PART D - CHAPTER 3

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MODELING

3.1 INTRODUCTION

Models can be used for risk assessment in the absence of empirical data, as a supplement to limited data, or to mathematically describe complex exposure situations. The use of predictive models may be required in the course of estimating human post-application exposures to pesticides to address data gaps as it is not always possible to collect adequate test data to fully address each scenario of concern. For example, the dilution and dissipation of chemicals in indoor air over time may be modeled or the dissipation rates of chemicals may be predicted based on physical-chemical properties. Additionally, modeling approaches may be required even when empirical data are available because of the complex nature of the postapplication risk assessment or the nature of the calculations required to adequately utilize the power of the available data. For example, attempting to account for the multiple potential activity and behavioral patterns that occur in a residential setting (e.g., time, location, and behavioral data inputs). The use of models potentially also has several other benefits including completing risk assessments early in the product development process, alleviating, in some cases, the need for conducting expensive and complex human exposure studies, and as tools for developing risk-based product support or enforcement policy approaches (e.g., develop relative risk rankings for chemical classes).

Generally, models transform known inputs or conditions into an exposure/risk analysis using mathematical algorithms created to predict an output for the given scenario. The mathematical algorithms that serve as the basis for models generally fit into two distinct categories including those that can predict chemical characteristics in the environment based on physical/chemical properties, and those that describe the treatment of existing data. Examples of predictive approaches based on the physical/chemical characteristics of a chemical would be the calculation of emission rates using molecular weight and vapor pressure or predicting environmental behavior (i.e., fate and transport) based on the principle of fugacity. Conversely, algorithms that describe the treatment of existing data could include sampling from a data distribution for stochastic modeling or development of an activity pattern scenario for a residential assessment based on a compilation of existing data.

Although models can be powerful tools for the risk assessment process. Assessors should be careful to abide by a “good modeling practice” approach and consider the level of validation as well as other risk characterization issues associated with any model that has been utilized to address an exposure scenario. Assessors should include discussions of risk characterization issues during the calculation process and more importantly while interpreting the results of an assessment. The “good modeling practice” approach

essentially mirrors the basic tenets of the Good Laboratory Practices (40CFR160) in that all assessments completed using a model should be mathematically transparent and reproducible by reviewers. Additionally, the rationale pertaining to how decisions regarding data inputs and the use of empirical data were made should be clear from any assessment. The level of validation of any selected model is a primary risk characterization issue for the Agency. Available information pertaining to the development and validation of the selected model should be included (at least in summary form) in any assessment as this will provide insight into the regulatory importance that should be associated to the assessment. Additionally, a discussion of the appropriateness of the model should also include several other risk characterization issues including a discussion of the anticipated levels of accuracy and precision, a discussion of the reliability of the inputs, and a discussion of any other critical issues that should be considered in the interpretation of the assessment. Assessors should also abide by other general requirements of the exposure assessment process including compliance with the U.S. EPA Exposure Assessment Guidelines (see Part D-Chapters 1 and 2 for further information).

This chapter provides a discussion of some of the parameters involved in modeling exposure to chemicals and an overview of some of the models that may be applicable to estimating postapplication exposure to chemicals. This chapter also provides more specific guidance on generally-accepted model validation criteria and recommendations on presenting an exposure assessment completed using a model. The intent of this chapter is not to provide an in-depth discussion of all of the models or issues that may be used to exhaustively address postapplication exposure issues. Such an in-depth analysis is left to each assessor, given the numbers and variety of the assessments that are anticipated by the Agency in response to Food Quality Protection Act requirements for chemicals in the residential marketplace and to address exposure issues related to those occupationally exposed in the agricultural and industrial/commercial marketplaces.

3.2 MODELING PARAMETERS

Modeling parameters can be divided into two categories: those that pertain to the estimation of the chemical concentration in a localized environment, and those that pertain to the estimation of individual exposure in an environment. This discussion of modeling parameters focuses on indoor air concentrations because, currently, modeling is most frequently used by EPA to estimate indoor air concentrations of pesticides (e.g., after the use of antimicrobials and after indoor crack-and-crevice application).

3.2.1 Estimation of Chemical Concentration

The concentration of a particular chemical in an indoor environment can be estimated by examining the chemical of concern and the environment in which it exists. Properties of interest are: the physical and chemical properties of the chemical of concern, the properties of the environment in which the chemical exists. For example, for an indoor environment, information about the environmental chamber (house), the airflow throughout the environmental chamber, and the effects of sources and sinks in the environment is needed. These parameters are generally inputs into the model and are, in some cases, essential for running the model.

One element of determining the concentration of a chemical in an environment is evaluating the physical and chemical properties of the chemical of concern. In general, a mass balance equation is used to determine the amount of the chemical present. The amount of chemical present is equal to the amount that was placed in the system minus the amount that has left the system. For example, the amount of pesticide remaining after application to a room is equal to the amount initially applied minus the amount that has dissipated. The remaining pesticide is in two forms: the liquid portion that has not evaporated, and the vapor portion that lingers in the air. Chemical properties—such as volatility, reactivity, and the ability of a chemical to decay and produce other chemicals—can be used to determine how much, if any, of the chemical has evaporated into the surrounding air. Knowing the amount of the chemical in the ambient air, the amount of the chemical remaining on the applied surface, and the airflow through the chamber, one can determine, using the mass balance equation, the amount of chemical present, which in turn can be related to an exposure concentration (CMA, 1993).

A second environmental property of consideration is the environment in which the chemical exists. In assessing indoor air concentrations, the characteristics of the environmental chamber, or house, being studied is of interest. The environmental chamber can consist of one room or many rooms. The size, or volume, of the environmental chambers is important in helping to determine the ratio of the vapor concentration of the chemical of concern to the amount of air available. Large or multi-roomed chambers may afford a larger volume of air in which to dilute hazardous vapors. The ambient temperature and pressure of the environmental chamber will also affect the amount of chemical released into the vapor phase, and where it may be located. The structural elements of a room, such as the placement of doors, windows, and stairs, also affect how chemical vapors will flow through a room and where these vapors may condense to form dermal hazards. All of these factors need to be considered when selecting and using a model (Austin et al., 1992).

Other factors that shape the environment being analyzed are fate and transport parameters. For indoor air, this can include the airflow in the environmental chamber and the occurrence of sources and sinks. The airflow assists in the evaporation of a chemical as well as its transport into and out of the environmental chamber. Airflow can be a function of changes in temperature and pressure. It can also be the result of mechanical turbulence (e.g., a fan or air conditioner). As mentioned above, the structural factors of an environmental chamber can affect the transport of vapors throughout a room. Pockets of chemical vapors could occur in corners or spaces throughout a room due to lack of airflow. If an environmental chamber has multiple rooms or is one large room, airflow characteristics may cause a gradient in vapor concentrations throughout the chamber. Therefore, it is important to understand the properties of the airflow (e.g., the velocity, direction, etc.) in an environmental chamber in order to ensure proper performance of the model (Austin et al., 1992; CMA, 1993).

Sources can be described as physical objects that release a chemical into the environment. Sinks, on the other hand, can be considered objects that trap, or remove, a chemical from the environment. The ability of these objects to affect the mass balance of a particular chemical is dependent on the physical, as well as the chemical, makeup of the objects. Source emission rates are used to provide information on how much of a particular chemical will be released into the air at given periods of time. The surface area, as well as the relative location of a source or sink, may be used in a model to determine the amount of a chemical that may pose a dermal threat (Austin et al., 1992; CMA, 1993).

3.2.2 Estimation of Human Exposure

Human exposure to a chemical can be estimated by defining those factors that pertain to the chemical of concern and the individual being exposed. The properties pertaining to the chemical of concern have already been discussed. The properties defining the exposed individual include the following: the exposed population, the exposure duration, the exposed individual's activity patterns, and the exposure routes.

The exposed population is the set of individuals being exposed to chemicals in the environmental chamber. The exposed population can be described by parameters such as age, sex, race, and occupation. Such parameters will help shape decisions on exposure duration and exposure route parameters described below. For example, an infant may be exposed to a chemical in a much different fashion than an elderly person. At the same time, a housewife may be exposed to a chemical for a much longer time than a woman who works at an office and is only exposed to the room for a few hours. Exposed populations may or may not be put directly into a computer model.

Exposure duration is how long an individual is exposed in an environmental chamber. This can be measured in hours per day, days per week, days per year, and so forth. This parameter will help determine the acute or short-term exposures, and the chronic or long-term exposures. This parameter is usually put into computer models.

Activity patterns are what an individual does in the environmental chamber. The patterns are directly related to the amount of the chemical to which an individual will come into contact. An individual sitting and watching television does not respire as rapidly as an individual who is exercising, and, therefore, will not inhale the same amount of a chemical in the air. However, if the chair of the person sitting is treated with the chemical of concern, the person sitting and watching television may be exposed dermally to the chemical of concern, while the exercising person is not. In addition, activity pattern data help to define the placement of an individual within the treated area relative to chemical concentrations in the environmental chamber. For example, for individuals residing in a home where pesticides have been applied in the basement, postapplication exposures may be the highest during activities conducted in the basement and lower when activities are performed in other parts of the house. Activity patterns may or may not be a direct input parameter for exposure models (Austin et al., 1992).

The last property considered in estimating human exposure is the exposure route of the chemical. The exposure route indicates how the chemical comes in contact with an individual. For the purposes of this discussion, inhalation, dermal contact, and ingestion are the exposure routes being considered.

3.3 EXAMPLES OF COMPUTER MODELS

Described below are two indoor air quality models, one dermal model, and a migration model that are currently used by EPA to estimate potential chemical exposure. These models were selected for discussion because they have been accepted and are currently supported by the EPA's Office of Pollution Prevention and Toxics (OPPT) for assessing new and existing chemicals. Additional, exemplary exposure-related models and software products that may be appropriate for assessing postapplication exposure to pesticides are briefly described in Appendix 3-A to this chapter. This appendix is not a comprehensive list and the mention of model and software names is not an endorsement. However, the Appendix provides a sampling of products that may have utility for postapplication exposure assessments. It is left to the reader to determine the appropriate model and software of choice for a given situation and to document the modeling approach and appropriate validation. Additional software systems, exposure-related databases and online systems are addressed by U.S. EPA (1992) and P.J. Hakkinen (1997).

Multi-Chamber Concentration and Exposure Model (MCCEM)

Description:

MCCEM is an interactive model developed for the EPA's, OPPT and updated for the Office of Research and Development (ORD) by Geomet Technologies, Inc. The model is used for assessing inhalation exposure to airborne concentrations of chemicals released from products in residences. It contains a database of house data needed to run an indoor air model—information such as air exchange rates, inter-room airflows, and house and room volumes. The user can enter source emission rates of pollutants into the model either as numbers or as formulas. MCCEM accounts for chemical decay and changing outdoor concentrations over time. It is capable of performing sensitivity analyses and Monte Carlo analyses (U.S. EPA, 1991).

Input parameters:

The following are input parameters for MCCEM: environmental chamber location, type of environmental chamber, geographic location, exposure duration, the number of exposures per year, the number of years of exposure, room size, pollutant concentration in outdoor air, inter-room airflow rates, emission rates, decay rates, chemical levels of concern, and the number of rooms being analyzed.

If the Monte Carlo analysis option is selected, the type of distribution and lower boundary of the distribution for the infiltration rate, source rate, decay rate, and outdoor concentration must also be provided.

MCCEM allows the user to explore the sensitivity of the model results to changes in one or more of the input parameters. If the sensitivity analysis option is selected, the multiplicative factor for the parameter of concern must be included. Parameters that can be modified in the sensitivity analysis include the infiltration rate, the source rate, the decay rate, and the outdoor concentration.

Default Values: MCCEM provides default values for the input parameters discussed above. When calculating the Lifetime Average Daily Dose (LADD) values, MCCEM assumes a default breathing rate of 20 cubic meters per day, a default body weight of 70 kilograms, and default average lifetime of 70 years.

Output Parameters:

MCCEM provides summary statistics (average concentration, standard deviation, maximum concentration and the percent of the values above the level of concern) for a chemical in each room, the percent of time an individual is in the environmental chamber, and the estimated LADD.

Output Products:

MCCEM can summarize inputs and outputs on the computer monitor. ASCII text files and data files are also created to provide the user the opportunity to further review the data.

SCREENING CONSUMER INHALATION EXPOSURE SOFTWARE (SCIES)

Description:

SCIES has been developed for the EPA's OPPT by Versar Inc. The model is used to assist in performing screening-level assessments of potential dose rates from inhalation of new and existing chemicals in consumer products. The model classifies consumer products in 10 categories and estimates potential average individual dose rates from inhaling each component of a consumer product based on the product category in which it has been placed. The model estimates potential dose rates for both the user of the product and passively exposed non-users. The model allows for the selection of default consumer product categories as well as a user-input scenario (U.S. EPA, 1994). EPA is currently in the process of developing the Consumer and Occupational Model (COM), which will incorporate a consumer inhalation exposure module similar to SCIES and will eventually replace the SCIES model in performing screening level assessments for new and existing chemicals at OPPT.

Input parameters:

The following parameters are input into SCIES: chemical name (optional), molecular weight of the chemical, vapor pressure, weight fraction of the chemical, the room where the product was used, and user occupancy patterns. In the user-input scenario, the following parameters may also be required: the annual frequency of use, the mass of the product used per event, the air exchange rate, the non-user inhalation rate, the user inhalation rate, the duration of use, room volume, and the environmental chamber volume.

Default Values:

SCIES provides default values for all of the parameters listed above in the user-input scenario. SCIES uses a two-room environmental chamber (the room where the product was released and the rest of the environmental chamber) and assumes the concentration of the product outside the environmental chamber is zero. Product use is restricted to rooms labelled "the kitchen" or "the bedroom".

Output Parameters:

SCIES provides data on the annual potential dose rates for active- and passive-exposed individuals, evaporation time, the amount of time following each use of the product, the interval between uses of the product, the average and peak predicted concentrations in the two rooms for users and non-users, and a summary of the hourly activity patterns for users and non-users throughout the environmental chamber.

Output Products:

SCIES can summarize the inputs and outputs for a model run on the computer monitor or send the summary to a printer. A text file can also be created so that the file can be imported into a word processing program (e.g., WordPerfect).

DERMAL

Description:

DERMAL is a dermal exposure model developed for EPA's OPPT by Versar Inc. to be used in performing screening-level assessments of the potential dose rates from dermal contact with consumer products containing new and existing chemicals. The model allows the user to select from 1 of 16 consumer product categories for screening-level estimates. The model also allows users to design their own scenarios for products not included in the model. The model is user-friendly and requires minimum input from the user (U.S. EPA, 1995). OPPT's COM will include a dermal exposure assessment module that will update and replace the DERMAL model. COM is currently under development by OPPT.

Input parameters:

DERMAL requires the following input parameters: median and high-end weight fraction of chemical in product; median and high-end skin surface area exposed; film thickness of liquid on skin; density of the product; dilution fraction; low, median, and high-end frequency of events; and, low, median, and high-end years of use of the product in a lifetime. For certain consumer products, more information on the exposed portion of skin and the amount of product contacting the hands may be required.

Default Values:

Default values exist for all of the input parameters, except for the weight fraction inputs, for the 16 consumer product categories in the DERMAL model. These default values can be changed during any model run.

Output Parameters:

DERMAL outputs the central, high-end, and bounding acute potential dose rates, and the central and high-end LADD. Output products: DERMAL allows the user to send all of the input and output data results to the screen, to a printer, or to a WordPerfect file.

AMEM (Arthur D. Little Migration Estimation Model)

Description:

AMEM (U.S. EPA, 1990) is a computer program that facilitates the rapid estimation of the fraction of additives originally in polymer sheets that will migrate under various conditions. With AMEM, one can estimate migration of additives to fluid and solid external phases. The Exposure Evaluation Division of the Office of Pollution Prevention and Toxics at the EPA assesses the potential for exposure to chemicals that are used as additives in polymeric materials or are the monomers or low molecular weight oligomers contained in polymers, by using AMEM or similar models. AMEM, which also has subroutines that estimate many physical properties (diffusion coefficients of additives in the polymers, in air, and in water; partition coefficients; and mass transfer coefficients), is coded in FORTRAN for operation on PCs.

Input Parameters:

The input parameters for AMEM include polymer thickness (cm); external phase type (air, water, or solid), and duration over which migration occurs (hrs). The diffusion coefficient (cm^2/s) of the chemical is also needed, and can be estimated by the model if the molecular weight of the migrant (g/mole) is known and the polymer type (e.g., silicone rubber, polystyrene, etc.) is selected from the model's menu. If partitioning effects and mass transfer resistance are considered, the user may also need to provide information on the saturation concentration of the migrant in the polymer (g/cm^3), vapor pressure (for air phases) (torr), melt temperature (for water phases) ($^\circ C$), surface length (cm), air or water flow velocity (cm/s), volume of external phase (m^3), and surface area of the polymer (cm^2).

Output Parameters:

The model provides information on the fraction of polymer migrated and the diffusion coefficient in the polymer (cm^2/s), if estimated. If partitioning effects and mass transfer resistance are considered, estimated partition coefficients and mass transfer coefficients will be provided.

3.4 VALIDATION OF PREDICTIVE PESTICIDE EXPOSURE MODELS

In general, predictive pesticide exposure models must be shown to produce results that reflect "real-world" data. It is not enough that a model developer put forward a model and state that it produces accurate real-world data simply because a model is based on detailed theoretical mathematical representations. Regulatory authorities have traditionally relied upon field studies, conducted in accordance with the appropriate guidelines, because the data generated by field studies are based upon measured concentrations. Although field study data may be limited in strength because the results may reflect only one specific location under one set of conditions, they can be considered valid for real-world conditions. Predictive models, in contrast, generate results that are based upon mathematical representations of physical, biological, and chemical processes. The confidence that regulatory authorities can place in predictive models is based upon the accuracy of the input parameters, and the degree to which the model has been proven to reproduce observed field-generated data. Thus, regulatory authorities require validation of predictive models through the generation of data that demonstrate that:

i) input variables are accurate and appropriate (which includes ensuring that the computer source code is properly debugged and that there is confirmation that the algorithms are mathematically correct), and

ii) results from predictive models are reliably comparable to those seen in field studies (i.e., "real world" data should be generated to confirm model output).

Field studies used for validation purposes must be representative of the various scenarios that a model may predict. Thus, it is not adequate to conduct a single validation study for a model that makes predictions for different types of formulations, hydrophobic and hydrophilic compounds, and various settings (e.g., single room vs. entire home). The validation data must reflect the various scenarios the model predicts.

In addition, validation studies must have been conducted using the same guidelines required for the conduct of the corresponding field studies (i.e., Series 875, Group B for residential pesticide exposure studies). Hence, issues such as the appropriate number of replicates and quality assurance are still of concern when validating a model. Validation studies that are not conducted according to the required regulatory guidelines for field studies cannot be considered valid in themselves and, as such, cannot be used to validate predictive models.

3.5 REPORTING CRITERIA FOR MODEL-BASED ASSESSMENTS

The reporting of all assessments should be based on the principles and requirements described in the *Data Reporting Guidelines* that have been developed for this document. These guidelines are presented in Appendix I. Assessors should also review and incorporate the general guidance pertaining to the exposure and risk assessment process that is described in Chapters 1 and 2 of Part D of this document (i.e., Chapter 1: Fundamentals of Exposure and Risk Assessment and Chapter 2: Calculations), and *The International Harmonization Position Paper: Guidelines For Using and Reporting PHED Data* (Final Draft of 9/19/1997).

Critical issues and requirements that are specific to reporting model-based assessments are summarized and presented below. These include:

- Providing an adequate description of the model used in the assessment including source, version number, and operational requirements (e.g., Windows or DOS-based).
- Providing an adequate description of the model inputs along with a description of any assumptions used.
- Developing risk characterization language that describes and quantifies the uncertainties associated with model inputs, model validation, the model algorithm, and for interpreting the resulting risk assessment.
- Providing a working copy of the model(s) used to accompany any exposure/risk assessment.
- Including all model inputs/outputs in any submission (e.g., hardcopy of input tables and outputs).

APPENDIX 3-A: EXPOSURE MODELS/SOFTWARE BIBLIOGRAPHY

The following paragraphs briefly discuss additional models and software products that may be relevant for assessing postapplication pesticide exposure or factors (e.g., physical/chemical properties) necessary for estimating these exposures. The products' capabilities and computer requirements, as well as available contacts are included. The list is not intended to be inclusive of all available models and software, but provides a sampling of products with potential utility for postapplication exposure assessments.

AERIS (Aid for Evaluating the Redevelopment of Industrial Sites)

AERIS is a soil toxicity model developed by SENES Consultants Ltd., Ontario, Canada. The model, which is specifically designed to meet the soil testing requirements for the Decommissioning Steering Committee in Canada, provides estimates of concentrations of chemicals in contaminated soil that are used to help establish cleanup guidelines or to indicate when remedial actions are required. Model inputs include site-specific data, physical and chemical properties, transport calculation methods, and exposure parameters. The model also estimates human exposures resulting from contaminated soil. The PC-based model includes a lookup database that contains physical and chemical properties of certain chemicals.

API DSS (American Petroleum Institute Decision Support System)

API DSS estimates exposure concentrations and subsequent risk from a suite of fate and transport models coupled with toxicity parameters. Relevant exposure pathways evaluated by the models include vapor intrusion (from soil) into homes, volatilized chemicals from bathroom showers, soil ingestion, and ingestion of food and water.

CalTOX (California Toxicity Model)

The Department of Toxic Substances Control (DTSC) of the California Environmental Protection Agency has the responsibility for managing the state's hazardous waste program. As part of this program, the DTSC funded the development of the CalTOX program (McKone, 1993a, 1993b, 1993c). CalTOX has been developed as a set of spreadsheet models and spreadsheet data sets to assist in assessing human exposures and defining soil cleanup levels at uncontrolled hazardous waste sites. CalTOX addresses contaminated soils and the contamination of adjacent air, surface water, sediments, and groundwater. The modeling components of CalTOX include a multimedia transport and transformation model, exposure scenario models, and add-ins to quantify uncertainty and variability. 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, soil, 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 CalTOX to estimate average daily doses within a human population. The exposure models encompass 23 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 dust, soils and so forth.

CHEMCAN

CHEMCAN, which is similar to CalTOX and USES, is a multiple media fugacity model designed to estimate the distribution of single chemicals in multiple media. Given emission rates and chemical properties, it estimates chemical concentrations in air, food, soil, and water. CHEMCAN was developed for Environment Canada.

CONSEXPO (CONSumer EXPOsure Model)

CONSEXPO (Van Veen, 1995) is a modeling approach based on simple exposure and uptake models. In order to cope with the diversity in consumer products, it is based on a model framework that provides a general setting for widely differing exposure situations. It also offers a number of predefined exposure and uptake models, which users can link to build a complete exposure and uptake model. The starting points are the inhalation, dermal, and ingestion exposure pathways. For each of these pathways, a limited number of models are available for exposure and uptake. The program reports several important exposure variables; namely, the per-event concentration, the yearly averaged concentration, the fraction taken up, the amount taken up during a year (per year and summed), and the uptake per kilogram of body weight per day. The program also allows for stochastic parameters, in order to propagate the effects of variable and/or uncertain parameters to the final exposure and uptake estimates. If stochastic parameters are included, the resulting distributions can be displayed and studied.

The CONSEXPO program is related to the USES programs (also discussed in this section). CONSEXPO can be operated as a stand-alone program or as part of the framework of USES. The computer system requirements for CONSEXPO are an Intel-based PC, Microsoft Windows 3.1, and at least 1 MB of available hard drive space. A math coprocessor is not mandatory, but is highly recommended.

CONTAMx

The National Institute of Standards and Technology (NIST) has, over the past several years, developed a series of public domain computer programs (CONTAM86, CONTAM87, CONTAM94) for calculating airflow and contaminant dispersal in multiple zone buildings. These programs take a multiple zone network approach to airflow analysis. Airflow paths include doorways, small cracks in the building envelope, and a simple model of the air handling system.

CONTAM94, the most recent version of CONTAMx, works on an Intel-based PC in the DOS environment. A graphical interface is used to create and edit building descriptions. Future versions of this program will include exposure assessment.

EASE (Estimation and Assessment of Substance Exposure)

The EASE system was developed by the United Kingdom Health and Safety Executive in conjunction with the Artificial Intelligence Applications Institute. EASE is a knowledge-based system that stores knowledge on specialized subjects along with the reasons for that knowledge. EASE estimates exposure of workers to notified substances. Particularly, it estimates inhalation exposure to dust and vapor and dermal exposure.

EML/IMES (Exposure Models Library/Integrated Model Evaluation System)

EML, developed by the EPA's Office of Research and Development, is a collection of exposure models distributed in a CD-ROM (U.S. EPA, 1996). The purpose of this disc is to provide a compact and efficient means for distributing exposure models, documentation, and the IMES. The disc contains over 120 models that may be used for transport modeling and exposure assessments. The model files may contain source and/or executable code, sample input, and other data files, sample output files, and, in many cases, model documentation in WordPerfect, ASCII text, or similar formats. IMES assists in selecting appropriate models, provides literature citations on model validations, and demonstrates model uncertainty protocols. The IMES software is an MS-DOS application, can be used on an Intel-based PC, and is capable of running on a network. Model codes and documentation can be downloaded from the CD-ROM to a hard drive. The most recent version, which is the third edition, has an HTML interface to view model directories and an internet source for some models.

For copies of the CD or for technical assistance, the contact person is Richard Walentowicz at the EPA's Office of Research and Development in Washington, D.C. (phone: 202-260-8922, E-mail: walentowicz.rich@epamail.epa.gov).

INDOOR/EXPOSURE/RISK (IAQ Model for Windows, RISK Version 1.0)

RISK is the third in a series of indoor air quality models developed by the Indoor Air/Radon Mitigation Branches of EPA's National Risk Management Research Laboratory. The first model, INDOOR, was designed to calculate the indoor pollutant concentrations from indoor sources. The second model, EXPOSURE, extended INDOOR to allow calculation of individual exposure. RISK extends EXPOSURE to allow analysis of individual risk to indoor pollutant sources. Risk estimates generated by models such as this one are useful mainly for the purpose of comparing scenarios rather than for determining absolute risks to individuals or populations.

RISK uses data on source emissions, room-to-room airflows, air exchange with the outdoors, and indoor sinks to predict concentration-time profiles for all the rooms. The concentration-time profiles are then combined with individual activity patterns to estimate exposure. Risk is calculated using a risk calculation framework. The model allows analysis of the effects of air cleaners located in the central air circulating system and/or individual rooms on Internal Air Quality (IAQ) and exposure. The model allows simulation of a wide range of sources, including long-term steady state sources, on/off sources, and decaying sources. Several sources are allowed in each room. The model allows the analysis of the effects of sinks and sink re-emissions on IAQ. The results of test house experiments were compared with model predictions. The agreement between predicted concentration-time profiles and the test house data was good. The model is designed to run in the Windows operating environment.

RISK can be ordered from the National Technical Information Service, 5285 Port Royal Road, Springfield, VA 22161 (Phone: 703-487-4650). The complete report is titled "IAQ Model for Windows, RISK Version 1.0: User Manual," (Order No. PB96-501 929).

MMSOILS (Multiple Media Soil Model)

MMSOILS estimates the human exposure and health risk associated with releases of contamination from hazardous waste sites. It is a multimedia model addressing the transport of a chemical in groundwater, surface water, soil erosion, the atmosphere, and accumulation in food. The human exposure pathways considered in the methodology include: soil ingestion, air inhalation of volatiles and particulates, dermal contact, ingestion of drinking water, consumption of fish, consumption of plants grown on contaminated soil, and consumption of animals grazing on contaminated pasture. For multimedia exposures, the methodology provides estimates of human exposure through individual pathways and combined exposure through all pathways considered. The risk associated with the total exposure dose is calculated based on chemical-specific toxicity data.

The methodology is intended to be used as a screening tool. It is critical that the results are interpreted in the appropriate framework. The intended use of the exposure assessment tool is for screening and relative comparison of different waste sites, remediation activities, and hazard evaluation. The methodology can be used to provide an estimate of health risks for a specific site, but the uncertainty of the estimated risk may be quite large (depending on the site characteristics and available data), and this uncertainty must be considered in any decision-making process.

MMSOILS was developed to operate on an Intel-based PC. Other minimum system requirements are 512 KB of available random access memory, one 3-1/2" or 5-1/4" floppy disk drive, one hard disk drive (2.0 MB storage available), and DOS 3.x or higher. Because of the extensive computations involved in MMSOILS, it will operate most effectively on a 386 or 486 series computer equipped with a math coprocessor.

PC-GEMS (Personal Computer - Graphical Exposure Modeling System)

GEMS supports exposure and risk assessments by providing access to single medium and multimedia fate and exposure models, physical and chemical properties estimation techniques, statistical analysis, graphics and mapping programs with related data on environments, sources, receptors, and populations. Under development since 1981, GEMS provides analysts with an interactive, easily learned interface to various models, programs, and data needed for exposure and risk assessments on the EPA's NCC VAX cluster. PC-GEMS is a stand-alone version of GEMS that can be run on a PC.

The environmental models in GEMS are atmospheric, surface water, land unsaturated (soil) and saturated (groundwater) zones, and multimedia in nature. Methods for estimating octanol-water partition and adsorption coefficients, bioconcentration factor, water solubility, melting and boiling point, vapor pressure, Henry's constant, acid dissociation constant, lake/stream volatilization rate, and atmospheric half-life are available. Data sets are related to environmental characteristics (climate, soil, rivers, groundwater, vegetation), source releases (POTWs and industrial water discharges, Census business patterns, RCRA permit sites), and receptors (population and household estimates for 1970, ‘80, ‘90, and ‘95 by small area census district; drinking water facilities). Mapping routines in GEMS support Tektronix 4014 and color 4105/06/25/35, and ASCII terminals or PCs. PC-GEMS supports Hercules, CGA, and EGA graphics.

PC-GEMS is available with air, surface water and groundwater models and associated environmental and 1980 population data encompassing most of the United States System requirements: IBM AT or compatible, Math Coprocessor (80187/80287/80387), 640K RAM, 20 Mb of dedicated disk space or Bernoulli cartridge.

RISKPRO

RISKPRO provides an integrated system that includes environmental modeling programs, site, and chemical tracking and supporting tools. Six programs are provided to simulate the transport and transformation of a chemical through air, water, and soil. The models interact with each other. Chemical property estimation and environmental databases are included.

RISKPRO is a compartmentalized system consisting of

(1) AUTOEST - a chemical property estimating program,
(2) ISCLT (Industrial Source Complex Long Term Model) - an air dispersion modeling program,
(3) PTPLU (Point Plume) - a single source Gaussian dispersion modeling program,
(4) SESOIL (Seasonal Soil Compartment Model) - a soil transport modeling program,
(5) AT123D - a groundwater transport modeling program, and
(6) EXAMS (Exposure Analysis Modeling System) - a surface water modeling program.

Also included within the system are several databases that include climate information for the United States, geographic information, census data, and a catalog of SMILES notations. RISKPRO was produced by General Sciences Corporation as an updated, user-friendly version of PCGEMS.

RISK*ASSISTANT

Developed by Hampshire Research Institute, RISK*ASSISTANT for Windows, a commercial product, provides a straightforward tool for evaluating complex risks, useful for both novice and professional risk assessors. The software provides information on hazard, exposure, and risk, and allows flexibility for tailoring the assessment to local sites. Risks from air, surface water, groundwater, soil, sediment, and food can be assessed. The software offers the choice of chemical and concentration data sets, alternative populations, exposure scenario factors, and toxicity data sets. Risks can be calculated for single scenarios (e.g., showering) or multiple scenarios (drinking water, showering, and eating local fish).

Sensitivity analyses can be performed to determine the effect of exposure variables on risk estimates. Transport models included are ISCLT2 (air dispersion model to predict chemical concentrations in the air surrounding points where toxic chemicals are released as air emissions) and STREAM (surface water model to predict the downstream concentrations of contaminants in rivers and streams). The software provides more than 15 MB of hydrology data on U.S. water bodies.

Databases in the software include hazard data for 650 chemicals. They provide EPA data on carcinogenic and noncarcinogenic toxicity, from the Integrated Risk Information System (IRIS) or Health Effects Assessment Summary Tables (HEAST). Other toxic hazard data bases can be easily incorporated.

SmartRISK

SmartRisk is a stand-alone commercial application designed for conducting human health risk assessments. Calculations follow the EPA paradigm: Hazard Identification, Exposure Assessment, Dose Assessment, Risk Characterization. Exposure is characterized through scenarios, and multiple pathways are considered. Exposure scenarios require exposure media contact, exposure durations, and exposure frequencies. All calculations are deterministic. Risk reports can be exported to a spreadsheet format in order to perform Monte Carlo Simulation using Crystal Ball or @RISK. For additional information, contact Pioneer Systems Development (phone: 206-822-4461; E-mail: pioneer@halcyon.com).

THERdbASE (Total Human Exposure Risk database and Advanced Simulation Environment)

THERdbASE is the result of a cooperative agreement with EPA's Office of Research and Development (National Exposure Research Laboratory, Las Vegas). THERdbASE is being developed as a PC-based computer modeling and database system that contains exposure- and risk-related information. The system provides an optimal framework for the construction of a suite of exposure- and risk-related models within the Modeling Engine by using information available in data files within the Database Engine.

Data can be viewed as a table, coded fields can be viewed as decoded fields, fields can be set to "show" or "hide" mode, and multiple data files can be viewed at the same time. In the "advanced" mode, user files can be edited. Data records can be queried and simple statistics (summary statistics: mean, standard deviation, minimum and maximum; percentile values at desired intervals; and linear regression on two numerical data fields) can be performed. Data can be printed, saved, or exported. New user files can be created and data can be imported.

Input to models is achieved through a standardized procedure. Inputs can be provided as single values, custom distributions (normal, lognormal, etc.), distributions based on data files present in THERdbASE, or specific percentile values. Efficient algorithms are provided to optimally access input data, to perform the numerical simulations, and to generate appropriate output data. Multiple model runs can be done through a batch process. Outputs from models are conducted as THERdbASE data files or as pre-set graphs.

In the Internet version of THERdbASE, the following data files are included:

- 1990 Bureau of Census Population Information
- California Adult Activity Pattern Study (1987-88)
- AT&T-sponsored National Activity Pattern Study (1985)
- 1992-94 National Human Activity Patterns Study (NHAPS)
- chemical agents from sources
- chemical agent properties
- air exchange rates
- information from EPA's TEAM (Total Exposure Assessment Methodology) studies
- information from EPA's NOPES (Non-Occupational Pesticides Exposure Study) studies
- human physiological parameters

In the Internet version of THERdbASE, the following models are included:

- location patterns
- chemical source release - instantaneous emission
- chemical source release - timed application
- indoor air (2-Zone)
- indoor air (N-Zone)
- exposure patterns for chemical agents
- Benzene Exposure Assessment Model (BEAM)
- source-based exposure scenario (inhalation + dermal)
- film thickness-based dermal dose
- PBPK-based dermal dose

The computer requirements of THERdbASE are an Intel-based 486 or higher PC, at least 8 MB of RAM, at least 40 MB of available disk space, a color VGA monitor, and Microsoft Windows 3.1. The most recent installable version of THERdbASE underwent beta-testing and a beta version is in the Internet (WWW site: http://www.hrcweb.lv-hrc.nevada.edu).

USES (Uniform System for the Evaluation of Substances) and EUSES (European USES)

USES (RIVM, 1994), was developed in the Netherlands by the National Institute of Public Health and Environmental Protection (RIVM); Ministry of Housing, Spatial Planning and Environment (VROM); and the Ministry of Welfare, health, and Cultural Affairs (WVC). USES provides a single framework for comparing the potential risks of different chemical substances released to multiple media of the environment.

It is an integrated modeling system that includes multiple environmental media and multiple human exposure pathways. The exposure assessment in USES starts with an estimate of substance emissions to water, soil, and air during the various life-cycle stages of a substance and follows its subsequent distribution in the total environment. The results of this type of multi-media assessment are the Predicted Environmental Concentrations (PECs) and an estimate of the daily intake by human receptors. In general, PECs are compared to "no-effects" levels for organisms in the environment, which are derived by extrapolating single-species toxicity tests to field situations. The estimated daily intake by humans is compared to the "no-observed-adverse-effect" level for mammals or to the "no-effect" level for humans.

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