# CalTOX, A Multimedia Total Exposure Model For Hazardous-Waste Sites

## Part I: Executive Summary

**Prepared for:**
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**Department of Toxic Substances Control**
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# Foreword

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

The reader will note that every page has a disclaimer regarding the use of these documents for regulatory action. DTSC has intentionally avoided issues relating to the application of the model to assess risk for regulatory action in this document. Every effort has been made to prevent non-scientific regulatory considerations from jeopardizing the scientific credibility of the model. However, these regulatory considerations must be addressed before the model can be used for regulatory action. CalTOX differs from current regulatory risk assessment practices in a number of areas. These differences include a stochastic method of estimating risk and a description of chemical transport in the environment that allows for source depletion. Existing risk assessment policy will not be adequate to guide the use of CalTOX in regulatory applications. Therefore, additional policy will have to be developed before the model can be implemented to assess risk for regulatory decision making. These technical reports should be viewed as describing the technical basis around which future policy will be developed. These reports do not contain that policy context and are insufficient for applying the model to assess risk as a basis for regulatory action. Therefore, **do not cite, quote or use these documents to support any regulatory action.**

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### ABSTRACT

CalTOX has been developed as a spreadsheet model to assist in health-risk assessments that address contaminated soils and the contamination of adjacent air, surface water, sediments, and ground water. The modeling effort includes a multimedia transport and transformation model, exposure scenario models, and efforts to quantify and reduce uncertainty in multimedia, multiple-pathway exposure models. This report provides an overview of the CalTOX model components, lists the objectives of the model, describes the philosophy under which the model was developed, identifies the chemical classes for which the model can be used, and describes critical sensitivities and uncertainties. The multimedia transport and transformation model is a dynamic model that can be used to assess time-varying concentrations of contaminants introduced initially to soil layers or for contaminants released continuously to air or water. This model assists the user in examining how chemical and landscape properties impact both the ultimate route and quantity of human contact. Multimedia, multiple pathway exposure models are used in the CalTOX model to estimate average daily potential doses within a human population in the vicinity of a hazardous substances release site. The exposure models encompass twenty-three exposure pathways. The exposure assessment process consists of relating contaminant concentrations in the multimedia model compartments 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.

## INTRODUCTION

Reports of environmental contaminants in air, drinking water, soil, and food result in public concern about the risks to human health posed by the chemical byproducts of industrial societies. Hazardous-waste sites that contain layers of contaminated soils are among the issues that are foremost in this area of public awareness. In order to address public concerns about the long-term residual health effects of contaminated sites (both before and after cleanup efforts), regulatory agencies make use of risk assessment. 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 hazardous-waste sites, and in particular to contaminated soils, risk assessment involves four inter-related steps. These are (1) determination of source concentrations or emissions characteristics, (2) exposure assessment, (3) toxicity assessment, (4) risk characterization.

These steps can be carried out with assistance from calculational models in order to project forward to define the risk associated with existing contaminated soil concentrations and to work backward to define what residual levels of contaminant concentration will pose negligible risk to any member of a potentially exposed populations.

CalTOX has been developed as a spreadsheet model to assist in making these types of calculations. With CalTOX, we can address contaminated soils and the contamination of adjacent air, surface water, sediments, and ground water. The modeling effort includes a multimedia transport and transformation model, exposure scenario models, and efforts to quantify and reduce uncertainty in multimedia, multiple-pathway exposure models.

The multimedia transport and transformation model is a dynamic model that can be used to assess time-varying concentrations of contaminants introduced initially to soil layers or for contaminants released continuously to air or water. 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 CalTOX to estimate average daily doses within a human population in the vicinity of a hazardous substances release sites. The exposure models encompass twenty-three exposure pathways. The exposure assessment process consists of relating contaminant concentrations in the multimedia model compartments 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 report is the first of three reports in the current (1992-1993) series of reports describing the CalTOX model and its development. This report is the executive summary. The second report (Part II) in this series describes the multimedia transport and transformation model. The third report (Part III) in this series describes the multiple-pathway exposure model. There is also a supplemental report describing the values and ranges of parameters used in the models and how the uncertainty and variability in these parameters can be used to assess outcome variability and uncertainty.

This report is divided into five sections. The first describes the objectives of the CalTOX model, its role in regulation, and the philosophy under which it was developed. The next summarizes the model components—the transport and transformation model and the human exposure models. The third section describes the inputs required to run the model and the process for propagating uncertainty and variability associated with inputs to estimates of variance in outputs of CalTOX. The fourth section describes the capabilities of the model by identifying the space and time scales for which it was intended; the chemical classes for which it was designed; and when the model should not be used. The last section provides a summary discussion regarding the use of CalTOX and identifies areas of future research and development.

## OBJECTIVES OF THE CALTOX MODEL

Decisions regarding the remedial actions required at hazardous waste sites regulated by the Department of Toxic Substances Control (DTSC) are made by the Site Mitigation Program staff. These decision makers, who serve as the risk managers, must consider multiple criteria in defining remedial actions. Protection of human health and the environment is one of theses criteria. Other criteria involve issues such as protection of water resources, cost, and feasibility. In addressing the risk to human health, the DTSC currently uses a guidance document on hazardous-waste-site risk assessment prepared by U.S. Environmental Protection (U.S. EPA, 1989). This document has been useful to the DTSC, but has a number of deficiencies. CalTOX builds on and extends the EPA guidance in order to eliminate many of these deficiencies. At this point in time CalTOX is directed primarily at human health as the endpoint of concern. Ecological risk and water-resource degradation are not explicitly addressed in the current model, but could be incorporated as model endpoints.

The major objective of CalTOX is to provide risk managers and other decision makers with a more complete picture of both how potential human exposure comes about and how precisely it can be quantified for soil-bound contaminants. In addressing this objective, CalTOX represents a major step forward in a number of areas. First, CalTOX increases the separation between risk assessment and risk management by addressing uncertainty and variability quantitatively. The frequent use of “reasonable maximal exposure” in risk assessments forces responsibility for making judgments on what is “reasonable maximal” on the risk assessor, when such a value judgment should be made by risk managers. CalTOX allows the risk assessor to focus on accurate, precise, and reliable estimates instead of struggling with “reasonable” estimates. Second, CalTOX is based on both conservation of mass and chemical equilibrium. The model addresses gains and losses and audits mass potential, thus eliminating the need to make assumptions that implicitly “double count” the spread of contaminants. For soil, water, and air compartments, the model computes time-varying chemical concentrations that result from a combination of transport and degradation processes. Third, the model makes the a distinction between environmental concentrations and exposure concentrations. Finally, the model provides methods for addressing all potential exposure pathways including the highly uncertain, but sometimes significant, indirect exposures such as those through food. We believe these extensions to current U.S. EPA methods are the next logical step in the evolution of risk assessment toward a more credible policy tool.

For the majority of waste sites regulated by the DTSC, we believe that uncertainty about underlying physical processes and uncertainties about the value of critical parameters are factors that mainly limit the precision of our risk estimates and thus contribute the most to uncertainty about risk. We consider model specification errors to be smaller contributors to uncertainty about the exposure component of risk (but not necessarily about dose-response component). Thus, CalTOX was designed to be a relatively simple model and transparent model, which we believe is appropriate for most of the sites regulated by DTSC. Even though large complex models may appear to be more credible and more "realistic," the reliability of such models is limited by the same parameter uncertainties that limit the reliability of CalTOX. Nonetheless, it is possible that sufficient chemical- and site-specific data will be obtained to justify the use of more complex models or that CalTOX may be inappropriate for use at some sites. In these cases alternative models may be used. In these cases, responsible parties will be expected to justify that the alternative model is more precise and more accurate than CalTOX and that sufficient data have been collected to employ the substitute model.

**Linking Sources with Multiple Environmental Media and Exposure Media**

In risk analysis, we use human-exposure assessments to translate contaminant sources into quantitative estimates of the amount of contaminant that comes in contact with the human-environment boundaries, that is, the lungs, the gastrointestinal tract, and the skin surface of individuals within a specified population. An assessment of intake requires that we determine how much crosses these boundaries. Exposure assessments often rely implicitly on the assumption that exposure can be linked by simple parameters to ambient concentrations in air, water, and soil. However, total exposure assessments that include time and activity patterns and micro-environmental data reveal that an exposure assessment is most valuable when it provides a comprehensive view of exposure pathways and identifies major sources of uncertainty. Thus, we see the need to address many types of "multiples" in the quantification of human exposure, such as multiple media (air, water, soil); multiple exposure pathways (or scenarios); multiple routes (inhalation, ingestion, dermal); multiple chemicals; multiple population subgroups; and multiple health endpoints. In order to address these issues CalTOX was designed to be comprehensive and flexible. Potential dose by route is linked to contaminant-specific, multimedia dispersion in the environment.

Environmental media include air, ground-surface soil, root-zone soil, plants, ground water and surface water in the contaminated landscape. Exposure pathways define a link between an environmental medium and an exposure medium. Exposure media include outdoor air, indoor air, food, household dust, homegrown foods, animal food products, and tap water. Exposure routes are inhalation, ingestion, and dermal uptake. Figure 1 illustrates the type of exposure "road map" we use to carry out a multimedia, multiple pathway, multi-route exposure / dose assessment.

**Sources, Exposure, Dose, and Risk**

Following the logic of Figure 1, we construct the distribution of individual lifetime risk, H(t), at some time t in the future within a population exposed for an exposure duration, ED (years), to a contaminant in soil at an initial (time zero) concentration, $C_s(0)$ [mg/kg(soil)], by summing the dose and effect over exposure routes, over environmental media, and over exposure pathways.

$$H(t) = C_s(0) \times \left\{ \sum_{\substack{j\ \text{routes},}} \ \sum_{\substack{k\ \text{environ-,} \\ \text{mental} \\ \text{media}}} \ \sum_{\substack{i\ \text{exposure} \\ \text{media}}} \left[ Q_j\left(ADD_{ijk}\right) \times \left( \frac{ADD_{ijk}}{C_k} \right) \times \Phi[C_s(0) \rightarrow C_k, t] \right] \right\} \quad (1)$$

where $\Phi[C_s(0) \rightarrow C_{k,} t]$ is the multimedia dispersion function that converts the contaminant concentration $C_s(0)$ mg/kg measured in soil today, into contaminant concentration $C_k$ at a time t in the future for a duration ED in environmental medium k (units of $C_k$ are mg/kg for soil, mg/m$^3$ for air, and mg/L for water). $(ADD_{ijk}/C_k)$ is the unit dose factor, which is the average daily potential dose (over a specified averaging time) from exposure medium i by route j (inhalation, ingestion, dermal uptake) attributable to environmental compartment k divided by $C_k$ when $C_k$ is constant over the duration ED. The exposure media summation is over number of exposure media that link potential dose by route j to contaminants in compartment k. $Q_j(ADD_{ijk})$ is the dose-response function that relates the potential dose, $ADD_{ijk}$, by route j to the lifetime probability of detriment per individual within the population, (mg/kg-d)$^{-1}$. When an environmental concentration is assumed constant over the exposure duration, ED, the population-averaged potential dose (for ingestion or inhalation routes) or absorbed dose (for dermal contact) is the average daily dose rate $(ADD_{jk})$, in mg/kg-d is given by

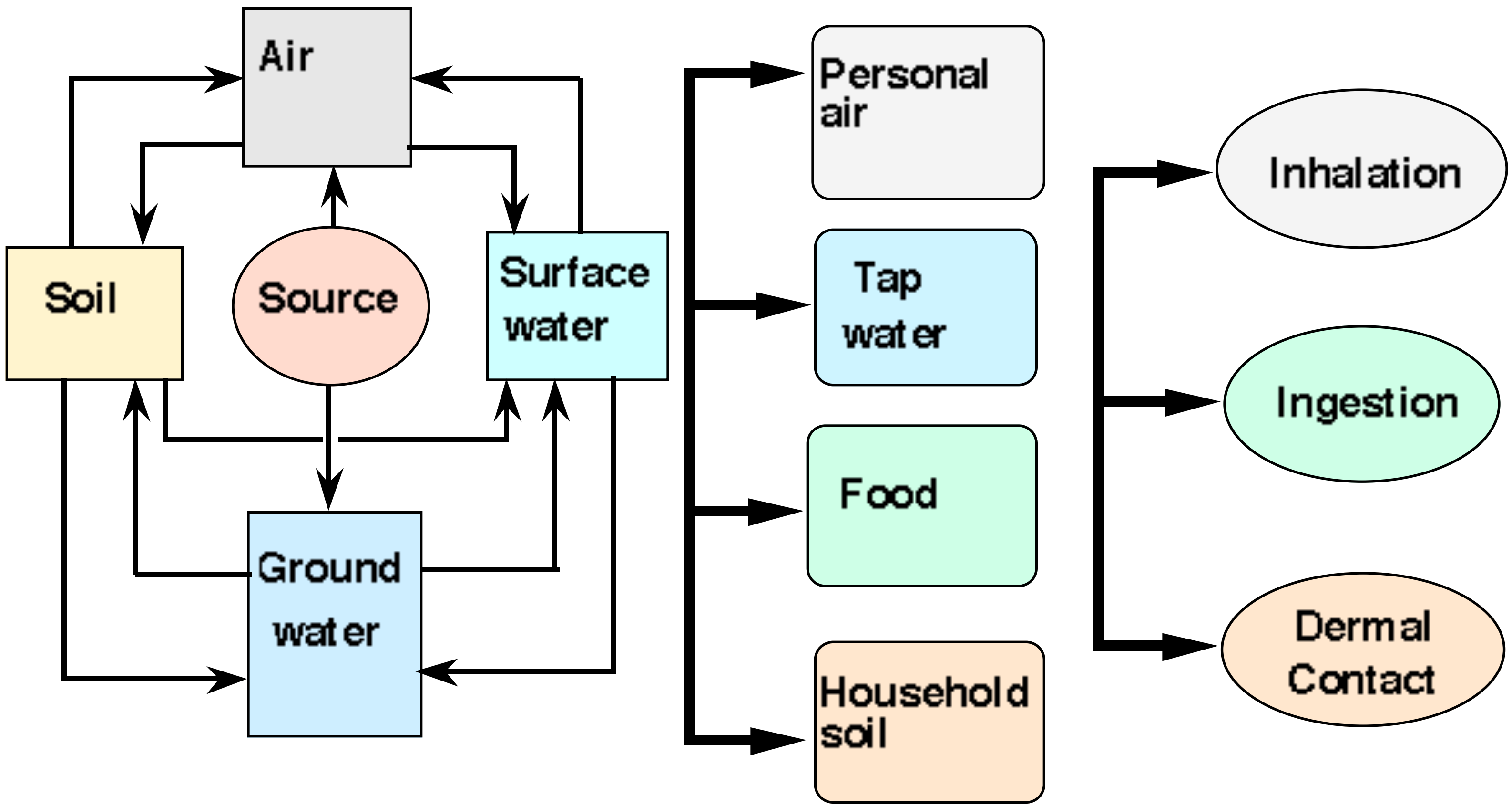


Figure 1. The potential interactions among source term, environmental media, exposure media, and exposure routes that must be addressed in a multimedia, multiple pathway, exposure assessment.

$$\mathrm{ADD_{ijk}} = \left[\frac{\mathrm{C_i}}{\mathrm{C_k}}\right] \times \left[\frac{\mathrm{IU_{ij}}}{\mathrm{BW}}\right] \times \frac{\mathrm{EF} \times \mathrm{ED}}{\mathrm{AT}} \times \mathrm{C_k} \qquad (2)$$

In this expression $[C_i / C_k]$ is the intermedia-transfer ratio, 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 $[IU_{ij} / BW]$ is the intake or uptake factor per unit body weight associated with the exposure medium i and route j. For exposure through the inhalation or ingestion route, $[IU_{ij} / BW]$ is 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, $[IU_{ij} / BW]$ is 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 individual, 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.

Equation (1) can be used to estimate potential risk at some time t in the future associated with a measured concentration $C_s$ taken today. This is the forward calculation of risk. However, CalTOX is designed to also carry out the reverse calculation. That is, what concentration in soil, $C_s(0)$ measured today is acceptable, given that our goal is to maintain our expectation of risk H(t) within the population at some time t in the future at or below a target risk $H^*(t)$? In this case we calculate a target cleanup goal $C_s^*(0)$ according to

$$C_s^*(0) = \frac{H^*(t)}{\sum\limits_{\substack{\text{j routes},}} \sum\limits_{\substack{\text{k environ-,}\\ \text{mental}\\ \text{media}}} \sum\limits_{\substack{\text{i exposure}\\ \text{media}}} \left[ Q_j \left( ADD_{ijk} \right) \times \left( \frac{ADD_{ijk}}{C_k} \right) \times \Phi[C_s(0) \rightarrow C_k, t) ] \right]} \quad . \qquad (3)$$

CalTOX was designed to make this calculation using a multimedia, multiple pathway approach. In addition, CalTOX is capable of accepting a Monte Carlo add-on function so that the risk in Equation (2) or the soil concentration in Equation (3) can be determined probabilistically. This allows the specification of a level of certainty associated with the target risk and the target cleanup level.

**Confronting Uncertainties**

Regulatory toxicology and risk assessment often operate under the premise that, with sufficient funding, science and technology will provide an obvious and cost-effective solution to the problems of cleaning up hazardous waste sites. However, in reality there are many sources of uncertainty and variability in the process of human health-risk assessment. Many of these uncertainties and variabilities are not reducible. Effective hazardous waste clean-up policies are possible under conditions of uncertainty, but such policies must take the uncertainty into account. There is a well-developed theory of decision making under uncertainty, which is described in Chernoff and Moses (1959), Lindley (1985), and Berger (1985) among others. One often used method for addressing uncertainty in risk assessments is the compounding upper bound estimates in order to make decisions based on a highly conservative estimate of exposure and risk. Such an approach is contrary to the principles of decision making under uncertainty (as described in the texts cited above). This approach leaves the decision maker with no flexibilty to address margins of error; to consider reducible versus irreducible uncertainty; to separate individual variability from true scientific uncertainty; or to consider benefits, costs, and comparable risks in the decision making process.

The principles of decision making under uncertainty are not necessarily complex. Often the principles of such decision making are simply common sense. But in any issue involving uncertainty, it is important to consider a variety of plausible hypotheses about the world; consider a variety of possible strategies for meeting our goals; favor actions that are robust to uncertainties; hedge; favor actions that are informative; probe and experiment; monitor results; update assessments and modify policy accordingly and favor actions that are reversible (Ludwig et al., 1993).

In order to make CalTOX consistent with such an approach, it was designed to have both sensitivity and uncertainty analyses incorporated directly into the model operation. Parameter values suggested for use in CalTOX are described in terms of mean values and a coefficient of variation in place of plausible upper values. Models are described in terms of the confidence intervals associated with model predictions. This is done to allow the users to produce more than a single number for an outcome such as a soil clean-up goal.

## The Peer Review Process for CalTOX

The scientific community relies heavily on peer review to verify the quality and validity of a scientifically based activity. In this regard, the CalTOX reports and the CalTOX model were given scientific peer review both within the academic community and among the various agencies with the California Environmental Protection Agency. The first drafts of the CalTOX model and reports were completed in the summer of 1992. This material was sent for academic peer review to eight different groups representing (1) university scientists in the fields of environmental science, environmental chemistry, civil engineering, soil science, exposure assessment, risk assessment, and decision analysis; (2) environmental scientists and risk assessors at the U.S. EPA; (3) environmental modelers at a consulting organization; and (4) environmental scientists and risk assessors at a U.S. Department of Energy National Laboratory. This review produced several pages of commentary and numerous specific comments. All of the comments were addressed with written responses and the reports and models were revised accordingly.

Following the academic peer review, revised documents were released in December of 1992. These documents along with academic reviews and the response to reviews were circulated throughout the California Environmental Protection Agency for reviews and comments. Again, many general commentaries and numerous specific comments were collected, summarized, and addressed. The current (third) versions of the CalTOX reports were revised in response to the comments received as part of this second review process.

## OVERVIEW OF THE COMPONENT MODELS OF CalTOX

There are two major model components within CalTOX and each can operate independently of the other. These two model components are the multimedia transport and transformation model, which is used to determine the dispersion of soil contaminants among soil, water, and air media and the human exposure model, which translates environmental media concentrations into estimates of human contact and potential dose. In the sections below, we provide an overview of these two models. A detailed description of the multimedia transport and transformation model is provided in the Part-II report. A detailed description of the human-exposure model is provided in the Part-III report. An identification of inputs to these models including ranges needed to represent uncertainty and variability are provided in a supplemental report describing the values and ranges of parameters to be used in the CalTOX model.

## The Multimedia Transport and Transformation Model

In response to the need for multimedia models in risk assessment, a number of multimedia transport and transformation models have recently appeared. 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 as a screening tool with the MCM model (Cohen and Ryan, 1985) and more recently with the spatial multimedia compartment model (SMCM) model (Cohen et al., 1990), which allows for nonuniformity in some compartments. 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.

### *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/m$^3$) through the fugacity capacity, $Z$ (mol/m$^3$-Pa),

$$C = fZ \quad . \tag{4}$$

$Z$ 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),

$$C_1 / C_2 = fZ_1 / fZ_2 = Z_1 / Z_2 = K_{12} \quad , \tag{5}$$

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.

*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 or depth of and method of incorporation for soil contaminants). 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.

CalTOX is a seven-compartment regional and dynamic 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, but CalTOX 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 CalTOX is illustrated in Figure 2. The seven CalTOX compartments are (1) air, (2) ground-surface soil, (3) plants, (4) root-zone soil, (5) the vadose-zone soil below the root zone, (6) surface water, and (7) sediments. The air, surface water, ground-surface-soil, plants, and sediment compartments are assumed to be in quasi-steady state with the root-zone-soil, and vadose-zone-soil compartments. Contaminant inventories in the root-zone soil and vadose-soil zone are treated as time-varying state variables. Contaminant concentrations in ground water are based on the leachate from the vadose-zone soil.

It is important to note that, in contrast to many models used for assessing environmental fate, CalTOX 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.

*Balancing Gains and Losses—Sources, Transport, and Transformation*

Mathematically, CalTOX 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. Quantities or concentrations within compartments are described by a set of linear, coupled, first-order differential equations. Illustrated in Figure 3 are the types of gains and losses that are considered in defining the inventory of each compartment in the CalTOX model. Contaminants are moved among and lost from each compartment through a series of transport and transformation processes that can be represented mathematically as first-order losses (that is the rate of loss is linearly proportional to the concentration or inventory). CalTOX simulates all decay and transformation processes (such as radioactive decay, photolysis, biodegradation, etc.) as first-order, irreversible removals. Mass flows among compartments include solid-phase flows, such as dust suspension or deposition, and liquid-phase flows, such as surface run-off and ground-water recharge. The transport of individual chemical species among compartments occurs by diffusion and advection at the compartment boundaries. Each chemical species is assumed to achieve chemical equilibrium among the

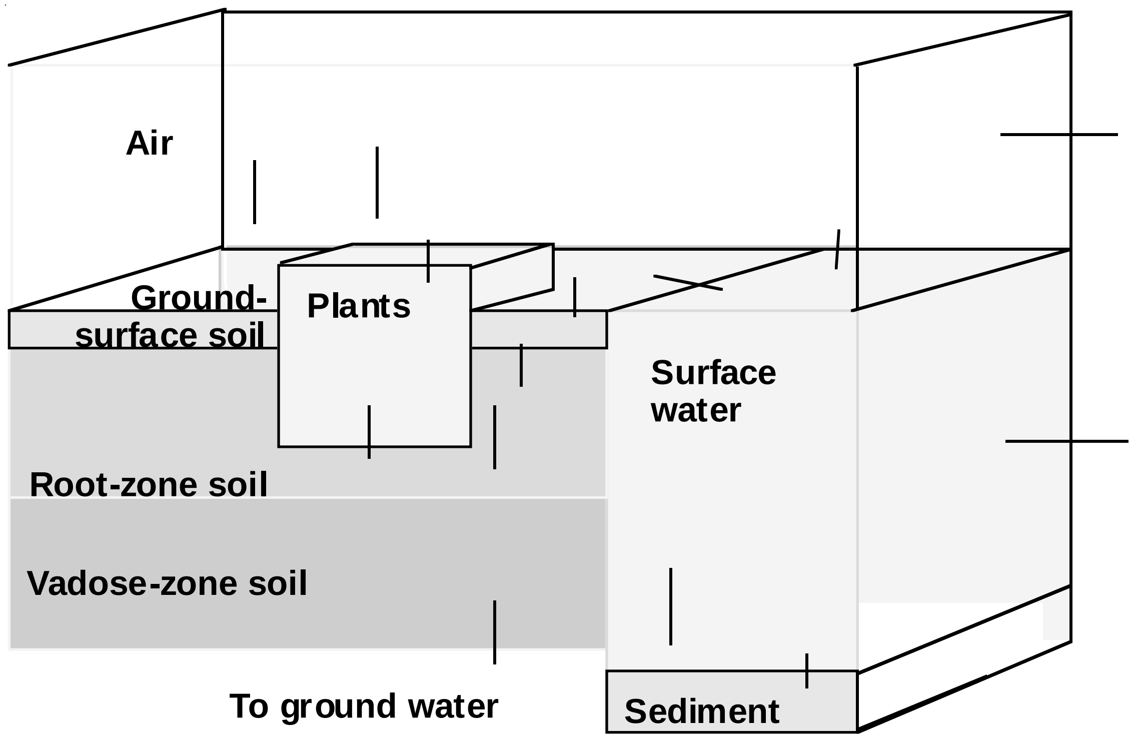


Figure 2. An illustration of mass-exchange processes modeled in the seven-compartment environmental transport and transformation model. (Ground water is not explicitly modeled in the system of equations but is used in the exposure calculations.)

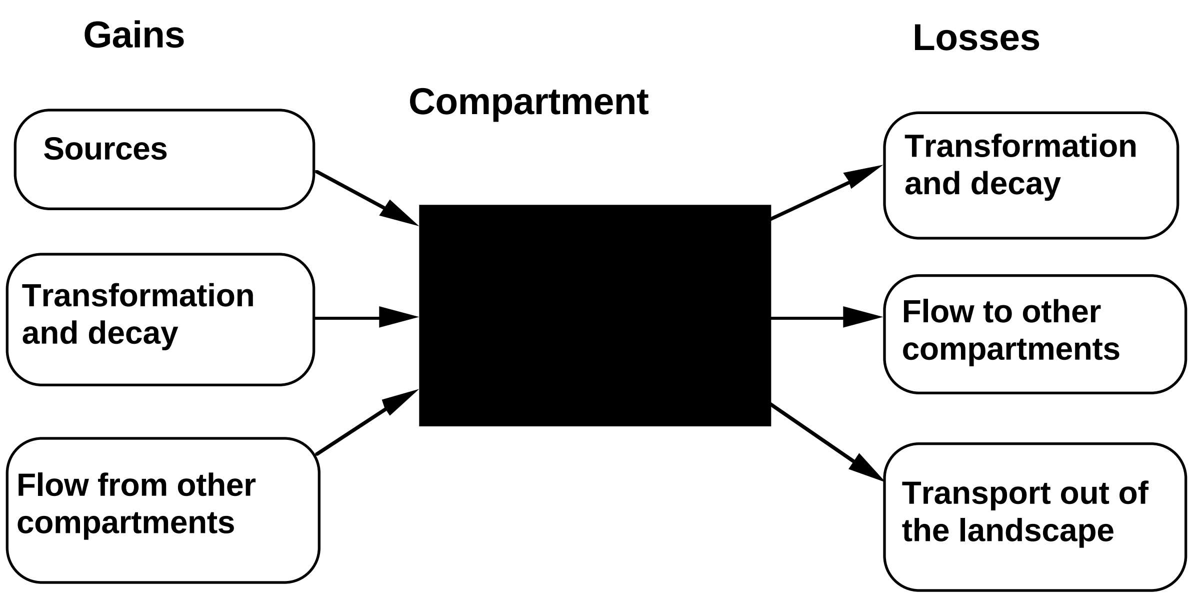


Figure 3. An illustration of the balancing of gains and losses in an environmental transport and transformation model, such as CalTOX.

phases within a single compartment. However, there is no requirement for equilibrium between adjacent compartments. As an example, one can consider the root-zone soil layer, which contains solids, liquids, and gases. An organic chemical added to the soil distributes itself among these three phases such that it achieves chemical and physical equilibrium. Among the potential transport pathways from the root-zone soil compartment are liquid advection (soil water runoff), solid-phase advection (erosion to surface water or dust stirred up and blown about), and diffusion from both the soil gas phase and soil water into the lower atmosphere.

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 exposure.

*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 (IAEA, 1989). 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 CalTOX 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 CalTOX 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.

**The Human Exposure Model**

Human exposures to chemicals can result from contact with contaminated soils, water, air, and food as well as with drugs and consumer products. Exposures may be dominated by contacts with a single medium or may reflect concurrent contacts with multiple media. Assessment of human exposure to environmental contaminants requires translating environmental concentrations into quantitative estimates of the amount of chemical that contacts individuals within an exposed population. Potential dose, expressed as average daily dose, is the amount of material per unit of body weight per day (mg/kg-d) that crosses the mouth of an exposed individual by inhalation or ingestion or enters the outer layer of the skin through dermal contact. Dose models used in CalTOX are based on those described by the U.S. Environmental Protection Agency (EPA, 1989; Federal Register, 1992) and by the California Department of Toxic Substances Control (DTSC, 1992a, 1992b).

The nature and extent of multimedia exposures depends largely on two things—(1) human factors and (2) the concentrations of a chemical substance in contact media. Human factors include all behavioral, sociological, and physiological characteristics of an individual that directly or indirectly affect his or her contact with the substances of concern. Important factors in this regard are contact rates with food, air, water, soils, drugs, etc. Activity patterns, which are defined by an individual's allocation of time spent at different activities and locations, are also significant because they directly affect the magnitude of inhalation and dermal exposures to substances present in different indoor and outdoor environments. From an exposure-assessment standpoint, our challenge is to estimate or measure a person's exposure as a function of relevant human factors and measured and/or estimated concentrations in contact media. Table I gives a matrix showing the many interrelationships (or pathways) that can exist between contaminated media and the three possible routes of exposure.

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

| **Exposure routes** | **Media** | | |
|---|---|---|---|
| | **Air (gases and particles)** | **Soil (ground-surface soil; root-zone soil)** | **Water (surface water and ground water)** |
| **Inhalation** | • Inhalation of gases and particles in outdoor air<br><br>• Inhalation of gases and particles transferred from outdoor air to indoor air | • Inhalation of soil vapors that migrate to indoor air<br><br>• 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<br><br>• Ingestion of meat, milk, and eggs contaminated by transfer of contaminants from air to plants to animals<br><br>• Ingestion of meat, milk, and eggs contaminated through inhalation by animals<br><br>• Ingestion of mother's milk | • Human soil ingestion<br><br>• Ingestion of fruits, vegetables, and grains contaminated by transfer from soil<br><br>• Ingestion of meat, milk, and eggs contaminated by transfer from soil to plants to animals<br><br>• Ingestion of meat, milk, and eggs contaminated through soil ingestion by animals<br><br>• Ingestion of mother's milk | • Ingestion of tap water<br><br>• Ingestion of irrigated fruits, vegetables, and grains<br><br>• Ingestion of meat, milk, and eggs from animals consuming contaminated water<br><br>• Ingestion of fish and sea food<br><br>• Ingestion of surface water during swimming or other water recreation<br><br>• Ingestion of mother's milk |
| **Dermal contact** | • (not included) | • Dermal contact with soil | • Dermal contact in baths and showers<br><br>• Dermal contact while swimming |

*Model Structure*

Multimedia, multiple pathway exposure equations are used in CalTOX to estimate average daily doses within a human population in the vicinity of a hazardous-substances-release site. The overall model encompasses twenty-three potential exposure pathway scenarios. The end product of these exposure assessments for contaminants at hazardous-waste sites is an estimation of the distribution of potential dose among the population at risk.

The multiple pathway exposure analysis in CalTOX begins with the assumption that through models or measurement, concentrations are available for ambient air, surface water, ground water, surface soil, and root-zone soil. The exposure assessment process consists of relating contaminant concentrations in these environmental media to contaminant concentrations in the contact media (personal air, tap water, foods, household dusts and soils, etc.).

Each of the exposure scenarios relating an average daily dose to an environmental medium concentration for a specific pathway is developed in the form of the following equation, which is essentially the same as Equation (2) above,

$$ADD = \text{Intake}_i = TF(k \rightarrow i) \times \left[\frac{IU_i}{BW}\right] \times \frac{EF \times ED}{AT} \times C_k \quad . \tag{6}$$

In this expression, the concentration of contaminant in an environmental medium k is assumed constant over the exposure duration. ADD is the average daily potential dose rate in mg/kg-d, which is the intake of a contaminant from exposure medium i; TF(k→i) is the intermedia-transfer factor, $[C_i/C_k]$, which expresses the ratio of contaminant concentration in the *exposure* medium i to the concentration in an environmental medium k and, as before $[IU_i/BW]$ is the intake or uptake factor per unit body weight associated with the exposure medium i. EF is the exposure frequency for the exposed individual, the number of days per year that an individual contacts the contaminated medium k; ED is the exposure duration for the exposed individual, y; and AT is the averaging time for the exposed individual, d.

The unit dose factor, UDF(k→i), [or potential dose factor PDF(k→i)] is defined as the ratio of dose through contact medium i relative to contaminant concentration in medium k, and is equal to $ADD/C_k$ for a given pathway. The UDFs are 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.

*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.

*Summary Comparison of Multiple-Pathway Exposure*

The CalTOX exposure model provides methods for integrating multiple-exposure routes from multiple-environmental media into a matrix of factors that relate concentrations of toxic chemicals to potential total human dose at toxic-substances-release sites. This type of matrix is used to generate the histogram shown in

Figure 4. The scenarios used to develop this particular histogram are for a representative volatile organic compound incorporated in the top several meters of soil. Here, we can see that, based on a multimedia, multiple-pathway, and multiple-route assessment, we get indications of where it is most valuable to focus our resources to more fully characterize distributions of population exposure. In this way we characterize total potential dose using comprehensive, simple, and possibly stochastic models to focus efforts on those exposure routes, media, and scenarios that require more realistic assessment of the distribution of dose within the population. This matrix allows us to make both route-to-route and medium-specific comparisons of total potential doses from multiple environmental media.

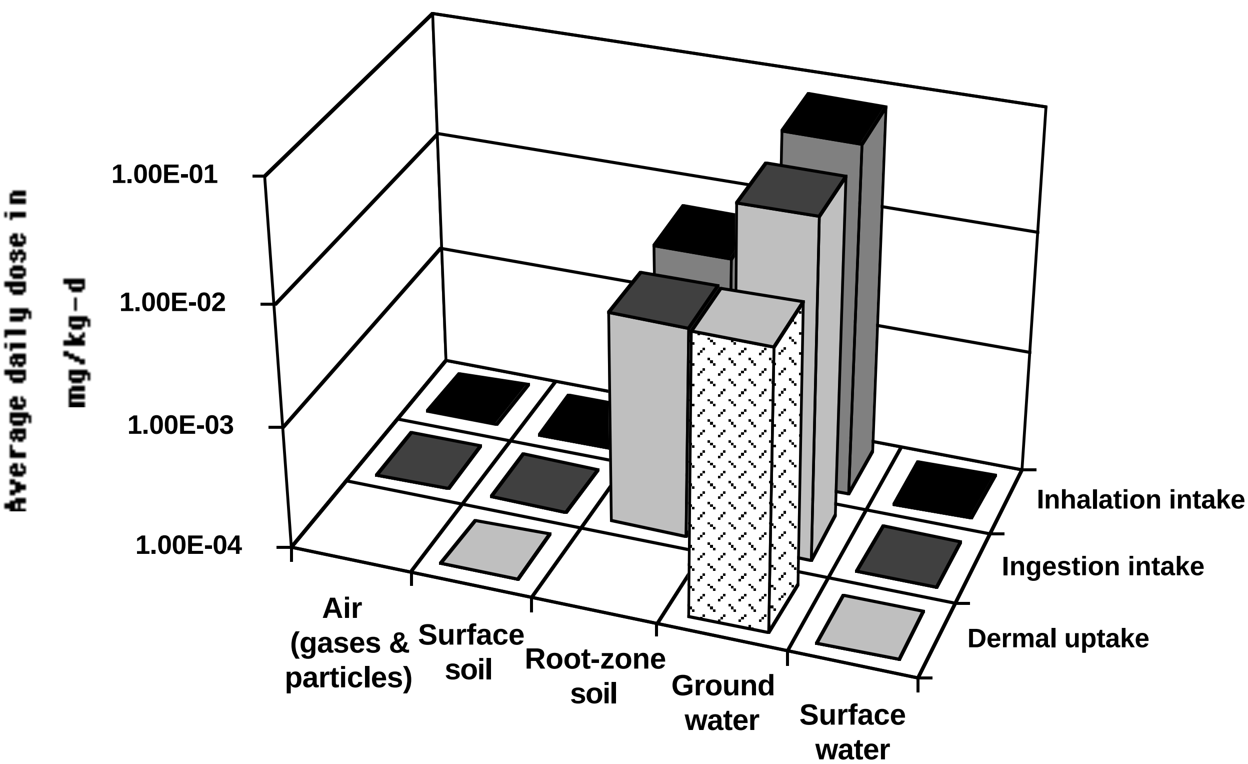


Figure 4. Disaggregation by exposure route and by exposure medium for the average daily potential dose to volatile organic compound in an example calculation of multimedia exposure.

## CalTOX INPUTS AND OUTPUTS

This section describes the inputs required to run the model. We also describe the process we use with CalTOX for propagating uncertainty and variability associated with model inputs into a distribution of output values.

### Inputs Required for the Transport and Transformation Model

The CALTOX 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 microenvironments 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 microenvironments, 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.

## Uncertainty and Variability of Inputs

One of the issues in model outcome uncertainty that must be confronted is how to distinguish between the relative contribution of true uncertainty versus inter-individual variability to outcome distribution of predicted population risk (Bogen and Spear, 1987). Uncertainty or model-specification error (e.g., statistical estimation error) can be modeled using a random variable with an identified probability distribution. In contrast, inter-individual variability refers to quantities that are distributed empirically within a defined population—such factors as food ingestion rates, exposure duration, and expected lifetime. Variability and true uncertainty have also been referred to as, respectively, *Type A* uncertainty, that "due to stochastic variability with respect to the reference unit of the assessment question," and *Type B* uncertainty, that "due to lack of knowledge about items that are invariant with respect to the reference unit of the assessment question" (IAEA, 1988). When both Type A and Type B uncertainties are negligible, we truly have a deterministic result, but this is rare in risk assessment. However, there are situations in which true (Type B) uncertainty is negligible relative to variability (Type A) uncertainty and in these situations, the outcome of a variance propagation analysis simply represents the expected statistical variation in dose or risk among the exposed population. When neither variability nor uncertainty are negligible, we have a situation in which there are multiple probability distributions representing variability, but the correct distribution is unknown because of uncertainties.

**Uncertainty and Sensitivity Analyses with CalTOX**

Uncertainty analysis as applied to mathematical models involves the determination of the variation or imprecision in an output function based on the collective variation of model inputs, whereas sensitivity analysis involves the determination of the changes in model response as a result of changes in individual model parameters. Iman and Helton (1988) have identified three approaches that are useful for assessing uncertainty and sensitivity in mathematical models. These are (a) differential analysis, (b) response-surface replacement, and (c) Monte-Carlo or modified-Monte-Carlo (i.e., latin-hypercube sampling) methods. In order to apply any of these methods, one can think of a model as producing an output Y, such as population-health risk, that is a function of several input variables, $X_i$, and time, t,

$$Y = f(X_1, X_2, X_3, \ldots X_k, t). \tag{7}$$

The variables, $X_i$, represent the various inputs to the risk-assessment model such as water concentration, exposure factors, metabolism parameters, cancer potency, etc. In an unmodified Monte Carlo method, as illustrated in Figure 5, each of the input parameters is represented by a probability-density function that defines both the range of values that the parameter can take on and the likelihood that the parameter has a value in any subinterval of that range. In an unmodified Monte Carlo method, simple random sampling is used to select each member of the input

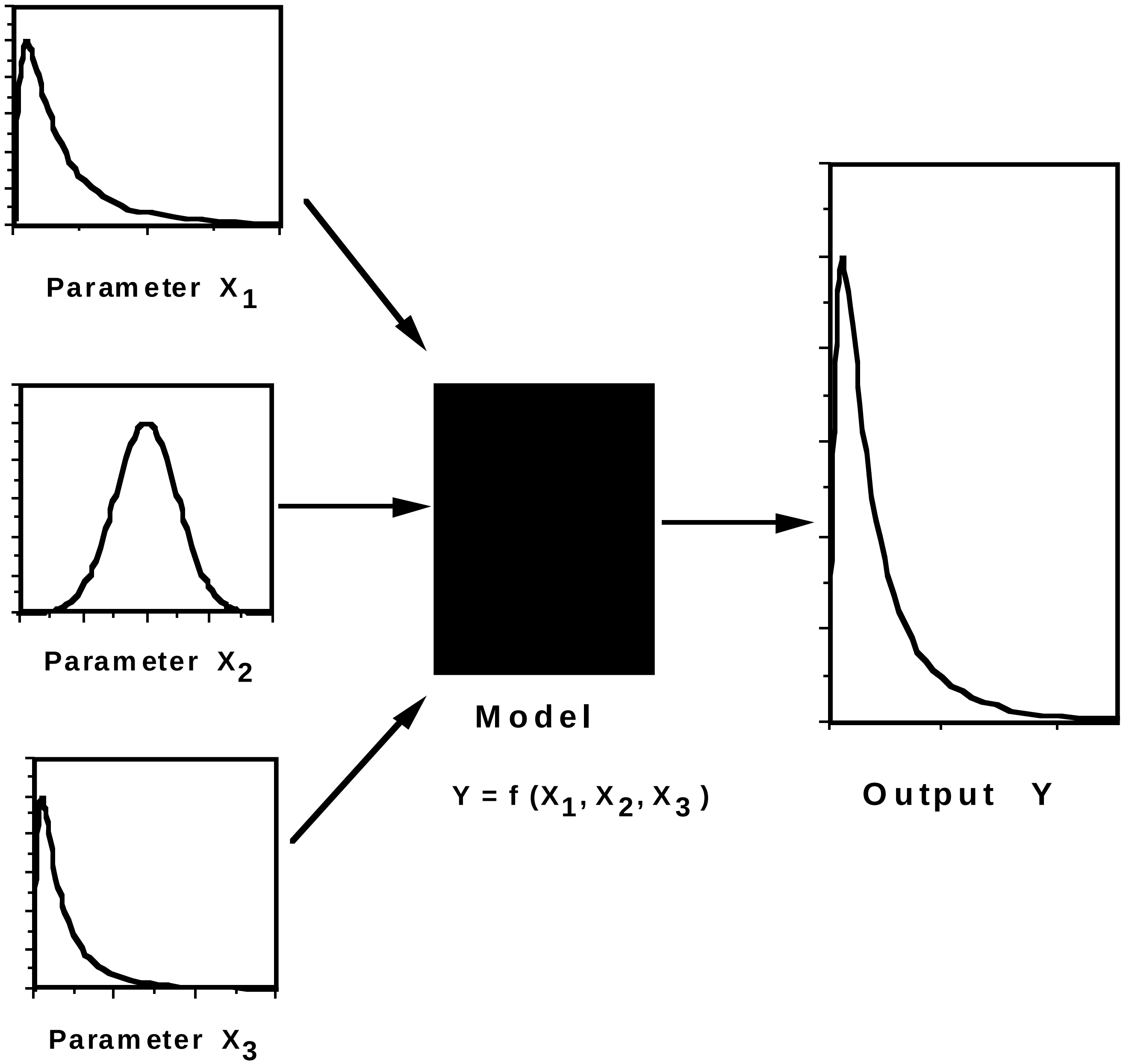


Figure 5. An illustration of an unmodified Monte Carlo sampling method, in which simple random sampling is used to select each member of a triplet; $X_1$, $X_2$, and $X_3$. These randomly-sampled triplets are used in a model that relates the output function, Y to each input parameter by some function, $f(X_1, X_2, X_3)$. When a sufficient number of samples is used, the variance of the output Y reflects the combined impact of the variances in $X_1$, $X_2$, and $X_3$ as propagated through the model $f(X_1, X_2, X_3)$.

parameter set. When a sufficient number of samples is used, the variance of the output Y reflects the combined impact of the variances in $X_1$, $X_2$, and $X_3$ as propagated through the model $f(X_1, X_2, X_3)$. Latin hypercube sampling (LHS) is a Monte Carlo method that uses stratified random sampling to select each member of an input set. Whereas for simple random sampling it is often a matter of chance how evenly the *n* selected values cover the range of parameter X, latin hypercube sampling places restrictions on possible unevenness. Additional information on latin hypercube sampling is available in Iman and Shortencarier (1984).

Describing uncertainty in the output variable, Y, involves quantification of the range of Y, its arithmetic mean value, the arithmetic or geometric standard deviation of Y, and upper and lower quantile values of Y, such as 5% lower bound and 95% upper bound. Convenient tools for presenting such information are the probability-density function (PDF) or the cumulative distribution function (CDF) for Y. However, the PDF or CDF of Y can often only be obtained when we have meaningful estimates of the probability distributions of the input variables $X_i$. If this information is missing or incomplete, one can still construct the CDF or PDF for Y, but should be careful to characterize it as a screening distribution for parameter uncertainty instead of characterizing it as a realistic representation of the uncertainty in Y.

## THE CAPABILITIES, LIMITATIONS, AND RELIABILITY OF CalTOX

CalTOX consists of two coupled but independent models—a multimedia transport and transformation model and a multiple pathway human exposure model. Mathematically, the CalTOX 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 space and time scales for which it was intended; the chemical classes for which it was designed; and when the model should not be used.

**Space and Time Scales**

CalTOX is a lumped systems, zero-(spatial)-dimension model. This means that it includes compartments to represent various components of the environment, but that there are no explicit vertical or horizontal dimensions in these compartments. However, because of the nature of these compartments, and the way mass exchange is modeled among these compartments, there are implicit transport vectors within the model. Transport in the soil column is implicitly vertical within CalTOX, chemicals move up toward the atmosphere and/or down to ground water. Once in the atmosphere contaminants either move vertically back to the ground-surface soil or to surface water or are blown by wind horizontally out of the landscape. Transport from soil to surface water is implicitly horizontal and at the surface. Implicit in CalTOX is the assumption that, in the unsaturated soil layers, vertical transport is much greater than horizontal. In level terrain, we estimate that this assumption holds for landscapes on the order of 1,000 $m^2$ or greater. CalTOX has more resolution of chemical transport in soils than in surface waters and is intended for landscapes in which there is a large ratio of land area to surface-water area. The CalTOX transport model was designed to be applied over long time periods, months to years, when seasonally and yearly averaged partition factors apply. The exposure model is intended for situations in which the environmental media concentrations are constant over the exposure duration.

**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 CalTOX 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 CalTOX Transport Model Should Not Be Used For

As is the case with any model, CalTOX 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 CalTOX transport model is intended for application over long time scales, several months to decades. It should be used cautiously for time periods less than one year and then only when properly time-averaged landscape properties are employed. When this is not the case, CalTOX can be used, but some adjustments must be made.

CalTOX should not be used for landscapes in which water occupies more than 10% of the land surface area. CalTOX 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. There is a warning in the spreadsheet model to advise the user when this happens.

CalTOX should not be used as substitute for measured data, where it is available. Also, it should not be used when a more detailed transport and transformation and/or exposure assessment has been conducted. However, it might be used as a complement to such assessments.

## DISCUSSION

In his treatise *Air, Water, and Places,* the ancient-Greek physician Hippocrates demonstrated that the appearance of disease in human populations is influenced by the quality of air, water, and food; the topography of the land; and general living habits (Wasserstein, 1982). This approach is still relevant more than two thousand years later and, indeed, the cornerstone of modern efforts to relate public health to environmental factors. What has changed is the precision with which we can measure and model these long-held relationships. Today, 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 CalTOX 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.

An exposure assessment can be carried out through modeling, sampling, or some modeling/sampling combination. Ultimately this characterization provides 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 unless we have a very large set of “pictures”. The goal of the CalTOX project is to maximize the amount of information obtained from each “picture”. This can be accomplished through an iterative set of models and samples. In such a system, the model used initially to characterize exposure must serve as a repository for much of the current knowledge of environmental pollution and exposure processes. In addition the models and surveys used in an exposure characterization must provide estimates of uncertainties and variance.

Overall variance in quantitative estimates of population exposure comes from several factors including (a) variability among individuals; (b) our ignorance regarding the processes of dispersion, transport, contact, and uptake; and (c) the reliability with which we can measure or quantify the parameters describing the exposure/uptake process. There are two obvious methods for reducing uncertainty—expanding the data and improving the precision of measurements and/or models. However, unless our strategy for reducing uncertainty recognizes that the cost of collecting data and building new models must be balanced by the value of the information obtained, we might squander limited resources for environmental research. The “value of information” approach is particularly important in defining the capabilities and limits of CalTOX. It is very important to minimize the cost of providing exposure information without jeopardizing the precision required of this information to meet the needs or objectives of the decision on when to terminate site clean-up.

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