day^{-1} , that express fraction per unit time of the inventory of compartment i that is transferred to compartment j . The compartment abbreviations are a for air, l for plant leaves, g for ground-surface soil, s for root-zone soil, r for plant roots, w for surface water, and d for sediments. The product of an N term and a T term is the rate of change of inventory in mol/d . $L_i N_i$ represents all losses from compartment i , mol/d . The term S_a , in equation [41] is the rate of contaminant input to the air compartment, mol/d . In the sections below, the transfer-rate constants are defined in terms of landscape properties, chemical properties, fugacity capacities, and other parameters used to construct them and the loss-rate constants are defined in terms of transfer- and transformation-rate constants.

In terms of fugacity, the balance in mol/d is expressed as a loss from a compartment i and transfer to a compartment j in the form

$$\text{loss} = \text{Area} \times v_{ij} \times Z_{ik} \times f_i \quad [48]$$

Table II. Summary of the processes by which contaminants are exchanged and lost among the seven CAirTOX compartments.

Compartment	Gains	Losses
(1) Air (both the gas phase and particles of the troposphere)	diffusion from soil diffusion from plants diffusion from surface water resuspension of deposited soil particles <i>contaminant sources</i>	diffusion to ground-surface soil diffusion to surface water diffusion to plants washout by rainfall convection losses deposition to soil deposition to plants deposition to surface water chemical/physical transformation
(2) Plant leaves	deposition of particles from air foliar uptake	diffusion from leaf surfaces washoff from leaf surfaces chemical/physical transformation
(3) Ground-surface soil	diffusion from air diffusion from root-zone soil washout from air by rainfall dry deposition of air particles <i>contaminant sources</i>	diffusion to air diffusion to root-zone soil advection to root-zone soil soil solution runoff erosion (mineral runoff) to surface water resuspension of soil particles chemical/physical transformation
(5) Root-zone soil	diffusion from ground-surface soil advection from ground-surface soil plant decomposition	diffusion to ground-surface soil infiltration (leaching) to vadose-zone soil chemical/physical transformation
(6) Plant roots	Translocation from leaves root-uptake from root-zone soil	translocation to leaves plant decomposition
(6) Surface water	diffusion from air washout by rainfall deposition of atmospheric particles soil solution runoff erosion (mineral runoff) diffusion from sediment sediment resuspension	sediment deposition diffusion to air diffusion to sediment surface-water outflow chemical/physical transformation
(7) Sediment layer	diffusion from surface water sediment deposition (from surface water)	diffusion to surface water sediment resuspension chemical/physical transformation

where *Area* in m² is that across which mass exchange occurs, v_{ij} is the advection or diffusion velocity from *i* to *j* at the exchange boundary, and Z_{ik} is the fugacity capacity of the moving phase *k* from *i* to *j*, and f_i represents the fugacity of compartment *i*. Equation [48] can also be written as

$$loss = T_{ij} N_i , \quad [49]$$

in which

$$N_i = Z_i f_i V_i , \quad [50]$$

$$T_{ij} = \frac{area \times v_{ij}}{V_i} \frac{Z_{ik}}{Z_i} = \frac{v_{ij}}{d_i} \frac{Z_{ik}}{Z_i}, \text{ and} \quad [51]$$

V_i is the compartment volume, d_i is the compartment depth or thickness, and Z_i is the total fugacity capacity of compartment *i*. This is the general approach used in the sections below to obtain the transfer-rate constants.

Air (a)

The air compartment is represented by a simple box model in which losses include deposition to soil, vegetation, and surface water; convective losses; and transformation losses. In the box model used for air, the inventory, N_a in mol, is described by solving equations [41] to [47]. L_a is the sum of all loss-rate constants from the air compartment,

$$L_a = T_{al} + T_{ag} + T_{aw} + T_{ao} + R_a , \quad [52]$$

where $L_a N_a$ is the sum of all losses from the air compartment, mol/d; $T_{la} N_p$, $T_{ga} N_g$, and $T_{wa} N_w$ are the gains from plant leaves, ground soil, and water, mol/d; T_{ag} , T_{al} , and T_{aw} are the rate constants for deposition losses, to ground soil, plant leaves, and water, day⁻¹; T_{ao} is the rate constant for convective losses, day⁻¹ and R_a is the rate constant for transformation losses, day⁻¹.

According to Benarie (1980), the long-term average pollutant concentration in a region bordered by a box model with volume V_a and pollution source, S_a in mol/d, is given by

$$C_{air} = N_a / V_a = \frac{c S_a}{Area \times v_w} , \quad [53]$$

where c is a unitless proportionality constant; $Area$ is the area of the region being modeled, and v_w is the long-term average wind speed in m/d. This implies that the inverse of the rate constant, T_{ao} , is the convective residence time and is given by the expression, $c d_a / v_w$, where d_a is the atmospheric mixing height. Based on a model for area sources developed by Turner (1970), the constant c can be estimated as $4.3 \sqrt{Area} / d_a$, where $\sqrt{Area}$ is the cross-sectional length of an assumed square area containing the source S_a . Making the appropriate substitutions gives the following expression for the convective loss-rate constant in the air compartment:

$$T_{ao} = \frac{0.23 v_w}{\sqrt{Area}} \quad [54]$$

The rate constant, T_{ag} , accounts for gross diffusion, rain-water washout, and particle-deposition losses from air to ground-surface soil.

$$T_{ag} = (1 - f_{arw}) \times \frac{(Y_{ag} + rain \times Z_{water} + v_d \times Z_{ap} \times \frac{\rho b_a}{\rho s_g})}{(Z_a \times d_a)} \quad [55]$$

In this expression, f_{arw} is the fraction of land area that is covered by surface water; ρb_a is the particle loading in the air, kg/m³, and ρs_g is the particle density, kg/m³. If the land-unit area is greater than or equal to 6×10^8 m², then the air-compartment mixing depth, d_a , is 700 m; if the area is less than 6×10^8 m², then d_a is $0.22 (\sqrt{Area})^{0.8}$ (Hanna et al., 1982). The net diffusion from air ground-surface soil is given by $Y_{ag}(f_a - f_g)$. Thus, $Y_{ag} f_a$ is the gross diffusion from air to soil and $Y_{ag} f_g$ is the gross diffusion from ground-surface soil to air.

The rate constant, T_{aw} , accounts for gross diffusion, rain-water washout, and particle deposition losses from air to surface water and has the form

$$T_{aw} = f_{arw} \times \frac{(Y_{aw} + rain \times Z_{water} + v_d \times Z_{ap} \times \frac{\rho b_a}{\rho s_g})}{(Z_a \times d_a)} \quad [56]$$

The rate constant T_{al} is derived in the next section.

Plant Leaves (l)

The plant leaves compartment interacts with the air, ground-surface, and plant roots compartments. Its inventory in steady-state, N_p in mol, is described by equation [42]. L_l is the sum of all loss-rate constants from the plants compartment,

$$L_l = T_{la} + T_{lg} + R_p \quad [57]$$

where $L_l N_l$ is the sum of all losses from the plant-leaves compartment, mol/d; $T_{al} N_a$, $T_{gl} N_g$, and $T_{rl} N_r$ are the gains from air, ground soil, and plant-roots compartments, mol/d; T_{la} and T_{lg} , are the rate constants for diffusion losses to air and for losses due to washoff from leaves and from plant senescence, day^{-1} ; and R_l is the rate constant for transformation losses, day^{-1} .

The expressions relating transfer of contaminants from air to plant leaves allows for transfer by deposition of the gas phase from air (deposition velocity v_{dg} in m/d) and deposition of particles,

$$T_{al} = (1-f_{arw}) \frac{(v_{dg} \times Z_{air}) + (F_v \times v_d \times Z_{ap} \times \rho_{ba} / \rho_{sg})}{Z_a \times d_a} \quad [58]$$

The expressions relating transfer of contaminants from plant leaves to air is defined by requiring that the net effect of gas deposition and transfer, T_{la} , from air to leaves will, at steady state, result in a concentration ratio $C_l(\text{mol}/\text{m}^3)/C_{air}(\text{mol}/\text{m}^3)$ equal to $K_{pa} \times \rho_p$,

$$T_{la} = (1-f_{arw}) \frac{v_{dg} \times Area}{K_{pa} \times \rho_p \times V_l} \quad [59]$$

The expression defining the transfer-rate constant from leaf surfaces to ground surface accounts for washoff and plant decay and is assumed to be 0.029 day^{-1} (based on a residence time of 35 d),

$$T_{lg} = 0.029 \quad [60]$$

The expressions relating transfer of contaminants from ground soil to plant leaves is defined by requiring that the net effect of T_{lg} and T_{gl} is to move the ratio of

plant contamination on leaves relative to surface soil in the direction of the rainsplash partition coefficient, which has units of kg(soil)/kg(plant),

$$T_{gl} = K_{ps}^{\text{rain}} T_{lg} \frac{V_l}{V_g} \quad [61]$$

T_{rl} is described in the section below on the plant-roots compartment.

Ground-Surface Soil (g)

The ground-soil compartment represents the thin surface layer of soil in which losses include diffusion to air, diffusion to root-zone soil, infiltration to root-zone soil, runoff to surface water, rainsplash to plant surfaces, and transformation processes. The inventory, N_g , in mol of contaminant in the ground-soil compartment is described by equation [43]. L_g is the sum of all loss-rate constants from the ground-surface-soil compartment,

$$L_g = T_{ga} + T_{gl} + T_{gs} + T_{gw} + R_g , \quad [62]$$

where $L_g N_g$ is the sum of all losses from the ground-soil compartment, mol/d; $T_{ag} N_a$, $T_{lg} N_l$, and $T_{sg} N_s$ are the gains from air, plant leaves, and root-soil compartments, mol/d; T_{ga} , T_{gl} , T_{gs} , and T_{gw} are the rate constants for resuspension losses to air, for losses due to rainsplash and resuspension transfer from ground soil to plant leaves, for gross diffusion losses to air and to root soil, for advection losses due to rain-water infiltration and for runoff losses to surface water, day⁻¹; and R_g is the rate constant for transformation losses, day⁻¹. These loss-rate constants are given by

$$T_{ga} = \frac{Y_{ag} + v_d \times \rho b_a \times \frac{Z_{gp}}{\rho s_g}}{Z_g \times d_g} , \quad [63]$$

$$T_{gs} = \frac{\text{recharge} \times Z_{\text{water}} + Y_{sg}}{Z_g \times d_g} , \quad [64]$$

$$T_{gw} = \frac{\text{runoff} \times Z_{\text{water}} + \text{erosion} \times \frac{Z_{gp}}{\rho s_g}}{Z_g \times d_g}, \text{ and} \quad [65]$$

$$\text{recharge} = \text{rain} \times (1 - f_{arw}) - \text{evapotrans} - \text{runoff} \quad [66]$$

Equation [63] reflects the assumption that resuspension of soil particles is, on average, equal to deposition. T_{sg} is taken up below in the section on the root-zone soil. Other parameters in these expressions have been defined previously.

Root-Zone-Soil compartment (s)

The root-zone-soil compartment represents the layer of soil in which losses include gross diffusion to ground-surface soil, uptake by vegetation, infiltration to vadose-zone soil, and transformation processes. The inventory, N_s in mol, of contaminant in the root-zone-soil compartment is described by equation [44]. L_s is the sum of all loss-rate constants from the root-zone-soil compartment,

$$L_s = T_{sr} + T_{sg} + T_{so} + R_s, \quad [67]$$

where L_s is the sum of all losses from the root-soil compartment, mol/d; T_{sg} is the gain by diffusion and infiltration from the ground-soil compartment, mol/d; T_{sr} , T_{sg} , and T_{sv} are the rate constants for uptake losses to plant roots, for gross diffusion losses to ground soil, and for diffusion and advection losses to deeper soil, day⁻¹; and R_s is the rate constant for transformation losses, day⁻¹. These loss-rate constants are given by

$$T_{sg} = \frac{Y_{sg}}{Z_s \times d_s} \quad [68]$$

$$T_{sr} = (1 - f_{arw}) \frac{\text{evapotrans} \times \text{Area} \times Z_{\text{water}}}{Z_s \times V_s} \quad [69]$$

$$T_{so} = \frac{\text{recharge} \times Z_{\text{water}}}{Z_s \times d_s} \quad [70]$$

T_{sr} relates to the transfer of soil solution into plant roots as a result of transpiration. Other parameters in these expressions have been defined previously.

Plant Roots (r)

The plant-roots compartment represents the portion of plants below the soil surface in which losses include translocation to plant leaves, transfer to soils through root decomposition, and biodegradation within the plant tissues. The inventory, N_r in mol, of contaminant in the root-zone-soil compartment is described by equation [45]. L_r is the sum of all loss-rate constants from the root-zone-soil compartment,

$$L_r = T_{rl} + T_{r1} + R_r, \quad [71]$$

where L_r represents total losses from the plant-roots compartment, mol/d; $T_{lr} N_l$ and $T_{sr} N_s$ are the gains from leaves by translocation and from root-zone soil by root uptake, mol/d; T_{rl} is the rate constants for losses from roots to leaves by translocation, day⁻¹; and R_r is the rate constant for transformation losses, day⁻¹. The expression relating transfer of contaminants from plant roots to root soil is defined by requiring that the net effect of T_{rs} and T_{sr} is to move the ratio of plant contamination in roots relative to root soil in the direction of the plant-soil partition coefficient, which has units of kg(soil)/kg(plant),

$$T_{rs} = \frac{T_{sr} \times V_s \times Z_s}{V_r \times Z_r} \quad [72]$$

T_{rl} relates to the transfer of root solution into plant leaves as a result of transpiration,

$$T_{rl} = (1-f_{arw}) \frac{\text{evapotrans} \times \text{Area} \times Z_{\text{water}}}{Z_r \times V_r} \quad [73]$$

Other parameters in these expressions have been defined previously.

The Surface-Water Compartment (w)

The surface-water compartment represents bodies of water in which losses include diffusion to air, diffusion to sediment, deposition to sediment, outflow to other surface-water bodies, and transformation processes. The inventory, N_w , in mol of contaminant in the surface-water compartment is described by equation [46]

and L_w is the sum of all loss-rate constants from the ground-surface-soil compartment,

$$L_w = T_{wa} + T_{wd} + T_{wo} + R_w , \quad [74]$$

where $L_w N_w$ is the sum of all losses from the surface-water compartment, mol/d; $T_{aw} N_a$ is the gain by diffusion and deposition from the air compartment, mol/d; $T_{gw} N_g$ is the gain by runoff from the surface-soil compartment, mol/d; $T_{dw} N_d$ is the gain by diffusion and deposition from the sediment compartment, mol/d; T_{wa} , T_{wd} , and T_{wo} are rate constants for gross diffusion loss to air, for deposition and gross diffusion losses to sediments, and for loss due to outflow, day⁻¹; and R_w is the rate constant for transformation losses, day⁻¹. The loss-rate constants are given by

$$T_{wa} = \frac{Y_{aw}}{Z_w \times d_w} , \quad [75]$$

$$T_{wd} = \frac{Y_{wd} + \text{deposit} \times Z_{dp}/\rho_{sd}}{Z_w \times d_w} , \quad [76]$$

$$T_{wo} = \text{outflow} \times \frac{[Z_{\text{water}} + (Z_{wp} \times \rho_{bw}/\rho_{sd})]}{Z_w \times d_w \times f_{arw}} , \text{ and} \quad [77]$$

$$\text{outflow} = \text{inflow} + \text{runoff} + \text{rain} \times (f_{arw}) - \text{evaporate} . \quad [78]$$

The Sediment-Zone Compartment (d)

The sediment compartment represents the sediment layer at the bottom of a surface-water column. In this compartment, losses include diffusion to water, resuspension of sediment particles, sediment burial, and transformation processes. The inventory, N_d in mol, of contaminant in the sediment compartment is described by equation [47]. L_d is the sum of loss-rate constants from the ground-surface-soil compartment,

$$L_d = T_{dw} + R_d , \quad [79]$$

$T_{wd} N_w$ is the gain by diffusion and deposition from the water compartment, mol/d; T_{dw} is rate constant for gross diffusion and particle resuspension losses to water, day⁻¹; and R_w is the rate constant for sediment burial and for transformation losses, day⁻¹. The loss-rate constant to water is given by

$$T_{dw} = \frac{Y_{wd} + \text{resuspend} \times Z_{dp} / \rho s_d}{Z_d \times d_d} \quad [80]$$

Other parameters used to describe the transport to and from the sediment compartment have been defined previously.

Solutions for the Molar Inventories

Equations [41] through [47] and matrix inversion methods are used to solve for the inventories, N_i , of contaminant in the seven compartments included in the model. These solutions give the following relationships,

$$N_a = C_a V_a \quad [81]$$

when the steady-state concentration, C_a , in mol/m³ in air is specified

and the inventories in other compartments are

$$N_l = N_a \frac{T_{al}}{L_l} + a_3 N_g \quad [82]$$

$$N_g = a_4 N_a \quad [83]$$

$$N_s = N_g \frac{T_{gs}}{L_s} \quad [84]$$

$$N_r = N_s \frac{T_{sr}}{T_{rl}} \quad [85]$$

$$N_w = a_1 N_a + a_2 N_g \quad [86]$$

$$N_d = N_w \frac{T_{wd}}{L_d} \quad [87]$$

where,

$$a_1 = \frac{T_{aw}}{\left[L_w - \frac{T_{dw}T_{wd}}{L_d} \right]} \quad [88]$$

$$a_2 = \frac{T_{gw}}{\left[L_w - \frac{T_{dw}T_{wd}}{L_d} \right]} \quad [89]$$

$$a_3 = \left[\frac{T_{sr}T_{gs}}{L_l L_s} + \frac{T_{gl}}{L_l} \right] \quad [90]$$

$$a_4 = \frac{\left[T_{ag} + \frac{T_{lg}T_{al}}{L_l} \right]}{\left[L_g - T_{lg}a_3 - \frac{T_{sg}T_{gs}}{L_s} \right]} \quad [91]$$

$$a_5 = \frac{\left[T_{aw} + a_4 T_{gw} \right]}{\left[L_w - \frac{T_{dw}T_{wd}}{L_w} \right]} \quad [92]$$

when the steady-state source, S_a , in mol/d to air is specified in place of C_a , then

$$N_a = S_a / \left[L_a - \frac{T_{la}T_{al}}{L_l} - a_3 a_4 T_{la} - a_4 T_{ga} - a_5 T_{wa} \right] \quad [93]$$

with equations [82] to [85] being applied as above.

PART II. MODEL INPUT AND DATA REQUIREMENTS

The CAirTOX multimedia transport and transformation model uses two sets of input data, one describing the properties of the contaminants and the other providing properties of the environment or landscape receiving the contaminants. Each of the inputs is described in terms of the physical process associated with the input and with an estimated coefficient of variation, which describes the uncertainty or variability associated with that parameter. The coefficient of variation or CV is the ratio of arithmetic standard deviation to arithmetic mean for a parameter that can have a range of values. Because the process of assigning CVs is itself an uncertain process, we use only five CV values corresponding to five uncertainty or CV classes to characterize these parameters. The term "CVa" represents a parameter that has a CV of 0.1 or less and is considered a highly reliable parameter that will contribute little to the overall uncertainty or variability of the final results so the uncertainty in the parameter need not be expressed. "CVb" represents a CV between 0.1 and 0.3 and indicates a parameter that has been measured or obtained from a highly reliable estimation method. A CV in this range reflects both the typical variability in the measurement and the uncertainty in extrapolating that value from an experimental setting to an environmental setting. "CVc" represents a CV between 0.3 and 3 (log mean CV of 1) and indicates a parameter for which a somewhat reliable estimation method exists. "CVd" represents a CV between 3 and 10 (log mean equal to 5) and is used for parameters for which the estimation method is much less reliable. "CVe" represents a CV between 10 and 15 (log mean equal to 12) and is used for parameters for which the estimated value is highly uncertain.

Chemical and Physical Data

The CAirTOX model also requires a set of physical-chemical properties inputs. These inputs and their approximate CVs are described in a companion report dealing with intermedia transfer factors.

Preliminary Landscape Properties for California

We have developed a landscape data set that is representative of California air/water sheds. In Table III, we summarize the landscape data that is used to represent this California landscape in the CAirTOX analyses. Also listed in this table are the CV classes associated with variability and uncertainty in this data.

Table III. The list of landscape properties used to carry out the environmental transport and transformation analysis for California residential sites.

Landscape Property	Value	Symbol	CV	Notes
Contaminated area in m^2	10^7	Area		
Annual average precipitation (m/d)	1.01×10^{-3}	rain	c	0.37 m/y
Flow of surface water into landscape (m/d)	0	inflow	n/a	0 m/y
Land surface runoff (m/d)	2.80×10^{-4}	runoff	c	0.1 m/y
Atmospheric dust load (kg/m^3)	6.15×10^{-8}	ρb_a	b	
Deposition velocity of air particles (m/d)	5.00×10^2	v_d	b	
Plant dry mass inventory ($kg[DM]/m^2$)	7.00×10^{-1}	bio_{inv}	b	
Plant dry-mass production ($kg[DM]/m^2-d$)	2.00×10^{-2}	bio_{prd}	b	
Plant dry mass fraction	2.00×10^{-1}	bio_{dm}	b	
Plant density kg/L	1.00	ρ_p	b	
Evapotranspiration from soil (m/d)	5.15×10^{-4}	evapotrans	c	0.19 m/y
Evaporation from surface water (m/d)	4.38×10^{-6}	evaporate	c	
Thickness of the ground-soil layer (m)	1.00×10^{-2}	d_g	c	
Soil particle density; ground-surface soil layer (kg/m^3)	2.40×10^3	ρs_g	a	
Water content in surface soil (volume fraction)	1.00×10^{-1}	β_g	b	
Air content in the surface soil (volume fraction)	2.00×10^{-1}	α_g	b	
Erosion of surface soil (kg/m^2-d)	3.30×10^{-3}	$erosion_g$	b	
Thickness of the root-zone layer (m)	2.00	d_s	b	
Soil particle density; root-zone soil layer (kg/m^3)	2.40×10^3	ρs_s	a	
Water content of root-zone soil layer (vol. fraction.)	2.00×10^{-1}	β_s	b	
Air content of root-layer (vol. fraction.)	1.00×10^{-1}	α_s	b	
Fraction of land area in surface water	8.15×10^{-3}	f_{arw}	b	
Average depth of surface waters (m)	6	d_w	c	

California Landscape properties (continued)

Landscape Property	Value	Symbol	CV	Notes
Suspended sediment in surface water (kg/m ³)	0.8	ρ_{bw}	c	
Suspended sediment deposition (kg/m ² /d)	1.05×10^1	deposit	b	
Thickness of the sediment layer (m)	5.00×10^{-2}	d_d	c	
Solid material density in sediment (kg/m ³)	2.40×10^3	ρ_{sd}	a	
Porosity of the sediment zone	2.00×10^{-1}	β_d	b	
Sediment resuspension rate (kg/m ² /d)	1.05×10^1	resuspend	d	
Ambient environmental temperature (K)	2.83×10^2	T	c	
Surface water current in m/d	0	current _w	c	
Organic carbon fraction in surface soil	1.20×10^{-2}	f_{ocg}	c	
Organic carbon fraction in root-zone soil	1.20×10^{-2}	f_{ocs}	c	
Organic carbon fraction in vadose zone	1.00×10^{-2}	f_{ocv}	c	
Organic carbon fraction in sediments	2.00×10^{-2}	f_{ocd}	c	
Boundary layer thickness in air above ground-surface soil (m)	0.005	δ_{ag}	b	
Yearly average wind speed (m/d)	1.50×10^5	v_w	b	1.74 m/s

The types of data needed to construct a landscape data set include meteorological data such as average annual wind speed, deposition velocities, air temperature, and depth of the mixing layer; hydrological data, such as annual rainfall, runoff, soil infiltration, ground-water recharge, and surface water depth and sediment loads; and soil properties, such as bulk density, porosity, water content, erosion rates, and root zone depth. Primary references for these data are van der Leeden et al. (1991), Soil Conservation Service (1975), the U.S. National Oceanic and Atmospheric Administration (1974), U.S. Department of Agriculture (1978), and Gleick (1987).

PART III. THE EXPOSURE PATHWAYS MODEL

The concentrations in air, water and soil used for an exposure assessment are those measured or estimated to be available in these environmental media at the nearest receptor point to the source (e.g., the hazardous-waste site). When an environmental concentration is assumed constant over time, the population-averaged potential dose (for ingestion or inhalation routes) or absorbed dose (for dermal contact) is expressed as an average daily dose rate (ADD), in mg/kg-d

$$ADD = \frac{C_i}{C_k} \times \left[\frac{IU_i}{BW} \right] \times \frac{EF \times ED}{AT} \times C_k \quad [94]$$

In this expression C_i/C_k is the intermedia-transfer factor, which expresses the ratio of contaminant concentration in the *exposure* medium i (i.e., personal air, tap water, milk, soil, etc.) to the concentration in an environmental medium k (ambient-air gases or particles, surface soil, root-zone soil, surface water, and ground water) and $[IU_i/BW]$ is the intake or uptake factor per unit body weight associated with the exposure medium i . For exposure through the inhalation or ingestion route, $[IU_i/BW]$ is I_i the intake rate per unit body weight of the exposure medium such as $m^3(\text{air})/\text{kg-d}$, $L(\text{milk})/\text{kg-d}$, or $\text{kg}(\text{soil})/\text{kg-d}$. For exposure through the dermal route, $[IU_i/BW]$ is replaced by UF_i , the uptake factor per unit body weight and per unit initial concentration in the applied medium ($L(\text{water})/\text{kg-d}$ or $\text{kg}(\text{soil})/\text{kg-d}$). EF is the exposure frequency for the exposed population, in days per year; ED is the exposure duration for the exposed population, in years; AT is the averaging time for the exposed population, in days; and C_k is the contaminant concentration in environmental medium k . The potential dose factor, $PDF(k \rightarrow i)$, is defined as the ratio of dose to concentration, as expressed in the following equation.

$$PDF(k \rightarrow i) = \frac{ADD}{C_k} = \frac{C_i}{C_k} \times \left[\frac{IU_i}{BW} \right] \times \frac{EF \times ED}{AT} \quad [95]$$

The PDF is used to make pathway and route-to-route comparisons in the absence of concentration values and allows one to consider the relative significance of several exposure pathways. With the PDF, we compare inhalation, ingestion, or dermal exposures to the same medium such as tap water and compare exposures through indirect pathways (such as food-chain transfers) to those from direct pathways such

as inhalation or ingestion. As an example, the PDF for a 70-kg individual ingesting 2 L/d of tap water 365 days per year for a lifetime is 2 L divided by 70 kg or 0.029 L/kg-d. This PDF and other PDFs like it can be used as the basis for determining the relative significance of dermal, inhalation, and other ingestion exposures attributable to tap water.

In summary, the exposure assessment process consists of relating contaminant concentrations in the environmental media—air, surface soil, root-zone soil, surface water, and ground water—to contaminant concentrations in exposure media with which a human population has contact (personal air, tap water, foods, household dusts and soils, etc.). The average daily dose is the product of the exposure concentrations in these contact media and an intake or uptake factor that relates the concentrations to the distributions of potential dose by the inhalation, ingestion, and dermal contact routes within the population. Listed in Table IV are the potential interactions among environmental media, exposure media, and exposure routes that are addressed in the models presented below.

Exposure factors

In constructing exposure models one needs to define the characteristics of individuals in various age/sex categories and the characteristics of the microenvironments in which they live or from which they obtain water and food. This section defines both the types of data needed to carry out the exposure assessment and how this data is obtained. For all exposure factors used in CAirTOX, we define both an arithmetic mean value and a coefficients of variation (CV), which is the arithmetic standard deviation divided by the arithmetic mean. In the sections below, we describe how we derived means and CVs for exposure duration and averaging time, anatomical and dietary properties, activity patterns and exposure times, household parameters, other human factors such as soil ingestion and breast milk intake, and parameters associated with food crops and food product animals.

Table IV. Matrix of exposure pathways linking environmental media, exposure scenarios, and exposure routes.

Exposure routes	Media		
	Air (gases and particles)	Soil (surface soil and root-zone soil)	Water (surface water)
Inhalation	<ul style="list-style-type: none"> • Inhalation of gases and particles in outdoor air • Inhalation of gases and particles transferred from outdoor air to indoor air 	<ul style="list-style-type: none"> • Inhalation of soil vapors that migrate to indoor air • Inhalation of soil particles transferred to indoor air 	<ul style="list-style-type: none"> • Indoor inhalation of contaminants transferred from tap water
Ingestion	<ul style="list-style-type: none"> • Ingestion of fruits, vegetables, and grains contaminated by transfer of atmospheric chemicals to plant tissues • Ingestion of meat, milk, and eggs contaminated by transfer of contaminants from air to plants to animals • Ingestion of meat, milk, and eggs contaminated through inhalation by animals • Ingestion of mother's milk 	<ul style="list-style-type: none"> • Human soil ingestion • Ingestion of fruits, vegetables, and grains contaminated by transfer from soil • Ingestion of meat, milk, and eggs contaminated by transfer from soil to plants to animals • Ingestion of meat, milk, and eggs contaminated through soil ingestion by animals • Ingestion of mother's milk 	<ul style="list-style-type: none"> • Ingestion of tap water • Ingestion of irrigated fruits, vegetables, and grains • Ingestion of meat, milk, and eggs from animals consuming contaminated water • Ingestion of fish and sea food • Ingestion of surface water during swimming or other water recreation • Ingestion of mother's milk
Dermal contact	(not considered)	<ul style="list-style-type: none"> • Dermal contact with soil 	<ul style="list-style-type: none"> • Dermal contact in baths and showers • Dermal contact while swimming

Exposure Duration and Averaging Time

In the basic exposure model, the exposure duration (ED) is the amount of time, in years, that the exposed population is assumed to be in contact with a specified environmental contaminant. The averaging time (AT) is the period, in days, over which exposure is averaged. More specifically, averaging time is the number of days from the total lifetime of an individual selected at random from the population over which human contact will be averaged so as to be representative of exposure in the total population. However, according to the EPA (1989a), because of the mobility of the U.S. population, the exposure duration at a specific site for an individual selected at random from the adjacent population is often significantly less than an average lifetime of 70 years. For all exposure calculations used to make chemical- and site-specific exposure estimates for noncarcinogens, the exposure duration, ED, and the exposure averaging time, AT, represent the same span of time (the units however are different, ED is in years and AT is in days). For carcinogens, the mean exposure duration, ED, is assumed to be 14 years with a CV of 1.15 (geometric mean and standard deviation of 9.0 and 2.5 respectively) (EPA, 1989b) and the averaging time, AT, is 25,550 days (70 years).

Anatomical and Dietary Properties

The potential dose calculation requires as input the *ratio* of intake to body weight *averaged* over the representative age group. In this section we describe how we developed mean values and CVs for air, water, and food intakes per unit body weight for children, for adults, and for a lifetime exposure.

Body Weight

We calculate the arithmetic-mean body weight and CV of body weight for three age groups—infant, child, and adult. The body weight for infants is needed for estimating exposures to contaminants in breast milk or other pathways that are unique to children in roughly the 0- to 1-year age group. Body weight for adults and children are needed to calculate lifetime-average contact rates per unit body weight and contact rates for an exposure duration of less than a full lifetime. The child age category applies to ages 0 to 15 years, but excludes breast-fed babies. General data on body-weight distributions by age and sex are available from the ICRP (1975), the U.S. EPA (1985, 1989a) and Najjar and Roland (1987). We used the Najjar and Roland (1987) data to develop the mean value and CV of body weight for ages 0 to 1, for ages 0 to 15, 15 to 70, and for lifetime. These values are listed in Table V.

Table V. Values of human anatomical and dietary properties for use as default values in the exposure calculations.^a

Parameter, symbol	Child ^b		Adult ^b		Combined ^b		Units
Body weight of infants age 0 to 1 y, BW	7.2	(0.3)	--		--	--	kg
Body weight of lactating women, BW _{mo}	--	--	65.4	(0.2)	--	--	kg
Body weight, BW	29	(0.24)	71	(0.2)	62	(0.2)	kg
Surface area, SA _b	0.032	(0.09)	0.024	(0.06)	0.026	(0.07)	m ² /kg
Working breathing rate, BR _w	--	--	0.030	(0.3)	--	--	m ³ /kg-h
Active breathing rate, BR _a	0.023	(0.3)	0.018	(0.3)	0.019	(0.3)	m ³ /kg-h
Resting breathing rate, BR _r	0.008	(0.3)	0.006	(0.2)	0.0064	(0.2)	m ³ /kg-h
Fluid intake, I _f	0.029	(0.2)	0.020	(0.2)	0.022	(0.2)	L/kg-d
Fruit and vegetable intake, I _{fv}	0.0075	(0.2)	0.0042	(0.2)	0.0049	(0.2)	kg/kg-d
Grain intake, I _g	0.0070	(0.2)	0.0028	(0.2)	0.0037	(0.2)	kg/kg-d
Exposed produce intake = $I_g + f_{fv}^{abg} \times I_{fv}$	0.011	(0.2)	0.0048	(0.2)	0.0060	(0.2)	kg/kg-d
Protected produce intake = $(1 - f_{fv}^{abg}) \times I_{fv}$	0.0040	(0.2)	0.0022	(0.2)	0.0026	(0.2)	kg/kg-d
Meat intake, I _{mt}	0.0043	(0.2)	0.0026	(0.2)	0.0030	(0.2)	kg/kg-d
Milk/Dairy intake, I _{mk}	0.017	(0.2)	0.0037	(0.2)	0.0065	(0.2)	kg/kg-d
Egg intake, I _{egg}	0.00061	(0.2)	0.00041	(0.2)	0.00046	(0.3)	kg/kg-d
Fish intake, I _{fsh}	0.00035	(0.4)	0.00028	(0.3)	0.00029	(0.4)	kg/kg-d

^a Listed are the arithmetic-mean value and (in parentheses) the estimated coefficient of variation (CV), equal to the standard deviation divided by the mean. Body weights are from Najjar and Roland (1987), breathing rates are from ICRP (1975), and food intakes are from Yang and Nelson (1986).

^b The child category covers ages 0 to 15, the adult category covers ages 16 to 70, the combined category is used to represent lifetime equivalent exposure and is obtained by multiplying the child category by 15/70, the adult category by 55/70, and then summing these products.

Breathing Rate

General data on breathing rates by age and sex are available from the EPA (1985, 1989a) and the ICRP (1975). Values in Table V are taken primarily from the ICRP (1975) with variances estimated by McKone and Daniels (1991). The working breathing rate is for 8 hours of work and, when combined with 8 hours of breathing at the active rate and 8 hours at the resting rate, gives a daily equivalent intake of 30 m³ for an adult (EPA, 1989a). Layton (1992) has derived breathing rates that are consistent with the quantities of oxygen needed to metabolize reported dietary intakes of fats, carbohydrates, and proteins. He has shown that the values in Table V could be high by a factor of from 20 to 30%. But this is within the CV reported here.

Body Surface Area

Information on the relation between human body weight and surface area has been published by the ICRP (1975) and the U.S. EPA (1989a). In the EPA report, it is suggested that surface area (SA) in m² can be estimated as 0.1 times body weight (BW) in kg raised to the 2/3 power. Using this formula, along with methods described in Bevington (1969), we estimate the mean value and standard deviation of surface area per unit body weight, SA_b in m²/kg, for children and adults using the formula

$$SA_b = \left[\frac{SA}{BW} \right] = 0.1 \times BW^{-1/3} \pm \left(0.1 \frac{\sigma_{BW}}{3} \right) BW^{-4/3} , \quad [96]$$

where the second term is the standard deviation of the surface area-body weight ratio. The resulting surface-area values and CVs are given in Table V.

Water Ingestion

Tap-water intake includes all household tap water that is consumed as a beverage or used to prepare foods and beverages. Yang and Nelson (1986) have published tap-water and total-fluid intakes in mL/d for the U.S. population by age, sex, and region of the country. Ershow and Cantor (1989) have published population-based estimates of sex-, region-, and season-averaged tap-water intakes per unit body weight by the U.S. population in mL/kg-d. From these two papers, we have derived intakes of tap water in L/kg-d for children, adults, and lifetime equivalent. The mean values of tap-water intake and CVs in these age groups are listed in Table V.

Food Intakes

For food intakes included in the exposure assessment, we calculate the arithmetic mean and standard deviation of each food intake per unit body weight in all age categories used and also combine these intake rates to determine the population average and standard deviation of each food intake per unit body weight. The following food groups are considered in the exposure assessment: meat including beef, pork, poultry, and other meats; milk and dairy products; eggs; leafy vegetables, such as cabbage, cauliflower, broccoli, celery, lettuce, and spinach; exposed produce, such as apples, pears, berries, cucumber, squash, grapes, peaches, tomatoes, string beans, etc.; protected produce or root crops, such as carrots, beets, turnips, potatoes, legumes, melons, citrus fruits, etc.; grains such as wheat, corn, rice, barley, millet, etc.; and fresh fish and seafood.

In the Nationwide Food Consumption Survey (NFCS) (USDA, 1983), the U.S. Department of Agriculture (USDA) used a stratified probability sample of households in the 48 conterminous states and the District of Columbia in each of four seasons from April 1977 through March 1978. The samples were designed to be representative of the United States and were classified according to geographic regions of the country; geographic divisions within each of the regions; and central city, suburban, and non-metropolitan populations. Data were collected for 30,770 individuals within 114 primary sampling units—indicating approximately 270 individuals per sampling unit. We calculate food intakes using results compiled by Yang and Nelson (1986), who analyzed the data from the USDA survey. According to Yang and Nelson (1986), 47% of all consumed produce (fruits and vegetables) consists of leafy vegetables and exposed produce, which intercept contaminants from the atmosphere. The remaining 53% of fruits and vegetables consists of protected produce or root crops, in which contaminant transfer to the edible portion is primarily by root uptake. All grain crops are assumed to be exposed primarily to air contaminants. For the food groups including milk, fruits and vegetables, grains, exposed produce and grains, protected produce, meat, eggs, and fish, we use the Yang and Nelson (1986) results to estimate the arithmetic mean and CV for daily intake per kg body weight for children, adults, and combined or lifetime-equivalent exposures. Table II lists these estimates. The variance of intake-per-body-weight ratio used to determine the CV is calculated under the assumption that food intake correlates with body weight to the two-thirds power. The mean and variance of body weight used in this estimate are taken from Table V.

Food Consumption Patterns

We consider *homegrown* foods those foods produced on the land associated with a household and, for the most part, consumed within that household; whereas *locally grown* foods are those that are produced in home gardens and commercial farms with air, soil, and/or water that have been contaminated by the local waste site and are consumed by the local population. Ideally, distributions describing local consumption of produce, grain, milk and dairy products, meat, eggs, and fish are needed to assess food-chain exposures. However, limited data are available on the amount of locally grown and consumed food products. The U.S. EPA (1989a) has compiled data for U.S. households on the fractions of consumed produce that comes from home gardens. For all categories of fruits and vegetables reported in this study, the fraction that is homegrown is in the range 0.04 to 0.75, and for the one grain listed (corn) the average fraction that is homegrown is 0.45 for 25% of the individuals surveyed (the other 75% did not consume homegrown corn). From these data we determined that the fraction of consumed fruits and vegetables that are homegrown is 0.24 with CV of 0.7, and that the fraction of consumed grains (mostly corn) that are homegrown is 0.11 also with a CV of 0.7. These values represent households with home gardens and not necessarily the average of total homegrown consumption in either the U.S. or California population.

The U.S. EPA (1989a) also reports that, in farm households that consume homegrown beef, the annual fraction of consumed beef that is homegrown is 0.44 with CV of roughly 0.5 and, in farm households that consume homegrown dairy products, the average fraction of consumed dairy products that are homegrown is 0.4 with CV of roughly 0.7. We applied the fraction of homegrown beef to all meat types. Because we could locate no information on consumption of homegrown eggs, we applied the same fraction as for dairy products.

According to U.S. EPA (1989a) data, recreational fishermen can consume as much as 30 to 140 g/d of fish and seafood. But these values do not necessarily apply to a specific body of water as is the case for our exposure assessment. The average consumption of fish and seafood in the U.S., as listed in Table V, is 18 g/d. To accommodate data regarding consumption of fish that is caught by recreational fishing, we assume that the fraction of fish consumed locally is a triangular distribution with a mean value of 0.7, a variance of 0.56, and CV of 0.3.

Fractions of consumed food that are from local supplies are listed in Table VI.

Table VI. Activity patterns, household parameters and other exposure factors.

Parameter name and symbol	Estimated mean value	Coefficient of variation	Units	Reference
Fraction of fruits and vegetables that are exposed produce, $f_{abv-grd}^v$	0.47	0.1	none	Yang and Nelson (1986)
Fraction of fruits and vegetables local, f_{local}^v	0.24	0.7	none	U.S. EPA (1989a)
Fraction of grains local, f_{local}^g	0.12	0.7	none	U.S. EPA (1989a)
Fraction of milk local, f_{local}^{mk}	0.4	0.7	none	U.S. EPA (1989a)
Fraction of meat local, f_{local}^{mt}	0.44	0.5	none	U.S. EPA (1989a)
Fraction of eggs local, f_{local}^{egg}	0.4	0.7	none	this report
Fraction of fish local, f_{local}^{fish}	0.7	0.3	none	U.S. EPA (1989a)
Exposure time, at home indoors, ET_h	16	0.14	h/day	U.S. EPA (1989a)
Exposure time, at home outdoors, ET_o	0.3	0.14	h/day	U.S. EPA (1989a)
Exposure time, in shower or bath, ET_{sb}	0.27	0.6	h/day	James and Knuiman (1987)
Exposure time swimming, ET_{sw}	0.5	0.5	h/d	U.S. EPA (1992a)
Exposure frequency, swimming, EF_{sw}	15	4	d/y	U.S. EPA (1992a)
Water ingestion while swimming, I_{sww}	0.0007	1	L/kg-d	U.S. EPA (1989b)
Fraction of water needs provided by ground water, f_{gw}^w	0.8	0.1	none	van der Leeden et al. 1990)
Water use in the shower, W_{shower}	8	0.4	L/min	James and Knuiman (1987)
Water use in the House W_{house}	40	0.4	L/h	van der Leeden, et al. (1990)
House air ventilation rate, VR_{house}	750	0.3	m ³ /h	McKone and Bogen (1992)
Bathroom air ventilation rate, VR_{bath}	1	0.4	m ³ /min	McKone and Bogen (1992)
Indoor soil-dust load, $dust_{in}$	3.0×10^{-8}	0.4	kg/m ³	Murphy and Yocom, 1986)
Soil ingestion by children 0 to 15 y, I_{sl}	2.2×10^{-6}	3	kg/kg-d	U.S. EPA (1989a)
Soil ingestion by adults 15 to 70 y, I_{sl}	1.4×10^{-7}	2	kg/kg-d	U.S. EPA (1989a)
Lifetime average soil ingestion, I_{sl}	3.5×10^{-7}	3	kg/kg-d	U.S. EPA (1989a)
Exposure frequency to soil, EF_{sl}	137	0.6	events/y	U.S. EPA (1992a)
Body surface fraction with soil contact	0.3	0.04	none	U.S. EPA (1992a)
Soil adherence to skin, Sl_{sk}	0.5	0.4	mg/cm ²	U.S. EPA (1992a)
Breast-milk ingestion by infants, I_{bm}	0.11	0.2	kg/kg-d	Butte et al. (1984), Whitehead and Paul (1981)

Activity Patterns and Exposure Times

CAirTOX requires as input the average number of hours per day spent indoors at home, spent outdoors at home, and spent in bathrooms (including showering and bathing time) during the exposure duration. We also use the number of days per year and hours per day spent in contact with surface water during swimming or other water recreation.

According to the U.S. EPA (1989a), the average time spent at home indoors is 16 h/d and the time spent at home outdoors is 0.3 h/d. We estimate the CV in these numbers to be 0.14. James and Knuiman (1987) analyzed data on domestic water use from 3,000 households in Australia and report the mean duration of a shower as 8 min with a geometric standard deviation (GSD) of roughly 1.8 (CV equal to 0.6). We double this time to account for additional time spent in the bathroom. The U.S. EPA (1992a) reports that swimming time ranges from a typical value of 0.5 h/d to an upper bound of 1 h/d and the frequency ranges from a typical value of 5 d/y to an upper bound of 150 d/y. From this we obtain a mean exposure time of 0.5 h/d with a CV of 0.5, and because of climate and proximity to water, we use 15 d/y (CV of 4) as representative of exposure frequency in California. Based on U.S. EPA (1989b) estimates, we use 0.0007 L/kg-h (CV equal to 1) as the ingestion rate of surface water by swimmers. Values and units of activity patterns and exposure times are listed in Table VI.

Household Parameters

Household factors relate to tap-water supply and use, room-ventilation rates, and dust concentrations within homes. In California, 70% of the water withdrawn by public-supply water systems and 90% of the water withdrawn in private domestic water systems is from ground water (van der Leeden et al. 1990). We assume the fraction of tap water withdrawn from ground water is 0.8 with a CV of 0.1. In their observation of Australian households, James and Knuiman (1987) found that the arithmetic-mean water use rate in showers is approximately 8 L/min with a GSD of roughly 1.4 (a CV of approximately 0.4). van der Leeden et al. (1990) report that water use in U.S. households, excluding outdoor uses, averages 240 L/d per person or 960 L/d per household of four. We use this value, converted to 40 L/h with a CV of 0.4 to represent water use in California homes. Room ventilation rates in the shower/bathroom and the remainder of the house are based on the assumption that the volumes of these compartments are 10 and 600 m³, respectively, and that the number of air changes per hour ranges from 2 to 10 in the bathroom and from 0.5 to

2 in the remainder of the house (McKone, 1987; McKone and Knezovich, 1991; McKone and Bogen, 1992). This yields a bathroom ventilation rate of $1 \text{ m}^3/\text{min}$ with a CV of 0.4 and a house ventilation rate of $750 \text{ m}^3/\text{h}$ with a CV of 0.3. House dust suspended in the indoor-air environment originates from three sources, (1) airborne particles that penetrate from outside air to indoor air; (2) surface soil and dust tracked into buildings on shoes or clothes, by pets, or other vectors; and (3) a variety of sources related to occupant activities, material degradation, and household products. Ambient levels of particles in outdoor air are on the order of 10 to $100 \text{ } \mu\text{g}/\text{m}^3$, with 60 as a representative value (Schroder and Lane, 1988). The concentration of indoor particles attributable to surface soil is on the order of $3.0 \times 10^{-8} \text{ kg (soil)}/\text{m}^3(\text{air})$ (Murphy and Yocom, 1986). We use this latter value as the indoor dust load that is attributable to household soil and assign a CV of 0.4.

Other Human Exposure Factors

Soil Ingestion and Soil Contact on Skin

General data on soil intake by age and sex have been reviewed or compiled by Paustenbach et al. (1986), LaGoy (1987), U.S. EPA (1989a), Calabrese et al. (1989), and Sedman (1989). The U.S. EPA (1989a) recommends that $0.2 \text{ g}/\text{d}$ be used as an average soil-ingestion rate for children under age 7 with $0.8 \text{ g}/\text{d}$ as an upper bound. Although the EPA report does not recommend rates to use for other ages, it does report four levels of soil ingestion for ages 0 to 18. One of these levels represents children with low soil-ingestion rates, two represent children with intermediate soil-ingestion rates, and one represents children with high soil-ingestion rates (U.S. EPA, 1989a). LaGoy (1987) suggests a soil-ingestion rate of $0.025 \text{ g}/\text{d}$ for adults. Combining the information in the EPA report with recommendations by Calabrese et al. (1991) and LaGoy (1987), we obtain soil-ingestion estimates of $2.2 \times 10^{-6} \text{ kg(soil)}/\text{kg-d}$ ($0.06 \text{ g}/\text{d}$ equivalent) with a CV of 3 for children 0 to 15 y, $1.4 \times 10^{-7} \text{ kg(soil)}/\text{kg-d}$ ($0.01 \text{ g}/\text{d}$ equivalent) with a CV of 2 for adults 15 to 70 y, and $3.5 \times 10^{-7} \text{ kg(soil)}/\text{kg-d}$ ($0.02 \text{ g}/\text{d}$ equivalent) with a CV of 3 for a lifetime equivalent during ages 0 to 70. These results are summarized in Table VI.

General data for soil deposition on skin surfaces are available from the U.S. EPA (1992a). According to this information, an adult with a body surface area of $18,000 \text{ cm}^2$ can have $5,000$ to $5,800 \text{ cm}^2$ exposed to contact with soil and have a soil-to-skin adherence of 0.2 to $1 \text{ mg}/\text{cm}^2$ with an exposure frequency of 40 to 350 events per year. From this information, we calculate a daily soil-contact rate over the

exposure duration (ED) as covering an average of 0.3 of the body surface (with CV of 0.04 for the value of this fraction), having a mean soil adherence of 0.5 mg/cm² with a CV of 0.4, and having a mean exposure frequency of 137 d/y with a CV of 0.6. These values are summarized in Table VI.

Ingestion of Breast Milk by Infants

Data on ingestion of breast milk by infants are available in Butte et al. (1984) and Whitehead and Paul (1981). We calculate the breast-milk ingestion per unit body weight for infants ages 0 to 12 months as 0.11 kg/kg-d with a CV of 0.2. This CV is based on the variability in ingestion factors for children and adults, such as milk, meat, and vegetation intakes.

Parameters Associated with Food Crops and Food-Producing Animals

To calculate human exposures to contaminants through the produce, meat, dairy-product, and egg pathways, we must quantify the ratio of fresh mass to dry mass of pasture and food crops; parameters that describe the diet, weight, water intake, soil intake, and inhalation rates of food-producing animals; the fat content of animal-based food products; the organic-carbon content of soils; and the fraction of contaminants in irrigation water that are retained in soil-pore water after application.

We assume the ratio of dry mass to fresh mass, bio_{dm} , for pasture and food crops is in the range 0.1 to 0.3, with mean value 0.2 and a CV of 0.2. Based on their review of ingestion and inhalation data for cattle, McKone and Ryan (1989) estimate arithmetic means and CVs (in parentheses) for vegetation intake as 17 (0.2) kg(dry mass)/d in dairy cattle and 12 (0.4) kg (dry mass)/d in beef cattle, for soil intake as 0.4 (0.7) kg(soil)/d in both dairy cattle and beef cattle, and for inhalation rates as 122 (0.3) m³/d in beef and dairy cattle. Altman and Dittmer (1968) report chicken feed requirements in the range 0.11 to 0.125 kg/d. Because chickens require grit in their diet to aid digestion and because it has been noted that 2% by weight of grit in diet is an optimum for chickens (NRC, 1984), we assume soil intake by chickens to be on the order of 2% of feed intake. Altman and Dittmer (1968) report that total water turnover (L/h) in mammals, such as cattle, can be estimated as 4.9 times body weight raised to the 0.86 power and that water turnover (in L/h) in bird species, such as chickens, can be estimated as 2.2 times body weight raised to the 0.61 power. With adult cattle weights in the range 500 to 1000 kg and adult chicken weights in the range 1.8 to 2.5 kg (Altman and Dittmer, 1968), we estimate the daily

Table VII. Parameters associated with food crops and food-producing animals.

Parameter description and symbol	Estimated mean value	Coefficient of variation	Units	Reference
Ratio of plant dry mass (DM) to fresh mass (FM), bio_{dm}	0.2	0.2	none	this report
Ingestion of pasture by beef cattle, I_{vbc}	60	0.4	kg[FM]/d	McKone and Ryan (1989)
Ingestion of pasture by dairy cattle, I_{vdc}	85	0.2	kg[FM]/d	McKone and Ryan (1989)
Ingestion of pasture by hens, I_{vh}	0.12	0.04	kg[FM]/d	Altman and Dittmer (1968)
Ingestion of water by dairy cattle, I_{wdc}	35	0.2	L/d	Altman and Dittmer (1968)
Ingestion of water by beef cattle, I_{wbc}	35	0.2	L/d	Altman and Dittmer (1968)
Ingestion of water by hens, I_{wh}	0.084	0.1	L/d	Altman and Dittmer (1968)
Ingestion of soil by cattle, I_{sc}	0.4	0.7	kg/d	McKone and Ryan (1989)
Ingestion of soil by hens, I_{sh}	0.0024	1	kg/d	NRC (1984)
Inhalation by cattle I_{nc}	122	0.3	m ³ /d	McKone and Ryan (1989)
Inhalation by hens, I_{nh}	2.2	0.3	m ³ /d	this paper
Fat content of milk	0.04	0.1	none	Travis and Arms(1988)
Fat content of meat	0.25	0.3	none	Travis and Arms(1988), Goldman et al. (1989).
Fat content of eggs	0.08	0.1	none	Goldman et al. (1989).
Fraction organic carbon in soil, f_{oc}	0.012	0.6	none	Soil Conservation Service (1975)
Fraction of the contaminant concentration in irrigation water retained in soil water, f_{ir}	0.25	1	none	this report

water intakes by cattle and chickens as, respectively, 35 L/d with a CV of 0.2 and 0.084 L/d with a CV of 0.1. We assume that inhalation rates in chickens are scaled to those for cattle and humans according to body weight to the 2/3 power to obtain the estimated inhalation rate for hens. From this information, we obtain arithmetic mean and CV values for the intakes of pasture (fresh mass), soil, water, and air by animals as listed in Table VII.

We assume that the fat content of meat averages 0.25 with range 0.1 to 0.4 and a CV of 0.3, that the fat content of whole milk averages 0.04 with range 0.03 to 0.05 and a CV of 0.1, and that the fat content of eggs averages 0.08 with a CV of 0.1 (Travis and Arms, 1988; Goldman et al., 1989). The fat content values that we use in the exposure model are listed in Table VII.

As a result of lower humidity and less rainfall, soils in the Western U.S. can have lower organic carbon contents than is typical of soils from regions east of the Mississippi River, and the reported fraction of organic carbon, f_{oc} , in the Western U.S. is in the range 0.0012 to 0.044 (Soil Conservation Service, 1975). As noted in Table VII, we use an average f_{oc} value of 0.012 with a CV of 0.6 to represent soils in California.

The fraction of the contaminant concentration in water used for irrigation that is retained in the water phase of soil on which that water is applied, f_{ir} , is used to calculate contamination of food crops by irrigation water. This factor includes the fraction of time that irrigated water is used to water the homegrown fruits, vegetables, and grains and the fraction of contaminant that is not lost by evaporation, biodegradation, or infiltration. We use 0.25 for this parameter and CV of 1 to reflect that this parameter is likely to be much lower than 1 but no greater than 1.

Multiple-Pathway Exposures and Total Dose: The Ingestion Route

In our multiple-pathway approach, total ingestion exposure is attributable to contaminated air, water, and soil. Concentrations of contaminants in six environmental media are used in the multiple-pathway assessment for ingestion exposures: (1) the contaminant concentration in ambient-air gases, C_a in mg/m³; (2) the concentration of contaminant bound to air particles, C_{ap} in mg/m³; (3) contaminant concentration in surface soil, C_g in mg/kg; (4) contaminant concentration in root-zone soil below the surface layer, C_s in mg/kg; (5) contaminant concentration in ground water, C_q in mg/L; and (6) contaminant concentration in surface water, C_w in mg/L. Total ingestion intake includes potential doses from the

ingestion of tap water; the ingestion of local or homegrown fruits, vegetables, grains, milk, meat, and eggs; ingestion of locally or recreationally caught fish; ingestion of soil; and the ingestion of surface water while swimming. In terms of the basic exposure model, expressed in equation [94], the ingestion intake of contaminants involves the intermedia transfer of contaminants from an environmental medium, k , to the exposure medium, i , which is the ingested water, produce, animal product, fish, or soil. The environmental medium, k , is one of the six media described above. For each pathway we derive an intermedia-transfer factor, C_i/C_k , to express this ratio. For the intake rate of the exposure medium per unit body weight, $[In_i/BW]$, we use the daily average ingestion rates per unit body weight as listed in Table V. The exposure frequency for all ingestion exposures is assumed to be 365 days per year. However, adjustments for dilution of the exposure media are made to account for seasonal unavailability of local foods and use of irrigation water.

In the sections below, C_{tw} represents the contaminant concentration in the environmental medium used to supply tap water, which is a combination of C_w , the contaminant concentration in surface water and C_g represents the contaminant concentration in ground water. Tap water concentration is calculated as

$$C_{tw} = f_{gw}^w \times C_g + (1 - f_{gw}^w) \times C_w , \quad [97]$$

where f_{gw}^w is the fraction of water needs provided by ground water as described in the section on exposure factors.

Ingestion of Tap Water

For tap water, the intermedia-transfer factor, C_i/C_k , is the ratio of contaminant concentration tap water, mg/L, to contaminant concentration, mg/L, in the nearest ground or surface water at the contaminated site and is assigned a default value of unity. When there is a mix of ground and surface water being used, the intermedia-transfer factors can be written as

$$C_{tw}/C_w = (1 - f_{gw}^w) . \quad [98]$$

The average daily dose (ADD) to contaminants in drinking water is calculated using the daily intake of tap water per unit body weight, I_{η} , for the individual exposed for the assumed exposure duration, ED, and is given by

$$\text{ADD}(\text{drinking water ingestion}) = I_{\eta} \times C_{\text{tw}} \quad [99]$$

The potential dose factors (PDFs), in L/kg-d, for this exposure pathway are simply the ratios of ADDs, in mg/kg-d, to water-supply concentrations, in mg/L multiplied by the fraction of water supplied by that water source.

Ingestion of Contaminated Homegrown Fruits, Vegetables, or Grains

We consider contamination of fruits, vegetables, and grains by air (both the gas phase and particles), water, surface soil, and root-zone soil. For these environmental media, the associated average daily doses are expressed as the average daily dose to the individual exposed for the assumed exposure duration, ED. For ingestion of contaminants through fruits, vegetables, or grains (FVG), the ratio of average daily dose (ADD), in mg/kg-d, of contaminants to water concentration, in mg/L; air concentration, in mg/m³; and soil concentration, in mg/kg, can be expressed using potential dose factors (PDF) with respective units of L/kg-d, m³/kg-d, and kg/kg-d,

$$\begin{aligned} \text{ADD}(\text{FVG ingestion}) = & \text{PDF}(\text{air gases to FVG}) \times C_a + \text{PDF}(\text{air particles to FVG}) \times C_{\text{ap}} \\ & + \text{PDF}(\text{surface water to FVG}) \times C + \text{PDF}(\text{ground soil to FVG}) \times C_g \quad [100] \end{aligned}$$

Contamination by Ambient-Air Contaminants

The ingestion intake of contaminants in fruits, vegetables, and grains contaminated by air involves the transfer of contaminants from air through deposition/resuspension of particle-bound contaminants or through foliar uptake of gas-phase contaminants. The intermedia-transfer factor, C_{plant}/C_a is the ratio of contaminant concentration in fresh produce, mg/kg(fresh mass), to contaminant concentration, mg/m³, in the gas phase of the ambient outdoor air and equal to the plant-air partition coefficient, $K_{\text{pa}}^{\text{gs}}$. The intermedia-transfer factor, $C_{\text{plant}}/C_{\text{ap}}$ is the ratio of contaminant concentration in fresh produce, mg/kg(fresh mass), to contaminant concentration, mg/m³, in the particle (or dust) phase of the ambient outdoor air and equal to the plant-air partition coefficient, $K_{\text{pa}}^{\text{pt}}$. Both $K_{\text{pa}}^{\text{gs}}$ and $K_{\text{pa}}^{\text{pt}}$ are discussed above and defined in terms of a mean value and a CV in Table V. The

inclusion of ingestion rates and exposure factors from Tables V and VI with these intermedia-transfer factors gives the PDFs for estimating doses through the air/plant/ingestion pathway,

$$\text{PDF(air gases to FVG)} = K_{pa}^{gs} \times \left(I_{fv} \times f_{abv-grd}^v \times f_{local}^v + I_g \times f_{local}^g \right) \text{ and} \quad [101]$$

$$\text{PDF(air particles to FVG)} = K_{pa}^{pt} \times \left(I_{fv} \times f_{abv-grd}^v \times f_{local}^v + I_g \times f_{local}^g \right) . \quad [102]$$

Contamination by Irrigation Water

For this exposure pathway, there are two intermedia-transfer factors, C_i/C_k , one for ground water and one for surface water. These ratios express the ratio of contaminant concentration in fresh produce, mg/kg(fresh mass), to contaminant concentration, mg/L, in the nearest ground or surface water at a contaminated site. For exposed produce these ratios are based on rainsplash and transfers to above-ground plant parts and are given by

$$C_{ep}/C_w = (1 - f_{gw}^w) \times (K_{ps}^{rain} + K_{ps}) \times K_D \times f_{ir} \quad (\text{for surface water}) \quad [103]$$

where C_{ep} refers to exposed produce. For protected produce and root crops, these ratios are based the root concentration factor, $K_{ps}(\text{roots})$, discussed above and are given by

$$C_{pp}/C_w = (1 - f_{gw}^w) \times K_{ps}(\text{roots}) \times K_d \times f_{ir} \quad (\text{for surface water}) \text{ and} \quad [104]$$

where C_{pp} refers to protected produce. Other partition coefficients and parameters used in this expression are discussed above and summarized in terms of mean values and coefficients of variation in a companion report on ITF factors. The inclusion of ingestion rates and exposure factors from Tables V and VI with the intermedia-transfer factor gives the following PDF for this exposure pathway,

$$\begin{aligned}
\text{PDF}(\text{surface water to FVG}) = & \left(1 - f_{gw}^w\right) \times \left\{ \left[I_{fv} \times f_{local}^v \right] \times \left[35 K_{ps} \times \left(1 - f_v^{abg}\right) \right. \right. \\
& \left. \left. + \left(K_{ps}^{rain} + K_{ps} \right) \times f_v^{abg} \right] \right. \\
& \left. + \left(I_g \times f_{local}^g \right) \times \left(K_{ps}^{rain} + K_{ps} \right) \right\} \times K_D \times f_{ir}
\end{aligned} \tag{105}$$

Parameters in these expressions are discussed above and summarized in Tables V through VII.

Contamination by Surface Soil

The ingestion intake of contaminants in fruits, vegetables, and grains contaminated by surface soil involves the transfer of contaminants from soil to plants. The intermedia-transfer factor, C_{ep}/C_{soil} , is the ratio of contaminant concentrations in exposed produce (ep) in mg/kg (fresh mass) to contaminant concentration, in mg/kg, in surface soil and equal to the rainsplash partition coefficient, K_{ps}^{rain} , which is discussed above and defined in terms of mean value and CV in Table V. The inclusion of ingestion rates for exposed produced from Table V and exposure factors from Table VI with this intermedia-transfer factor gives the following PDF for exposure through the soil/plant/ingestion pathway for homegrown fruits, vegetables, and grains,

$$\text{PDF}(\text{surface soil to FVG}) = K_{ps}^{rain} \times \left[\left(I_{fv} \times f_{fv}^{abg} \times f_{local}^v \right) + \left(I_g \times f_{local}^g \right) \right] . \tag{106}$$

Contamination by Root-Zone Soil

The ingestion intake of contaminants in fruits, vegetables, and grains contaminated by root-zone soil involves the transfer of contaminants from soil to both exposed produce (ep) and protected produce (pp). The corresponding intermedia-transfer factors, C_{ep}/C_s and C_{pp}/C_s , are the ratios of contaminant concentration in exposed and protected produce, mg/kg (fresh mass), to contaminant concentration, mg/kg, in root-zone soil and equal to K_{ps} and $K_{ps}(\text{roots})$, respectively. These factors are discussed above and defined in terms of mean value and CV in Table V. The inclusion of ingestion rates of exposed and protected produce from Table V and exposure factors from Table VI with these intermedia-transfer factors gives the following PDF for exposure through the root-soil/plant/ingestion pathway for homegrown fruits, vegetables, and grains,

$$\begin{aligned} \text{PDF}(\text{root - zone soil to FVG}) = & K_{ps} \times \left[\left(I_{fv} \times f_{local}^v \times f_{fv}^{abg} \right) + \left(I_g \times f_{local}^g \right) \right] \\ & + K_{ps}(\text{roots}) \times I_{fv} \times f_{local}^v \times \left(1 - f_{fv}^{abg} \right) . \end{aligned} \quad [107]$$

Ingestion of Contaminated Meat, Milk, and Eggs

Ingestion doses to humans through local or homegrown meat, milk, and/or eggs is based on potential contamination from air gases, air particles, surface soil, root-zone soil, surface water, and ground water. For these environmental media, the associated average daily doses are expressed as the average daily dose to the individual exposed for the assumed exposure duration, ED. The ratio of average daily dose (ADD) of contaminants, in mg/kg-d, to soil concentrations, in mg/kg; air concentrations, in mg/m³; and water concentrations, in mg/L, can be expressed using potential dose factors (PDF) with respective units of kg/kg-d, m³/kg-d, and L/kg-d,

$$\begin{aligned} \text{ADD}(\text{milk, meat, eggs}) = & [\text{PDF}(\text{air gas to milk}) + \text{PDF}(\text{air gases to meat}) \\ & + \text{PDF}(\text{air gases to eggs})] \times C_a + [\text{PDF}(\text{air particles to milk}) \\ & + \text{PDF}(\text{air particles to meat}) + \text{PDF}(\text{air particles to eggs})] \times C_{ap} \\ & + [\text{PDF}(\text{surface water to milk}) + \text{PDF}(\text{surface water to meat}) \\ & + \text{PDF}(\text{surface water to eggs})] \times C_w \\ & + [\text{PDF}(\text{surface soil to milk}) + \text{PDF}(\text{surface soil to meat}) \\ & + \text{PDF}(\text{surface soil to eggs})] \times C_g + [\text{PDF}(\text{root-zone-soil to milk}) \\ & + \text{PDF}(\text{root-zone-soil to meat}) + \text{PDF}(\text{root-zone-soil to eggs})] \times C_s . \end{aligned} \quad [108]$$

Contamination by Transfer from Air to Animal Products

Contaminants in air can be transferred from air to meat-, milk-, and egg-producing animals both directly by inhalation and indirectly by animal ingestion of plants that have taken up contaminants from air. We consider the gas phase of the air and air particles separately. For the gas phase of ambient air, the intermediate transfer factors, C_{meat}/C_a , C_{milk}/C_a , and C_{egg}/C_a express the ratio of contaminant concentration in fresh food product, mg/kg(fresh mass), to contaminant concentration, mg/m³, in ambient air gases,

$$C_{\text{meat}}/C_a = [I_{\text{nc}} + K_{\text{pa}}^{\text{gs}} \times I_{\text{vbc}}] \times B_t \quad \text{for meat,} \quad [109]$$

$$C_{\text{milk}}/C_a = [I_{\text{nc}} + K_{\text{pa}}^{\text{gs}} \times I_{\text{vdc}}] \times B_k \quad \text{for milk, and} \quad [110]$$

$$C_{\text{egg}}/C_a = [I_{\text{nh}} + K_{\text{pa}}^{\text{gs}} \times I_{\text{vh}}] \times B_e \quad \text{for eggs.} \quad [111]$$

For particle-bound contaminants in ambient air, the intermedia-transfer factors, C_{meat}/C_a , C_{milk}/C_a , and C_{egg}/C_a express the ratio of contaminant concentration in fresh food product, mg/kg(fresh mass), to contaminant concentration, mg/m³, attached to particles in ambient air,

$$C_{\text{meat}}/C_{\text{ap}} = [I_{\text{nc}} + K_{\text{pa}}^{\text{pt}} \times I_{\text{vbc}}] \times B_t \quad \text{for meat,} \quad [112]$$

$$C_{\text{milk}}/C_{\text{ap}} = [I_{\text{nc}} + K_{\text{pa}}^{\text{pt}} \times I_{\text{vdc}}] \times B_k \quad \text{for milk, and} \quad [113]$$

$$C_{\text{egg}}/C_{\text{ap}} = [I_{\text{nh}} + K_{\text{pa}}^{\text{pt}} \times I_{\text{vh}}] \times B_e \quad \text{for eggs.} \quad [114]$$

I_{nc} and I_{nh} are the daily inhalation rates by, respectively, cattle and egg-laying hens in m³/d and I_{vdc} , I_{vbc} , and I_{vh} are the daily intakes of pasture by, respectively, beef cattle, dairy cattle, and egg-laying hens in kg(dry mass)/d. These and other parameters have been defined previously and are listed in Table VII.

In order to calculate the exposure to the local population that results from intermedia transfers from ambient air as derived above, we combine these intermedia-transfer factors with intake rates and local consumption fractions to obtain the following PDFs,

$$\text{PDF(air-gases to meat)} = I_{\text{mt}} \times [I_{\text{nc}} + K_{\text{pa}}^{\text{gs}} \times I_{\text{vbc}}] \times B_t \times f_{\text{local}}^{\text{mt}}, \quad [115]$$

$$\text{PDF(air-gases to milk)} = I_{\text{mk}} \times [I_{\text{nc}} + K_{\text{pa}}^{\text{gs}} \times I_{\text{vdc}}] \times B_k \times f_{\text{local}}^{\text{mk}}, \quad [116]$$

$$\text{PDF(air-gases to eggs)} = I_{\text{egg}} \times [I_{\text{nh}} + K_{\text{pa}}^{\text{gs}} \times I_{\text{vh}}] \times B_e \times f_{\text{local}}^{\text{egg}}, \quad [117]$$

$$\text{PDF(air-particles to meat)} = I_{mt} \times [I_{nc} + K_{pa}^{pt} \times I_{vbc}] \times B_t \times f_{local}^{mt} , \quad [118]$$

$$\text{PDF(air-particles to milk)} = I_{mk} \times [I_{nc} + K_{pa}^{pt} \times I_{vdc}] \times B_k \times f_{local}^{mk} , \text{ and} \quad [119]$$

$$\text{PDF(air-particles to eggs)} = I_{egg} \times [I_{nh} + K_{pa}^{pt} \times I_{vh}] \times B_e \times f_{local}^{egg} . \quad [120]$$

The fractions of meat, milk, or eggs obtained from local sources is the fraction of the exposed population's intake of meat, milk, or eggs that comes from animals that are exposed to ambient air with contaminant concentrations C_a and C_{ap} .

Contamination by Transfer from Water to Animal Products

The ingestion intake of contaminants in local or homegrown milk, meat, and eggs involves the transfer of contaminants from water to animal products both through the direct ingestion of water by the animals and through ingestion of pasture and feed contaminated by the use of contaminated irrigation water. The intermedia-transfer factors, C_{meat}/C_w , C_{milk}/C_w , and C_{egg}/C_w , express the ratio of contaminant concentration in fresh food product, mg/kg (fresh mass), to contaminant concentration, mg/L, in the nearest surface water at the contaminated site and the intermedia-transfer factors, C_{meat}/C_q , C_{milk}/C_q , and C_{egg}/C_q , express the ratio of contaminant concentration in fresh-food product, mg/kg (fresh mass), to contaminant concentration, mg/L, in the nearest ground water at the contaminated site. These intermedia ratios are given by the expressions,

$$C_{meat}/C_w = \left[(1 - f_{gw}^w) \times I_{wbc} + \left(I_{vbc} \times \frac{C_{ep}}{C_w} \right) \right] \times B_t \quad \text{for meat,} \quad [121]$$

$$C_{milk}/C_w = \left[(1 - f_{gw}^w) \times I_{wdc} + \left(I_{vdc} \times \frac{C_{ep}}{C_w} \right) \right] \times B_k \quad \text{for milk,} \quad [122]$$

$$C_{egg}/C_w = \left[(1 - f_{gw}^w) \times I_{wh} + \left(I_{vh} \times \frac{C_{ep}}{C_w} \right) \right] \times B_e \quad \text{for eggs,} \quad [123]$$

where, I_{wbc} , I_{wdc} , and I_{wh} are the daily intakes of water by, respectively, beef cattle, dairy cattle, and egg-laying hens in L/d and I_{vbc} , I_{vdc} , and I_{vh} are the daily intakes of

pasture by, respectively, beef cattle, dairy cattle, and egg-laying hens in kg(dry mass)/d. The intermedia-transfer factors, C_{ep}/C_w and C_{ep}/C_w are the intermedia-transfer factor for pasture or feed and are modeled as exposed produce and set equal to the terms derived above for intermedia transfer from irrigation water to exposed produce. Other factors have been defined previously.

In order to calculate the exposure to the local population that results from intermedia transfers from ground and surface water as derived above, we use the following PDFs,

$$\begin{aligned} \text{PDF}(\text{surface water to meat}) &= I_{mt} \times f_{\text{local}}^{\text{mt}} \times (1 - f_{\text{gw}}^w) \\ &\times \left\{ I_{wbc} + \left[I_{vbc} \times (K_{ps}^{\text{rain}} + K_{ps}) \times K_D \times f_{ir} \right] \right\} \times B_t , \end{aligned} \quad [124]$$

$$\begin{aligned} \text{PDF}(\text{surface water to milk}) &= I_{mk} \times f_{\text{local}}^{\text{mk}} \times (1 - f_{\text{gw}}^w) \\ &\times \left\{ I_{wdc} + \left[I_{vdc} \times (K_{ps}^{\text{rain}} + K_{ps}) \times K_D \times f_{ir} \right] \right\} \times B_k , \end{aligned} \quad [125]$$

$$\begin{aligned} \text{PDF}(\text{surface water to eggs}) &= I_{egg} \times f_{\text{local}}^{\text{egg}} \times (1 - f_{\text{gw}}^w) \\ &\times \left\{ I_{wh} + \left[I_{vh} \times (K_{ps}^{\text{rain}} + K_{ps}) \times K_D \times f_{ir} \right] \right\} \times B_e , \end{aligned} \quad [126]$$

The fractions of meat, milk, or eggs obtained from local sources are the fractions of the exposed population's intakes of meat, milk, or eggs that comes from animals that ingest water having estimated concentrations of C_w or C_q .

Contamination by Transfer from Surface Soil to Animal Products

Contaminants in surface soil can enter meat, milk, or eggs through either the direct ingestion of soil by animals or the ingestion by animals of pasture vegetation that has taken up a contaminant from surface soil through rainsplash. The intermedia-transfer factors, C_{meat}/C_g , C_{milk}/C_g , and C_{egg}/C_g express the ratio of contaminant concentration in fresh-food product, mg/kg(fresh mass), to contaminant concentration, mg/kg, in the surface soil associated with the contaminated site. These intermedia ratios are given by the expressions,

$$C_{\text{meat}}/C_g = [I_{sc} + (K_{ps}^{\text{rain}} \times I_{vbc})] \times B_t \quad \text{for meat,} \quad [127]$$

$$C_{\text{milk}}/C_g = [I_{sc} + (K_{ps}^{\text{rain}} \times I_{vdc})] \times B_k \quad \text{for milk, and} \quad [128]$$

$$C_{\text{egg}}/C_g = [I_{sh} + (K_{ps}^{\text{rain}} \times I_{vh})] \times B_e \quad \text{for eggs,} \quad [129]$$

where I_{sc} and I_{sh} are the daily intakes of soil by, respectively, cattle and egg-laying hens in kg/d. Other factors have been defined previously.

In order to calculate the exposure to the local population that results from intermedia transfers from surface soil as derived above, we combine these intermedia-transfer factors with intake rates and local consumption fractions to obtain the following PDFs.

$$\text{PDF}(\text{surface soil to meat}) = I_{mt} \times f_{\text{local}}^{\text{mt}} \times [I_{sbc} + (K_{ps}^{\text{rain}} \times I_{vbc})] \times B_t \quad [130]$$

$$\text{PDF}(\text{surface soil to milk}) = I_{mk} \times f_{\text{local}}^{\text{mk}} \times [I_{sdc} + (K_{ps}^{\text{rain}} \times I_{vdc})] \times B_k \quad [131]$$

$$\text{PDF}(\text{surface soil to eggs}) = I_{egg} \times f_{\text{local}}^{\text{egg}} \times [I_{sh} + (K_{ps}^{\text{rain}} \times I_{vh})] \times B_e \quad [132]$$

The fractions of meat, milk, or eggs obtained from local sources is the fraction of the exposed individual's intake of meat, milk, or eggs that comes from animals exposed to soil having an estimated contaminant concentration C_g .

Contamination by Transfer from Root-Zone Soil to Animal Products

Contaminants in surface soil can enter meat, milk, or eggs through either the either ingestion by animals of pasture vegetation or feed derived from vegetation that has taken up a contaminant from root soil. The intermedia-transfer factors, C_{meat}/C_s , C_{milk}/C_s , and C_{egg}/C_s express the ratio of contaminant concentration in fresh food product, mg/kg(fresh mass), to contaminant concentration, mg/kg, in the root-zone soil associated with the contaminated site. These intermedia ratios are given by the expressions,

$$C_{\text{meat}}/C_s = K_{ps} \times I_{vbc} \times B_t \quad \text{for meat,} \quad [133]$$

$$C_{\text{milk}}/C_s = K_{ps} \times I_{vdc} \times B_k \quad \text{for milk, and} \quad [134]$$

$$C_{egg}/C_s = K_{ps} \times I_{vh} \times B_e \quad \text{for eggs,} \quad [135]$$

which include parameters that have all been defined previously. In order to calculate the exposure to the local population that results from intermedia transfers from root-zone soil as derived above, we combine these intermedia-transfer factors with intake rates and local-consumption fractions to obtain the following PDFs.

$$\text{PDF}(\text{root-zone soil to meat}) = I_{mt} \times f_{local}^{mt} \times K_{ps} \times I_{vbc} \times B_t \quad [136]$$

$$\text{PDF}(\text{root-zone soil to milk}) = I_{mk} \times f_{local}^{mk} \times K_{ps} \times I_{vdc} \times B_k \quad [137]$$

$$\text{PDF}(\text{root-zone soil to eggs}) = I_{egg} \times f_{local}^{egg} \times K_{ps} \times I_{vh} \times B_e \quad [138]$$

The fractions of meat, milk, or eggs obtained from local sources is the fraction of the exposed individual's intake of meat, milk, or eggs that comes from animals exposed to root-zone soil having an estimated contaminant concentration C_s .

Ingestion of Contaminated Fish

Ingestion doses to humans through locally caught fish is based on potential contamination from surface water with contaminant concentration, C_w in mg/L. The intermedia-transfer factor between fish and surface water is the bioconcentration factor, BCF. The average daily dose to an individual within the exposed population during the exposure duration, ED, is

$$\text{ADD}(\text{fish ingestion}) = I_{fsh} \times \text{BCF} \times f_{local}^{fsh} \times C_w \quad [139]$$

The fraction of fish from local waters, f_{local}^{fsh} , is the fraction of a representative individual's annual intake of fish that comes from local sources that are contaminated by runoff from the contaminated site and have an estimated water concentration, C_w . The PDF for this exposure pathway is the ratio of ADD to C_w and is equal to the product, $I_{fsh} \times \text{BCF} \times f_{local}^{fsh}$.

Soil Ingestion by Human

For household soil, the intermedia-transfer factor, C_i/C_k , is the ratio of contaminant concentration in household surface soil, mg/kg, to contaminant concentration, mg/kg, in the surface soil of the contaminated site and is assigned a default value of unity. The average daily dose (ADD) to contaminants through soil ingestion is calculated using soil ingestion per unit body weight for the individual exposed for the assumed exposure duration, ED, and is given by

$$\text{ADD}(\text{soil ingestion}) = I_{sl} \times C_g . \quad [140]$$

The PDF in kg/kg-d for this exposure pathway is simply the ratio of average daily dose (ADD), in mg/kg-d, to surface-soil concentration, C_g , in mg/kg and equal to I_{sl} .

Ingestion of Surface Water During Swimming

For a recreational surface-water body, the intermedia-transfer factor, C_i/C_k is the ratio of contaminant concentration in the recreational water, C_w in mg/L, to contaminant concentration, mg/L, in the surface water that is contaminated either directly or through contaminant runoff. This ratio is assigned a default value of unity. The average daily dose (ADD) to contaminants through swimming-water ingestion is calculated using swimming ingestion per unit body weight, L/kg-d, for the individual exposed for the assumed exposure duration, ED, times the exposure frequency of swimming, EF_{sw} in d/y, and is given by

$$\text{ADD}(\text{swimming-water ingestion}) = I_{sww} \times EF_{sw} \times C_w . \quad [141]$$

Parameters in this expression are defined in terms of expected value and CV in Table VI. The PDF, in L/kg-d, for this exposure pathway is simply the ratio of average daily doses (ADD), in mg/kg-d, to surface water concentration, C_w in mg/L and equal to $I_{sww} \times EF_{sw}$.

Multiple Pathway Exposures and Total Dose: The Inhalation Route

In the total-dose assessment-model used in CAirTOX, we consider for the inhalation route all transfers of contaminants from contaminated environmental media to personal air. Personal air is the envelope of air contacted by an individual during a 24-h period and is based on both activity patterns and time-weighted

breathing rates. Concentrations of contaminants in six environmental media are used in the multiple pathway assessment for inhalation exposures: (1) the contaminant concentration in ambient air gases, C_a in mg/m^3 ; (2) the concentration of contaminant bound to air particles, C_{ap} in mg/m^3 ; (3) contaminant concentration in surface soil, C_g in mg/kg ; (4) contaminant concentration in root-zone soil below the surface layer, C_s in mg/kg ; (5) contaminant concentration in ground water, C_q in mg/L ; and (6) contaminant concentration in surface water, C_w in mg/L . In terms of the basic exposure model, expressed in equation [94], the inhalation intake of contaminants involves the intermedia transfer of contaminants from the environmental medium, k , which is one of the six media described above to the exposure medium i , which is personal air. For each pathway we derive an intermedia-transfer factor, C_i/C_k to express this ratio. For the intake rate of the exposure medium per unit body weight, $[I_n/BW]$, we use the daily average inhalation rates per unit body weight listed in Table V. The exposure frequency for all inhalation exposures is assumed to be 365 days per year.

Inhalation of Contaminants in Ambient Air

Inhalation exposure is based on the average concentration in an exposed individual's personal air. In the case of ambient air, there are two intermedia-transfer factors, C_i/C_k . The first is the ratio of contaminant concentration in the personal air breathed by individuals to the contaminant concentration in the gas phase of ambient air, C_a in mg/m^3 . The second is the ratio of contaminant concentration in the personal air to the concentration in ambient-air of particle-bound contaminant, C_{ap} in mg/m^3 . We assume that, for both gases and particles, the ambient-air concentrations exist both indoors and outdoors so that the ratio C_i/C_k is equal to the total hours per day spent at by an individual at a household either indoors or outdoors divided by 24, that is $(ET_h + ET_o)/24$. ET_h and ET_o are summarized in Table VI. The average daily potential doses to these gas-phase and particle-phase contaminants are related to the active and resting breathing rates listed in Table V, under the assumption that one spends 8 h breathing at the resting rate and 16 h breathing at the active rate (ICRP, 1975). This results in a average daily potential dose estimates of the form,

$$\text{ADD(ambient-air gases)} = (16 \text{ BR}_a + 8 \text{ BR}_r) \times \frac{(ET_h + ET_o)}{24} \times C_a \quad \text{and} \quad [142]$$

$$\text{ADD(ambient-air particles)} = (16 \text{ BR}_a + 8 \text{ BR}_r) \times \frac{(\text{ET}_h + \text{ET}_o)}{24} \times C_{ap} . \quad [143]$$

The PDFs for these exposures are the ratio of ADD to ambient-air concentration and are the same for both particles and gases.

Inhalation of Contaminants Transferred from Soil to Indoor Air

Contaminants in soil can be transferred from soil to indoor air either by tracking of surface soil as dust into the house on shoes, clothing, or pets or by the migration of vapors into the house from soil below the house. These two scenarios can increase indoor concentrations to levels higher than those associated with the migration of ambient-air contaminants into the house as described above.

Dust migration from Surface Soil

This scenario is used to account for exposures that occur when contaminated soil is tracked into the home by shoes of occupants and by pets. The scenario is used for situations in which the household is proximate to a site with contaminated soil. The source of contaminated soil is assumed to be surface soil with contaminant concentration C_g in mg/kg. The intermedia-transfer factor is equal to the contaminant concentration in personal air, C_{pair} , in mg/m³ attributable to surface soil divided by the contaminant concentration, C_g (mg/kg) in surface soil and is given by the expression,

$$C_{pair}/C_g = \text{dust}_{in} \times \text{ET}_h/24 , \quad [144]$$

where dust_{in} is the particle concentration (or dust load) inside a home in kg/m³, ET_h is the number of hours per day an individual spends at home, and $\text{ET}_h/24$ is the assumed fraction of personal air that is contacted at home. These parameters are discussed in the section on household parameters and listed in Table VI. Under the assumption that one spends 8 h per day breathing at the resting rate and 16 h per day breathing at the active rate (ICRP, 1975), we estimate the average daily potential dose, ADD, in mg/kg-d, from tracked-in soil as

$$\text{ADD(tracked-in soil)} = (16 \text{ BR}_a + 8 \text{ BR}_r) \times \text{dust}_{in} \times \text{ET}_h/24 \times C_g . \quad [145]$$

The PDF for this exposure is the ratio of ADD to surface-soil concentration.

Vapor migration from Root-Zone Soil

This scenario is used to represent exposure in homes built near or over contaminated soil such that the base of the foundation is within approximately 1 m of the contaminated root-zone soil. The intermedia-transfer factor for this pathway is equal to the magnitude of contaminant concentration in the gas phase of personal air, C_{air} in mg/m^3 , attributable to soil-gas migration divided by the contaminant concentration in dry root-zone soil, C_s in mg/kg , and this ratio is given by

$$C_{air}/C_s = \alpha_{inair} \times ET_h/24 , \quad [146]$$

where α_{inair} is the partition coefficient for indoor-air concentration relative to soil concentration as described previously in the section on partition factors and listed in Table V, and $ET_h/24$ is used as described above in the soil-tracking scenario. Under the assumption that an exposed individual spends 8 h per day breathing at the resting rate and 16 h per day breathing at the active rate (ICRP, 1975), we estimate the average daily potential dose, ADD, in $\text{mg}/\text{kg-d}$, from soil-vapor migration as

$$\text{ADD}(\text{soil-vapor migration}) = (16 BR_a + 8 BR_r) \times \alpha_{inair} \times ET_h/24 \times C_s . \quad [147]$$

The PDF for this exposure is the ratio of ADD to root-zone soil concentration.

Inhalation of Contaminants Transferred from Water to Indoor Air

When surface water that provides a source of tap water for a household contain volatile contaminants, these contaminants can be transferred from tap water to personal air by showers, baths, and other household-water uses. In this case the environmental medium is surface water and the exposure medium is personal air. The intermedia-transfer factor for these transfers is equal to the contaminant concentration in personal air, C_{pair} , in mg/m^3 attributable to surface water divided by the contaminant concentrations C_w and is given by the expression

$$\begin{aligned}
C_{\text{pair}} / C_w = & (1 - f_{\text{gw}}^w) \times \left\{ \frac{W_{\text{shower}} \times \phi_x(\text{bath/shower})}{VR_{\text{bath}}} \times ET_{\text{sb}} \times BR_a \right. \\
& + \left. \frac{W_{\text{house}} \times \phi_x(\text{house})}{VR_{\text{house}}} \times [(ET_h - 8) \times BR_a + 8 \times BR_r] \right\} \\
& \times [16 \times BR_a + 8 \times BR_r]^{-1}
\end{aligned} \quad [148]$$

where ET_h is the number of hours per day an individual spends at home, ET_{sb} is the number of hours per day spent in the bathroom or shower, $ET_{\text{sb}} \times BR_a / [16 BR_a + 8 BR_r]$ is the assumed fraction of personal air that is contacted in the shower or bathroom, and $[(ET_h - 8) \times BR_a + 8 BR_r] / [16 BR_a + 8 BR_r]$ is the assumed fraction of personal air contacted in the home outside of the bathroom and shower. These fractions are based on the assumption that one spends 8 h per day breathing at the resting rate and 16 h per day breathing at the active rate (ICRP, 1975). Other parameters in these equations are discussed in the section on household parameters and listed in Table VI. We multiply the expressions above by daily air intake per unit body weight to obtain estimates of average daily potential doses, ADD, in mg/kg-d, associated with inhalation of waterborne contaminants transferred to personal air from either ground or surface water as

$$ADD(\text{surface water to personal air}) = (16 BR_a + 8 BR_r) \times (C_{\text{pair}} / C_w) \times C_w \quad \text{and} \quad [149]$$

The PDFs for these exposures are the ratios of ADDs to, respectively, surface-water and ground-water concentration.

Multiple-Pathway Exposures and Total Dose: The Dermal-Uptake Route

In the total-dose-assessment model developed for CAirTOX, we consider for the dermal-uptake-route transfers of contaminants from contaminated environmental media into the outer-skin layer, the stratum corneum.

Concentrations of contaminants in two environmental media are used in the multiple-pathway assessment for dermal exposures: (1) contaminant concentration in surface soil, C_g in mg/kg and (2) contaminant concentration in surface water, C_w in mg/L. In terms of the basic exposure model, expressed in equation [94], the uptake of contaminants into skin involves the intermedia transfer of contaminants

from the environmental medium, k , which is one of the three media described above, to the exposure medium, i , which is household soil, tap water, or swimming water. For each pathway we derive an intermedia-transfer factor, C_i/C_k , to express this ratio.

Dermal Contact While Swimming or Bathing

For human exposures during swimming, both the environmental medium and the exposure medium are surface water and the intermedia-transfer factor is unity. Dermal uptake from surface or ground water that provide sources of tap water involves the intermedia transfer from surface or ground water to tap water and the intermedia-transfer factors, C_{tw}/C_w and C_{tw}/C_g , are, respectively, the fraction of tap water obtained from surface water, $1-f_{gw}^w$, and the fraction of tap water obtained from ground water, f_{gw}^w .

The average daily potential dose, ADD in mg/kg-d, to an individual whose exposure time swimming is ET_{sw} h/d and whose exposure frequency swimming is EF_{sw} d/y is given by

$$ADD(\text{dermal uptake swimming}) = \frac{UF_{sw}}{BW} \times \frac{EF_{sw}}{365 \text{ d/y}} \times C_w, \quad [150]$$

where UF_{sw} expresses the dermal uptake during the exposure time ET_{sw} in mg/d per unit concentration (mg/L) in the water and is given by

$$\frac{UF_{sw}}{BW} = AR_{\text{water}} \times 1.0 \times SA_b \times 10 \text{ L/cm}^2, \quad [151]$$

where 1.0 is the fraction of total body surface area, SA_b [$\text{m}^2/\text{kg}(\text{BW})$], assumed to be in contact with water during swimming, and AR_{water} expresses the ratio of the absorbed dose per event of duration ET_{sw} [this absorbed dose is referred to as DA_{event} by U.S. EPA (1992)] to exposure-medium concentration and is equal to uptake per unit area of skin per unit concentration in water, mg/cm^2 per mg/cm^3 . Other parameters in this equation are discussed in the sections above on human anatomical data and activity patterns. Dividing equation [150] by C_w gives the PDF for this exposure pathway.

For an individual whose exposure time showering or bathing is $ET_{sb}/2$ hours per day (since ET_{sb} is the total time spent in the bathroom and half of that time is

assumed spent in either the shower or bath) and whose exposure frequency showering and bathing is assumed to be one event per day for 365 d/y, the average daily dose, ADD in mg/kg-d, is given by

$$\text{ADD}(\text{shower/bath dermal uptake}) = (1 - f_{gw}^w) \times \frac{UF_{sb}}{BW} \times C_w \quad [152]$$

where UF_{sb} expresses the dermal uptake during the exposure time $ET_{sb}/2$ in mg/d per unit concentration (mg/mL) in the water. As was the case for swimming exposure, the term $\frac{UF_{sb}}{BW}$ is given by equation [151]. Dividing equation [152] by C_w gives the surface-water PDF for this exposure pathway.

The parameter AR_{water} can be divided by the exposure time to obtain the effective permeability (cm/h) of a contaminant from water into the stratum corneum. Based on the work of McKone and Howd (1992), we estimate AR_{water} for organic chemicals in terms of the skin-water partition coefficient, K_m , and the skin thickness δ_{skin} , in cm, as

$$AR_{\text{water}} = \frac{\delta_{\text{skin}} K_m}{2} , \quad [153]$$

when the lag time, LT in h, is less than or equal to the exposure time, ET (either ET_{sb} or ET_{sw}), and

$$AR_{\text{water}} = \frac{\delta_{\text{skin}} K_m}{2} + (ET - LT) \times K_p^w , \quad [154]$$

when the exposure time is greater than the lag time. Based on McKone and Howd, (1992), the skin thickness, δ_{skin} , is taken as 0.0025 cm, the lag time, LT in h, is given by

$$LT = \frac{(0.0017 + 0.00067 K_{ow}^{0.8})}{6 K_p^w} , \quad [155]$$

where K_{ow} is the octanol-water partition coefficient and K_p^w is the steady-state permeability coefficient in cm/h for a contaminant from water on skin through stratum corneum and can either be based on a measured value or estimated as

$$K_p^w = MW^{-0.6} \times \left[\frac{2.4 \times 10^{-6} + 3.0 \times 10^{-5} K_{ow}^{0.8}}{\delta_{skin}} \right], \quad [156]$$

where MW is the molecular weight of the chemical in question. Equation [156] is taken from McKone and Howd (1992), who recommend that it be used for compounds with $MW \leq 280$. For compounds with $MW > 280$, an expression suggested by the U.S. EPA (1992) is used,

$$K_p^w = 0.0019 \times K_{ow}^{0.71} \times 10^{(-0.0061 \times MW)}. \quad [157]$$

Equation [157] is only recommended for compounds with $MW > 280$, since its estimation error is lower than that associated with equation [156] (McKone and Howd, 1992). However, following the guidance of the U.S. EPA (1992), we do not allow the value of K_p^w to exceed 1 cm/h, since no value higher than this has been measured experimentally. When equation [156] or [157] predict a value higher than 1 cm/h, we use 1 cm/h as a default.

Dermal Contact with Soil

For exposures to contaminants in soil on human skin, the environmental medium is surface soil, with concentration, C_g (mg/kg), and the exposure medium is household soil and the intermedia-transfer factor between household soil and environmental soil is assumed to be unity.

For an individual whose soil exposure time is ET_{sl} in h/d and whose exposure frequency is 1 event per day, the average daily dose, ADD in mg/kg-d, is given by

$$ADD(\text{dermal uptake from soil}) = \frac{UF_{sl}}{BW} \times \frac{EF_{sl}}{365} \times (1 \text{ event/d}) C_g, \quad [158]$$

where BW is the body weight of the exposed individual, EF_{sl} is the exposure frequency in d/y, and UF_{sl} expresses the dermal uptake during the exposure time,

ET_{sl} . UF_{sl} has units of kg/d, which is the mg/d per unit concentration of contaminant, in mg/kg, in the surface-soil medium and is given by

$$\frac{UF_{sl}}{BW} = AR_{soil} \times SA_b \times 0.3 \times 15 \text{ kg/cm-m}^2, \quad [159]$$

where 0.3 is the fraction of the total body surface area, SA_b [$\text{m}^2/\text{kg}(\text{BW})$], assumed to be in contact with soil during contact, 15 kg/cm-m^2 is a conversion factor based on a soil density of 1500 kg/m^3 , and AR_{soil} expresses the ratio of the absorbed dose per event of duration ET_{sl} to exposure medium concentration and is equal to uptake per unit area of skin per unit concentration in soil, mg/cm^2 per mg/cm^3 . Based on the work of McKone and Howd (1992), we approximate AR_{soil} as

$$AR_{soil} = \delta_{soil} \times \left\{ 1 - \exp \left(\frac{-K_p^s \times ET_{sl}}{\delta_{soil}} \right) \right\}, \quad [160]$$

where K_p^s is the permeability of a contaminant from soil into and through the stratum corneum in cm/h , and δ_{soil} is the thickness of the soil layer on skin. Based on a soil loading of 0.5 mg/cm^2 (as described in the section on exposure parameters) and a soil density of 1500 mg/cm^3 , we calculate δ_{soil} as $3 \times 10^{-4} \text{ cm}$. We assume the exposure time per exposure event, ET_{sl} , is equal to $ET_h/2$, that is half the exposure time at home. The soil-skin permeability in cm/h is derived from the water-skin permeability, K_p^w , according to

$$K_p^s = \frac{K_D}{K_m} \times K_p^w \times 1.7, \quad [161]$$

where K_m is the skin-water partition coefficient and K_D is the soil-water partition coefficient discussed in the section on partition coefficients, and the factor 1.7 accounts for the difference in thickness between fully hydrated skin in contact with water and less-hydrated skin in contact with soil (McKone and Howd, 1992). Other parameters in these equations are discussed in the sections above on human anatomical data and exposure factors. Making the appropriate substitutions and dividing equation [97] by C_g gives the PDF for this exposure pathway.

Contamination of Mother's Milk

Lactating women can transfer to breast milk their intake of contaminants from all intake routes—ingestion, inhalation, and dermal contact. Thus, ingestion of mother's milk by infants can be an important exposure in many situations. This possibility is addressed by calculating the average daily dose to the infant from ingestion of mother's milk. In terms of the basic exposure model, expressed in equation [94], the ingestion intake of contaminants through breast milk involves the transfer of contaminants from each environmental medium, k , air, water, and soil. For this exposure scenario there are three intermedia-transfer factors, C_i/C_k , that express the ratio of contaminant concentration breast milk, $C_{bm k}$ in mg/kg, to contaminant concentration in, respectively, air (mg/m³), water (mg/L), and soil (mg/kg). For each medium, k , this intermedia-transfer factor is given by

$$C_{bm k}/C_k = \text{PDF}(\text{by mother from medium } k) \times BW_{mo} \times B_{bm k} \quad [162]$$

where PDF is the average daily potential dose factor to the mother from all pathways linked to medium k , BW_{mo} is the mother's body weight, equal to 65.4 kg with CV 0.2 (Najjar and Roland, 1987). $B_{bm k}$ is the milk-concentration-versus-intake biotransfer factor, described above and listed in Table V. The average daily dose to the infant, ADD(infant) in mg/kg-d, is

$$\text{ADD}(\text{infant}) = [C_{bm k}/C_{air} + C_{bm k}/C_{water} + C_{bm k}/C_{soil}] \times I_{bm} \times \frac{ED}{AT} \quad [163]$$

where I_{bm} is the intake of breast milk per unit body weight per day by infants, kg(milk)/kg-d as discussed above and listed in Table VI. We estimate the ADD for this exposure with ED equal to one year and AT set to 365 d to estimate dose to the infant for noncarcinogens and AT set to 25,550 days (70 years) for carcinogens. The PDFs for infant exposures are the ratios of ADDs of contaminants to the infant, in mg/kg-d, to contaminant concentrations in water in mg/L, in soil in mg/kg, and in air in mg/m³. These ratios are based on the summation, taken independently from each medium, of all potential exposures to the mother through inhalation, ingestion, and dermal contact exposure.

PART IV. SUMMARY COMPARISON TO HRA WITH EXAMPLES

In this part of the report, we compare the existing HRA approach and predictions and the CAirTOX exposure equations and predictions. We provide a summary table for the exposure scenarios in CAirTOX and compare these to the exposure scenarios in HRA.

The matrix of equations in Table VIII summarizes the expressions for the PDFs developed in this report. Parameters used in these expressions are defined and assigned values in Tables V through VII.

The Health Risk Assessment (HRA) computer program has been developed by the State of California Air Resources Board (ARB) and the Office of Environmental Health Hazard Assessment (OEHHA). This program is used to carry out multiple pathway exposure assessment. HRA assists the evaluation of health risks associated with toxic chemical emissions to air and allows users to assess the potential for exposure to air emissions through inhalation as well as non-inhalation exposure routes. HRA has been used to carry out risk assessments for facilities subject to the California Air Toxics "Hot-Spots" Program and for municipal waste incinerators and medical wastes incinerators. HRA can calculate cancer risk and cancer burden and hazard indices for non-cancer health effects. The program requires as input atmospheric dispersion modeling results for the air shed in the vicinity of the facility being assessed. CAirTOX is intended to expand on the approach use in HRA. In order to make clear the differences in exposure pathways used in these two models, Table IX repeats the matrix of scenarios shown in Table IV as those covered by CAirTOX. The unshaded listings are exposure pathways included in both models and the shaded pathways are those included only in CAirTOX.

Table VIII. Summary of the potential-dose factor (PDF) expressions developed in this report; parameters used in these expressions are summarized in Tables V through VII.

EXPOSURE pathways	Air (gaseous)	Air (dust)	Ground-surface soil	Root-zone soil	Surface water
Personal air	$\frac{\text{m}^3/\text{kg-d}}{(16 \text{ BR}_g + 8 \text{ BR}_i) \times \frac{(\text{ET}_h + \text{ET}_c)}{24}}$	$\frac{\text{m}^3/\text{kg-d}}{(16 \text{ BR}_g + 8 \text{ BR}_i) \times \frac{(\text{ET}_h + \text{ET}_c)}{24}}$	$\frac{\text{kg}/\text{kg-d}}{(16 \text{ BR}_g + 8 \text{ BR}_i) \times \frac{\text{dust}_{10} \times \text{ET}_h}{24}}$	$\frac{\text{kg}/\text{kg-d}}{(16 \text{ BR}_g + 8 \text{ BR}_i) \times \frac{\alpha_{\text{air}} \times \text{ET}_h}{24}}$	$\frac{L/\text{kg-d}}{(16 \text{ BR}_g + 8 \text{ BR}_i) \times (C_{\text{path}}/C_w)}$ (see equation (148))
Tap water (ingestion)	..	..	..	..	$I_h \times (1 - f_{\text{gw}}^w)$
Tap water (dermal)	..	..	..	..	$(1 - f_{\text{gw}}^w) \times \frac{\text{UF}_{\text{sb}}}{B W}$
Exposed produce	$K_{\text{pa}}^{\text{g}} \times \left(I_{\text{rv}} \times f_{\text{rv}}^{\text{abg}} \times f_{\text{local}}^{\text{v}} + I_g \times f_{\text{local}}^{\text{g}} \right)$	$K_{\text{pa}}^{\text{p}} \times \left(I_{\text{rv}} \times f_{\text{rv}}^{\text{abg}} \times f_{\text{local}}^{\text{v}} + I_g \times f_{\text{local}}^{\text{g}} \right)$	$K_{\text{ps}}^{\text{rain}} \times \left[\left(I_{\text{rv}} \times f_{\text{rv}}^{\text{abg}} \times f_{\text{local}}^{\text{v}} \right) + \left(I_g \times f_{\text{local}}^{\text{g}} \right) \right]$	$K_{\text{ps}} \times \left[\left(I_{\text{rv}} \times f_{\text{rv}}^{\text{v}} \times f_{\text{local}}^{\text{v}} \right) + \left(I_g \times f_{\text{local}}^{\text{g}} \right) \right]$	$\left(1 - f_{\text{gw}}^w \right) \times \left[\left(I_{\text{rv}} \times f_{\text{local}}^{\text{v}} \right) \times f_{\text{v}}^{\text{abg}} + \left(I_g \times f_{\text{local}}^{\text{g}} \right) \right]$ $\times \left(K_{\text{ps}}^{\text{rain}} + K_{\text{ps}} \right) \times K_D \times f_{\text{ir}}$
Unexposed produce	..	..	..	$K_{\text{ps}} (\text{roots}) \times I_{\text{rv}} \times f_{\text{local}}^{\text{v}} \times \left(1 - f_{\text{rv}}^{\text{abg}} \right)$	$\left(1 - f_{\text{gw}}^w \right) \times \left[I_{\text{rv}} \times f_{\text{local}}^{\text{v}} \times \left(1 - f_{\text{v}}^{\text{abg}} \right) \right] \times K_{\text{ps}} (\text{roots})$ $\times K_D \times f_{\text{ir}}$
Meat	$I_{\text{mt}} \times \left[I_{\text{inc}} + K_{\text{pa}}^{\text{g}} \times I_{\text{vdc}} \right] \times B_i \times f_{\text{local}}^{\text{mt}}$	$I_{\text{mt}} \times \left[I_{\text{inc}} + K_{\text{pa}}^{\text{p}} \times I_{\text{vdc}} \right] \times B_i \times f_{\text{local}}^{\text{mt}}$	$I_{\text{mt}} \times f_{\text{local}}^{\text{mt}} \times K_{\text{ps}} \times I_{\text{vdc}} \times B_i$	$I_{\text{mt}} \times f_{\text{local}}^{\text{mt}} \times I_{\text{vdc}} + \left(K_{\text{ps}}^{\text{rain}} \times I_{\text{vdc}} \right) \times B_i$	$I_{\text{mt}} \times f_{\text{local}}^{\text{mt}} \times f_{\text{gw}}^w \times \left[I_{\text{vdc}} + \left(K_{\text{ps}}^{\text{rain}} + K_{\text{ps}} \right) \times \left[I_{\text{vdc}} + \left(K_{\text{ps}}^{\text{rain}} \times I_{\text{vdc}} \right) \right] \times B_i \right]$
Milk	$I_{\text{mk}} \times \left[I_{\text{inc}} + K_{\text{pa}}^{\text{g}} \times I_{\text{vdc}} \right] \times B_k \times f_{\text{local}}^{\text{mk}}$	$I_{\text{mk}} \times \left[I_{\text{inc}} + K_{\text{pa}}^{\text{p}} \times I_{\text{vdc}} \right] \times B_k \times f_{\text{local}}^{\text{mk}}$	$I_{\text{mk}} \times f_{\text{local}}^{\text{mk}} \times K_{\text{ps}} \times I_{\text{vdc}} \times B_k$	$I_{\text{mk}} \times f_{\text{local}}^{\text{mk}} \times \left[I_{\text{vdc}} + \left(K_{\text{ps}}^{\text{rain}} \times I_{\text{vdc}} \right) \right] \times B_k$	$I_{\text{mk}} \times f_{\text{local}}^{\text{mk}} \times f_{\text{gw}}^w \times \left[I_{\text{vdc}} + \left(K_{\text{ps}}^{\text{rain}} + K_{\text{ps}} \right) \times \left[I_{\text{vdc}} + \left(K_{\text{ps}}^{\text{rain}} \times I_{\text{vdc}} \right) \right] \times B_k \right]$
Eggs	$I_{\text{egs}} \times \left[I_{\text{inh}} + K_{\text{pa}}^{\text{g}} \times I_{\text{vh}} \right] \times B_e \times f_{\text{local}}^{\text{egs}}$	$I_{\text{egs}} \times \left[I_{\text{inh}} + K_{\text{pa}}^{\text{p}} \times I_{\text{vh}} \right] \times B_e \times f_{\text{local}}^{\text{egs}}$	$I_{\text{egs}} \times f_{\text{local}}^{\text{egs}} \times K_{\text{ps}} \times I_{\text{vh}} \times B_e$	$I_{\text{egs}} \times f_{\text{local}}^{\text{egs}} \times \left[I_{\text{vh}} + \left(K_{\text{ps}}^{\text{rain}} \times I_{\text{vh}} \right) \right] \times B_e$	$I_{\text{egs}} \times f_{\text{local}}^{\text{egs}} \times f_{\text{gw}}^w \times \left[I_{\text{vh}} + \left(K_{\text{ps}}^{\text{rain}} + K_{\text{ps}} \right) \times \left[I_{\text{vh}} + \left(K_{\text{ps}}^{\text{rain}} \times I_{\text{vh}} \right) \right] \times B_e \right]$ $\times K_D \times f_{\text{ir}} \times B_e$
Fish and seafood	..	..	I_{f}^{f}	..	$I_{\text{fsh}} \times \text{BCF} \times f_{\text{local}}^{\text{fsh}}$
Household soil (ingestion)	..	..	..	..	..
Household soil (dermal)	..	..	$\frac{\text{UF}_{\text{f}}^{\text{f}} \times \text{EF}_{\text{f}}}{B W \times 365 \text{ d/y}}$	..	$I_{\text{sww}} \times \text{EF}_{\text{sw}}$
Swimming water (ingestion)	..	..	..	..	$\frac{\text{UF}_{\text{sw}}^{\text{f}} \times \text{EF}_{\text{sw}}}{B W \times 365 \text{ d/y}}$
Swimming water (dermal)	..	..	..	..	..

Table IX. Matrix of exposure pathways used in CAirTOX and HRA to link environmental media, exposure scenarios, and exposure routes. Those pathways included only in CAirTOX are shaded and those included in both HRA and CAirTOX are not shaded.

Exposure routes	Media		
	Air (gases and particles)	Soil (surface soil and root-zone soil)	Water (surface water)
Inhalation	<ul style="list-style-type: none"> • Inhalation of gases and particles in outdoor air • Inhalation of gases and particles transferred from outdoor air to indoor air 	<ul style="list-style-type: none"> • Inhalation of soil vapors that migrate to indoor air • Inhalation of soil particles transferred to indoor air 	<ul style="list-style-type: none"> • Indoor inhalation of contaminants transferred from tap water
Ingestion	<ul style="list-style-type: none"> • Ingestion of fruits, vegetables, and grains contaminated by transfer of atmospheric chemicals to plant tissues • Ingestion of meat, milk, and eggs contaminated by transfer of contaminants from air to plants to animals • Ingestion of meat, milk, and eggs contaminated through inhalation by animals • Ingestion of mother's milk 	<ul style="list-style-type: none"> • Human soil ingestion • Ingestion of fruits, vegetables, and grains contaminated by transfer from soil • Ingestion of meat, milk, and eggs contaminated by transfer from soil to plants to animals • Ingestion of meat, milk, and eggs contaminated through soil ingestion by animals • Ingestion of mother's milk 	<ul style="list-style-type: none"> • Ingestion of tap water • Ingestion of irrigated fruits, vegetables, and grains • Ingestion of meat, milk, and eggs from animals consuming contaminated water • Ingestion of fish and sea food • Ingestion of surface water during swimming and other water recreation • Ingestion of mother's milk
Dermal contact	(not considered)	<ul style="list-style-type: none"> • Dermal contact with soil 	<ul style="list-style-type: none"> • Dermal contact in baths and showers • Dermal contact while swimming

Another way to compare CAirTOX and HRA is to consider how the quantitative results of the models differ for specific chemicals. Tables X and XI list potential doses by route and pathway predicted by HRA and CAirTOX using similar landscape characteristics and chemical properties for dioxins and furans (TCDD) and inorganic arsenic. In this simulation the air concentration was fixed at $10^{-9} \mu\text{g}/\text{m}^3$ for TCDD and $10^{-3} \mu\text{g}/\text{m}^3$ for arsenic. In comparing these results, we note that

- (1) the inhalation doses are comparable for both chemicals;
- (2) surface-water-ingestion doses are similar between the two models for arsenic but not for TCDD;
- (3) for both arsenic and TCDD, CAirTOX predicts higher potential does for home-grown produce than HRA;

Table X. Comparison of potential doses (mg/kg-d) to TCDD predicted by HRA and CAirTOX under similar landscape conditions and with an air concentration of $10^{-12} \text{ mg}/\text{m}^3$.

	HRA	CAirTOX
INHALATION	2.8×10^{-13}	3.5×10^{-13}
INGESTION:		
Water	2.2×10^{-12}	7.0×10^{-15}
Exposed produce	—	9.5×10^{-11}
Unexposed produce	—	8.4×10^{-14}
Garden products	5.7×10^{-13}	—
Meat	1.6×10^{-11}	2.3×10^{-11}
Milk	1.9×10^{-11}	7.0×10^{-11}
Eggs	n/a	6.0×10^{-13}
Fish	1.1×10^{-11}	6.7×10^{-13}
Soil	2.1×10^{-13}	4.2×10^{-15}
Total INGESTION	4.9×10^{-11}	1.9×10^{-10}
DERMAL UPTAKE	2.0×10^{-13}	2.6×10^{-12}
BREAST MILK	3.6×10^{-13}	2.0×10^{-11}
<i>Dose SUM</i>	5.0×10^{-11}	2.1×10^{-10}

Table XI Comparison of potential doses (mg/kg-d) to inorganic arsenic predicted by HRA and CAirTOX under similar landscape conditions and with an air concentration of 10^{-6} mg/m³.

	HRA	CAirTOX
INHALATION	2.8×10^{-7}	3.6×10^{-7}
INGESTION:		
Water	5.0×10^{-6}	1.0×10^{-5}
Exposed produce	—	1.0×10^{-5}
Unexposed produce	—	2.2×10^{-5}
Garden products	1.5×10^{-6}	—
Meat	2.0×10^{-7}	6.4×10^{-7}
Milk	7.7×10^{-8}	4.2×10^{-7}
Eggs	n/a	1.1×10^{-8}
Fish	9.4×10^{-9}	1.0×10^{-5}
Soil	1.3×10^{-6}	2.5×10^{-8}
Total INGESTION	8.1×10^{-6}	5.2×10^{-5}
DERMAL UPTAKE	2.8×10^{-8}	2.1×10^{-7}
BREAST MILK	n/a	2.2×10^{-9}
Dose SUM	8.1×10^{-6}	5.3×10^{-5}

- (4) for TCDD predictions of doses through meat are comparable and predictions of doses through milk differ by roughly a factor of 3 between the two models;
- (5) for arsenic, predictions of doses through meat are roughly a factor of 3 higher in CAirTOX and predictions of doses through milk are roughly a factor of 5 higher in CAirTOX;
- (7) for TCDD, predictions of doses through fish are a factor of 16 higher in HRA than in CAirTOX (this is due primarily to the modeling of particle deposition in CAirTOX and the absence of this modeling in HRA);
- (8) for arsenic, predictions of doses through fish are a factor of 1000 higher in CAirTOX than in HRA (this is due primarily to the modeling of particle runoff in CAirTOX and the absence of this modeling in HRA);

- (9) for both chemicals, soil-ingestion exposure is roughly a factor of 100 higher in HRA relative to CAirTOX;
- (10) dermal uptake of TCDD is comparable in the two models and, for arsenic, a factor of 10 higher in CAirTOX;
- (11) predicted breast milk dose to TCDD is 100 times higher in CAirTOX than in HRA (this is due primarily to the inclusion of more pathways for transferring contaminants from soil and food to human breast milk in CAirTOX); and
- (12) the total dose predicted from all pathways differs between the two models by roughly a factor of 5 or less for both compounds.

PART V. CRITICAL SENSITIVITIES AND UNCERTAINTIES

There are five factors that determine the precision or reliability of an environmental transfer model. These are (1) specification of the problem (scenario development), (2) formulation of the conceptual model (the influence diagram), (3) formulation of the computational model, (4) estimation of parameter values, and (5) calculation and documentation of results including uncertainties. Parameter uncertainties and model sensitivities are addressed in a supplemental report on model inputs (including ranges and coefficients of variability). However, it should be recognized at the outset that there are some important inherent sensitivities and uncertainties in the CAirTOX multimedia approach.

Many of the model sensitivities are highly dependent on the chemical properties of the chemical species being modeled. Nonetheless, in all cases the model is very sensitive to source terms. All model predictions are directly proportional to the initial inventory or input rates used. For many applications of a model such as CAirTOX source data has large variability and/or uncertainty. This is particularly the case for contaminant measurements in soils. For most chemicals, another important model sensitivity is to the magnitude of the transformation rates in soils, air, surface water, and/or sediments. These rate constants can have a large impact on the predicted persistence of any chemical species and are often the most uncertain inputs to the model. For volatile chemicals, the model is sensitive to the magnitude of the air-water partition coefficient. For semi-volatile chemicals and inorganic species the model is more sensitive to the soil-water partition coefficients. It is assumed that these partition processes are linear and reversible. When this is

not the case, the reliability of the model is reduced because of the uncertainties about how far soil partition processes are from this ideal behavior.

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