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CAirTOX, An Inter-Media Transfer Model for Assessing Indirect Exposures to Hazardous Air Contaminants

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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.[1] CAirTOX follows an approach that has been incorporated into the CalTOX model, which was developed for the California Department of Toxic Substances Control.[2-4] 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. The capacity to explicitly address uncertainty has been incorporated into the model in two ways. First, the spreadsheet form of the model makes it compatible with Monte-Carlo add-on programs that are available for uncertainty analysis. Second, all model inputs are specified in terms of an arithmetic mean and coefficient of variation so that uncertainty analyses can be carried out.[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 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.

This paper is divided into five parts. The first part provides an overview of the multimedia transport and transformation model used to determine the fate of air emissions. The second provides a description of the multiple-pathway exposure scenarios and exposure algorithms. The third part identifies inputs and data needs for CAirTOX and critical sensitivities and uncertainties. The fourth part addresses the capabilities, limitations, and reliability of the proposed model. The last section provides discussion and conclusions regarding the application of CAirTOX to toxic chemical emissions to air.

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 an air shed. 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.[5] 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[6] 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 [7,8] and Mackay and Paterson[9,10]. Cohen and his co-workers introduced the concept of the multimedia compartment model, MCM,[11] as a screening tool and more recently introduced the spatial multimedia compartment model (SMCM) model[12], which allows for nonuniformity in some compartments. However, neither of these models explicitly addresses human exposure. Another multimedia screening model, called GEOTOX[13,14], 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 1. The seven CAirTOX compartments are (1) air, (2) ground-surface soil, (3) root-zone 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.[8] 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.[7-10] 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/m^3) through the fugacity capacity, Z (mol/m^3-Pa),

$$C = fZ \; . \tag{1}$$

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),

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

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/m^2-d, across an interface is given by

$$flux = Y_{12} \, (f_1 - f_2) \; , \tag{3}$$

where Y_{12} is the fugacity mass-transfer coefficient across the boundary between medium 1 and medium 2 with units mol/(m^2-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 $(f_1\text{-}f_2)$ 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.

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

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

$$flux = Z_{water}\,[F^{W}_{12}\, f_1 - F^{W}_{21}\, f_2] + Z_{1p}\, F^{P}_{12}\, f_1 - Z_{2p}\, F^{P}_{21}\, f_2 \ , \tag{5}$$

where Z_{water} is the fugacity capacity of water, mol/m^3-Pa; F^{W}_{12} is the flux of water from medium 1 to 2, m^3/m^2-d; F^{W}_{21} is the flux of water from medium 2 to 1, m^3/m^2-d; Z_{1p} and Z_{2p} are, respectively, the fugacity capacities of the solid phases of media 1 and 2, mol/m^3-Pa; F^{P}_{12} is the flux of solids from medium 1 to 2, m^3/m^2-d; and F^{P}_{21} is the flux of solids from medium 2 to 1, m^3/m^2-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. Methods for estimating the intermedia transfer factors needed for the CAirTOX model are described by McKone et al.[15]

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.

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 1 lists the gains and losses considered for each compartment. The following equations express losses and gains for each of the seven CAirTOX compartments.

$$S_a + T_{la} N_l + T_{ga} N_g + T_{wa} N_w = L_a N_a \qquad \text{(air)} \tag{6}$$

$$T_{al} N_a + T_{gl} N_g + T_{rl} N_r = L_l N_l \qquad \text{(plant leaves)} \tag{7}$$

$$T_{ag} N_a + T_{lg} N_l + T_{sg} N_s = L_g N_g \qquad \text{(ground-surface soil)} \tag{8}$$

$$T_{gs} N_g = L_s N_s \qquad \text{(root-zone soil)} \tag{9}$$

$$T_{sr} N_s = L_r N_r \qquad \text{(plant root)} \tag{10}$$

$$T_{aw} N_a + T_{gw} N_g + T_{dw} N_d = L_w N_w \text{ and} \qquad \text{(surface water)} \tag{11}$$

$$T_{wd} N_w = L_d N_d \qquad \text{(sediments)} \tag{12}$$

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 (6) is the rate of contaminant input to the air compartment, mol/d. 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* and is in the form

$$loss = Area \times v_{ij} \times Z_{ik} \times f_i \ , \tag{13}$$

where *Area* in m^2 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 (13) can also be written as

$$loss = T_{ij} \, N_i \ , \tag{14}$$

in which

$$N_i = Z_i \, f_i \, V_i \ , \tag{15}$$

$$T_{ij} = \frac{area \times v_{ij}}{V_i}\frac{Z_{ik}}{Z_i} = \frac{v_{ij}}{d_i}\frac{Z_{ik}}{Z_i}, \text{ and} \qquad (16)$$

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 CAirTOX to obtain the transfer-rate constants. Equations (6) through (12) and matrix inversion methods are used to solve for the inventories, N_i, of contaminant in the seven compartments included in the model.

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

$$\mathrm{ADD} = \left[\frac{C_i}{C_k}\right] \times \left[\frac{IU_i}{BW}\right] \times \frac{EF \times ED}{AT} \times C_k \ . \qquad (17)$$

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(air)/kg-d, L(milk)/kg-d, or kg(soil)/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(water)/kg-d or kg(soil)/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→i), is defined as the ratio of dose to concentration, as expressed in the following equation.

$$\mathrm{PDF}(k \rightarrow i) = \frac{ADD}{C_k} = \left[\frac{C_i}{C_k}\right] \times \left[\frac{IU_i}{BW}\right] \times \frac{EF \times ED}{AT} \qquad (18)$$

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 2 are the potential interactions among environmental media, exposure media, and exposure routes that are addressed in CAirTOX.

Exposure factors

In constructing exposure models one needs to define the characteristics of individuals in various age/sex categories and the characteristics of the micro environments in which they live or from which they obtain air, 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.

Ingestion

The intakes of food and beverages often constitute the primary input parameters for characterizing exposures that occur via ingestion. Hence, dietary information is needed for the population(s) that are or could be exposed to the substance(s) addressed in an exposure assessment. In the U.S. a stratified random sample of the population is conducted every ten years to ascertain average dietary intakes for a three-day period. Ingestion of soil represents another possible exposure pathway to environmental contaminants.

Inhalation

Inhalation exposures are often difficult to quantify because of the spatial and temporal variations in the concentrations of air contaminants. Because the concentrations of many substances vary considerably between indoor and outdoor air, it is often crucial to determine the amounts of time that individuals spend in specific indoor and outdoor environments. Estimates of inhalation exposures to contaminated particles and gases require as input the breathing rates associated with different physical activities.

Dermal Uptake

Quantitative estimates of dermal uptake exposure are frequently required for exposure assessments that address contaminants in dusts or soils and bath, shower, and swimming water. Often these estimates include a rather large uncertainty because we must deal with the transport of chemicals within the skin layer, the interaction of the soil or water layer on the skin with the skin surface, and the dynamic conditions always involved in scenarios addressing soil and water contact with the skin. Dermal exposure to environmental contaminants can occur during a variety of activities and can be associated with several environmental media—for example contact with contaminated water during bathing, washing, or swimming; contact with contaminated soil during work, gardening, and recreation outdoors; and contact with sediment during wading and fishing.

CAIRTOX INPUTS AND OUTPUTS

Inputs Required for the Transport and Transformation Model

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.

The needed physical-chemical properties include molecular weight; octanol-water partition coefficient; melting point; solubility, Henry's law constant or vapor pressure, diffusion coefficients in pure air and water; and the organic-carbon partition coefficient, K_{OC}, and/or sorption coefficient, K_D. Also required are media-specific transformation rates, which are rate constants that express the rate of chemical transformations in each compartment.

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.

Inputs Required for the Human Exposure Model

In constructing exposure models one needs to define the characteristics of individuals in various age/sex categories and the characteristics of the micro environments in which they live or from which they obtain water and food. The types of data needed to carry out the exposure assessment include exposure duration and averaging time, anatomical and dietary properties, food consumption patterns, 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 producing animals. In addition, the calculation of intermedia transfer factors requires that a number of partition factors be available.

Exposure duration 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 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 over which human contact will be averaged so as to be representative of potential risk.

Anatomical and dietary properties include body weight, body surface area, and the ratio of intakes to body weight averaged over the representative age groups. Food consumption patterns are distributions describing local and homegrown consumption of produce, grain, milk and dairy products, meat, eggs, and fish.

Activity patterns provide the average number of hours per day spent indoors at home, spent outdoors at home, and spent in micro environments, such as bathrooms (including showering and bathing time) during the exposure duration. Exposure times are the number of days per year and hours per day spent in contact with soil during recreation and home gardening and in contact with surface water during swimming or other water recreation. Household factors relate to tap-water supply and use, room-ventilation rates, and dust concentrations within homes. Soil ingestion rates and soil contact on skin are also needed.

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 as soil-pore water after application.

The multiple pathway models require that one measure or estimate partition coefficients of contaminants between several pairs of environmental media. This list of partition coefficients includes those between water and octanol, water and organic carbon, soil and soil water, air and plants, soil and plants, animal intake and food, surface water and fish, mother's uptake and breast milk, tap water and indoor air, soil-gas and indoor air, human skin and soil, and human skin and water.

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 references 1 and 15 (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. 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.

THE CAPABILITIES, LIMITATIONS, AND RELIABILITY OF CAIRTOX

CAirTOX consists of two coupled but independent models—a multimedia transport and transformation model and a multiple pathway human exposure model. Mathematically, the CAirTOX transport model addresses the inventory of a chemical in each compartment and the likelihood that, over a given period of time, that chemical will remain in the compartment, be transported to some other compartment, or be transformed into some other chemical species. The exposure model links environmental media concentrations with exposure media concentrations and determines the potential for human dose. This section describes the capabilities of the model by identifying the chemical classes for which it was designed and when the model should not be used.

Chemical Classes

The are many classes of chemicals that must be addressed in environmental transport/transformation models, including organic chemicals, metals, inorganic chemicals, and radionuclides. These chemicals species can also be categorized according to the physical state in which they are introduced to the environment (gas, liquid, or solid), according to whether they dissociate in solution (ionic or nonionic) and according to the charge distribution on the molecule (polar or nonpolar). The traditional fugacity approach is most appropriate for nonionic, organic chemicals in a liquid or gaseous state. However, with modifications for condensation of solids on air particles, this approach can be made appropriate for solid-phase organic chemicals. Additional adjustments make possible the treatment of inorganic species, metals, and fully ionized organic species. Metals (such as mercury) and inorganic chemicals with a relatively large vapor pressure pose special problems, which are not addressed here. Special modeling problems also occur with mixed polarity, dissociating organic species, such as surfactants. The CAirTOX model, in descending order of reliability, is capable of handling nonionic organic chemicals, radionuclides, fully dissociating organic and inorganic chemicals, and solid-phase metal species. With careful attention to inputs, the model can be used for partially dissociated organic and inorganic species. The model has not been designed to work with surfactants, inorganic chemicals species with high vapor-pressure-to-solubility ratios, and volatile metals such as mercury.

What the CAirTOX Transport Model Should Not Be Used For

As is the case with any model, CAirTOX was designed for use in a limited range of spatial scales, time scales, geographic conditions, and chemical classes. As has been noted above it is not for surfactants or volatile metals. It should be used for partially ionized organic chemicals only when great care is exercised to adjust the partition coefficients to make sure they are appropriate for the pH of the landscape under consideration. The CAirTOX transport model is intended for application over long time scales, several months to years. CAirTOX should not be used for landscapes in which water occupies more than 10% of the land surface area. CAirTOX is designed for modeling very low concentrations of contamination. When contaminant concentration exceeds the solubility limit in any phase, the results of the model are no longer valid. CAirTOX should not be used as substitute for measured data, where it is available.

DISCUSSION AND CONCLUSIONS

Environmental scientists recognize that plants, animals, and humans encounter environmental contaminants via complex transfers through air, water, and food and use multimedia surveys and models to evaluate these transfers. The goal of CAirTOX is to identify an appropriate combination of survey methods and predictive models that provide a sufficient level of resolution and low cost needed to meet the objectives of risk managers. These integrated efforts can work like road maps to identify pathways and populations for which informed decisions can be made or for which more detailed analyses are needed.

Ultimately, environmental samples are a set of static pictures used to characterize a dynamic world. Unless these "pictures" can be guided by an appropriate theoretical framework, they are of little value in decision making unless we have a very large set of "pictures". The goal of the CAirTOX model is to maximize the amount of information obtained from each "picture". In such a system, the CAirTOX model must serve as a repository for much of the current knowledge of environmental pollution and exposure processes. We envision that CAirTOX can provide a "portfolio analysis" approach to human exposure in contaminated air sheds. That is, the exposure assessor should first develop a preliminary exposure matrix based on a portfolio of scenarios to match potential dose by route to contaminant-specific, multimedia dispersion in the environment. The result is a multimedia, multiple-pathway, and multiple-route assessment and gives indications of where it is most valuable to focus our resources to more fully characterize distributions of population exposure. This "value of information" approach is particularly important when there is a need to minimize the cost of providing exposure information without jeopardizing the precision required of this information to give the regulator confidence about the protection of public health.

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Table 1. 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 ***contaminant sources***	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 ***contaminant sources***	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

Table 2. 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	•Inhalation of gases and particles in outdoor air •Inhalation of gases and particles transferred from outdoor air to indoor air	•Inhalation of soil vapors that migrate to indoor air •Inhalation of soil particles transferred to indoor air	•Indoor inhalation of contaminants transferred from tap water
Ingestion	•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	•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	•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)	•Dermal contact with soil	•Dermal contact in baths and showers •Dermal contact while swimming

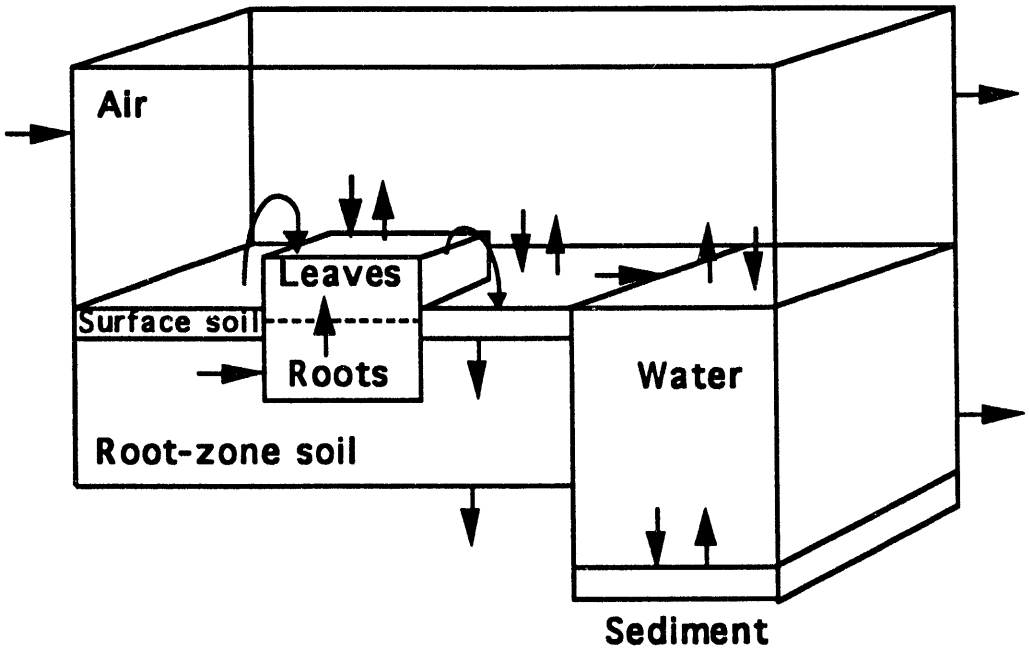

Figure 2. Mass-exchange processes modeled in a seven-compartment environmental transport model.

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