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CalTOX, A Multimedia Total-Exposure Model for Hazardous-Wastes Sites

Part I: Executive Summary

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Prepared for:
The Office of Scientific Affairs
Department of Toxic Substances Control
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Part I: Executive Summary

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FOREWORD

The Department of Toxic Substances Control (DTSC), within the California Environmental Protection Agency, has the responsibility for managing the State's hazardous-waste program to protect public health and the environment. The Office of Scientific Affairs (OSA) within the DTSC provides scientific assistance in the areas of toxicology, risk and environmental assessment, training, and guidance to the regional offices within DTSC. Part of this assistance and guidance is the preparation of regulations, scientific standards, guidance documents, and recommended procedures for use by regional staff, local governmental agencies, or responsible parties and their contractors in the characterization and mitigation of hazardous-waste-substances-release sites. The CalTOX model 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 multimedia transport and transformation models, exposure scenario models, and efforts to quantify and reduce uncertainty in multimedia, multiple-pathway exposure models. This report provides an executive summary of the model development process and is the first of a series of three reports describing the development and use of CalTOX model.

TABLE OF CONTENTS

Abstract 1
Introduction 2
Objectives of the CalTOX Model 3
Linking Sources with Multiple Environmental Media and Exposure Media 4
Sources, Exposure, Dose, and Risk 5
Confronting Uncertainties 8
The Peer Review Process for CalTOX 9
Overview of the Component Models of CalTOX 10
The Multimedia Transport and Transformation Model 10
Fugacity Models 11
Model Structure 12
Balancing Gains and Losses—Sources, Transport, and Transformation 13
Critical Sensitivities and Uncertainties 15
The Human Exposure Model 15
Model Structure 16
Ingestion 18
Inhalation 18
Dermal Uptake 19
Summary Comparison of Multiple-Pathway Exposure 19
CalTOX Inputs and Outputs 20
Inputs Required for the Transport and Transformation Model 20
Inputs Required for the Human Exposure Model 21
Uncertainty and Variability of Inputs 22
Uncertainty and Sensitivity Analyses with CalTOX 23
The Capabilities, Limitations, and Reliability of CalTOX 25
Space and Time Scales 25
Chemical Classes 26
What the CalTOX Transport Model Should Not Be Used For 26
Discussion 27
Acknowledgments 28
References 29

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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.

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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

In order to meet the risk management needs of the California Environmental Protection Agency, we believe it is not necessary to develop ever larger and more complex deterministic models. What is needed instead are scientifically defensive exposure models that incorporate uncertainty and population-distribution data.

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.

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

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, $(mg/kg\text{-}d)^{-1}$.

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

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

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.

uncertainty; to separate individual variability from true scientific uncertainty; or to consider benifits, 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 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),

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

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),

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

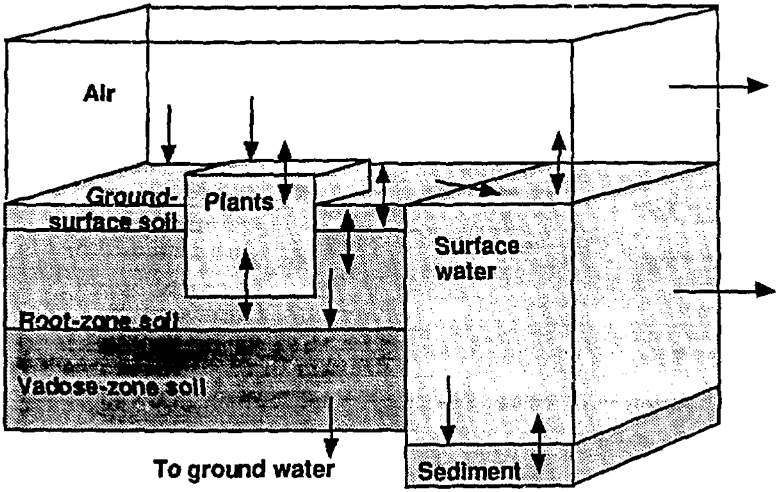

Figure 1. An illustration of mass-exchange processes modeled in the seven-compartment environmental transport and transformation model. (Ground water is not explicitly modeled in the system of equations but is used in the exposure calculations.)

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 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

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 •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 included)	•Dermal contact with soil	•Dermal contact in baths and showers •Dermal contact while swimming

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.

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 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 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 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 compliment 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"

REFERENCES

Bogen, K. T., and R.C. Spear (1987) "Integrating Uncertainty And Interindividual Variability In Environmental Risk Assessments." *Risk Analysis* 7, 427-436.

Berger, J.O. (1985) Statistical Decision Theory and Bayesian Analysis (Springer, New York).

Chernoff, H. and L.E. Moses (1959) *Elementary Decision Theory* (Wiley, New York; reprinted by Dover, New York, 1986).

Cohen, Y., and P. A. Ryan (1985) "Multimedia Modeling of Environmental Transport: Trichloroethylene Test Case," *Environ. Sci. Technol.* 9, 412–417.

Department of Toxic Substances Control (DTSC) (1992a) *Guidance for Site Characterization and Multimedia Risk Assessment for Hazardous Substances Release Sites, Volume 2, Chapter 2 Documentation of Assumptions Used in the Decision to Include and Exclude Exposure Pathways*, a report prepared for the State of California, Department of Toxic Substances Control, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-CR-103462.

Department of Toxic Substances Control (DTSC) (1992b) *Guidance for Site Characterization and Multimedia Risk Assessment for Hazardous Substances Release Sites, Volume 2, Chapter 3, Guidelines for the Documentation of Methodologies, Justification, Input, Assumptions, Limitations, and Output for Exposure Models*, a report prepared for the State of California, Department of Toxic Substances Control, by Lawrence Livermore National Laboratory, Livermore, CA, UCRL-CR-103460.

Federal Register (1992) "Guidelines for Exposure Assessment; Notice," Environmental Protection Agency, *Federal Register* 57(104), 22888-22938, May 29.

International Atomic Energy Agency (IAEA) (1989) *Evaluating the Reliability of Predictions Made Using Environmental Transport Models*, Safety Series 100, (International Atomic Energy Agency, Vienna)

U.S. Environmental Protection Agency (U.S. EPA) (1989) *Risk Assessment Guidance for Superfund Volume I Human Health Evaluation Manual (Part A)*, Office of Emergency and Remedial Response, EPA/540/1-89/002.

Wasserstein, A. (1982) *Galen's commentary on the Hippocratic Treatise, Airs, Waters, Places*, (English translation and notes) Proceedings of the Israel Academy of Sciences and Humanities VI, 3 (Israel Academy of Sciences and Humanities, Jerusalem).

Whicker, F.W. and T.B. Kirchner (1987) "PATHWAY: A Dynamic Food-Chain Model to Predict Radionuclide Ingestion After Fallout Deposition," *Health Phys.* **52**, 717-737.

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