United States
Environmental Protection
Agency

Office Of Air Quality
Planning And Standards
Research Triangle Park, NC 27711

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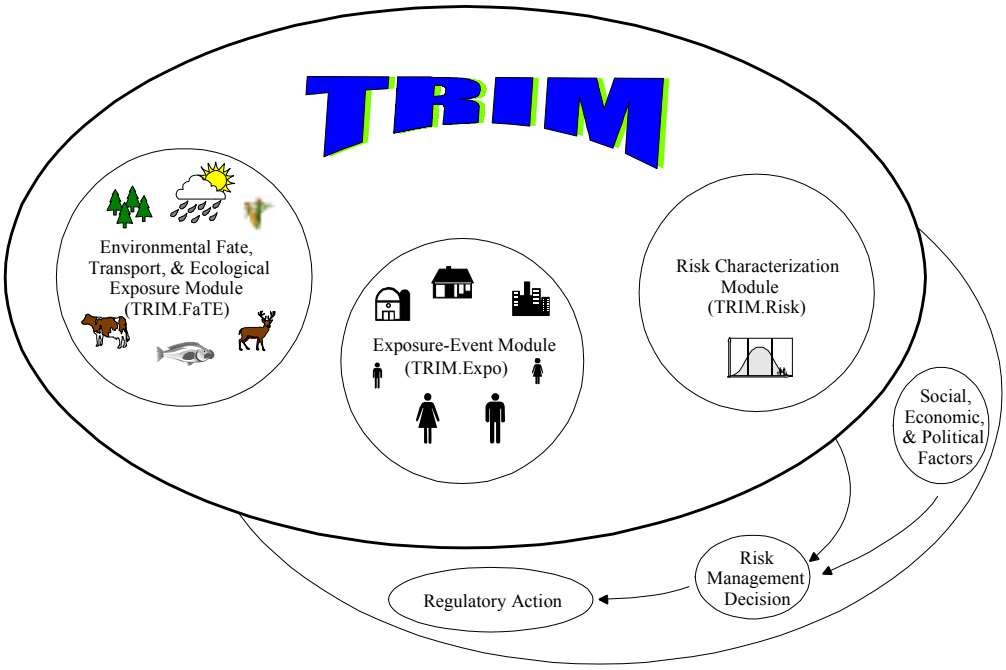
November 1999

Air

# TRIM
## Total Risk Integrated Methodology

# STATUS REPORT

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# Disclaimer

This report has been reviewed and approved for publication by the U.S. Environmental Protection Agency's Office of Air Quality Planning and Standards. Mention of trade names or commercial products is not intended to constitute endorsement or recommendation for use.

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# Acknowledgments

As described in this report, the Office of Air Quality Planning and Standards (OAQPS) of the U.S. Environmental Protection Agency is developing the Total Risk Integrated Methodology. The principal individuals and organizations in the TRIM development effort and in the preparation of this report are listed below. Additionally, valuable technical support for report development was provided by ICF Consulting.

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# Preface

This document, the 1999 *Total Risk Integrated Methodology (TRIM) Status Report*, is part of a series of documentation for the overall TRIM modeling system. The purpose of this report is to provide a summary of the status of TRIM and all of its major components, with particular focus on the progress in TRIM development since the 1998 *TRIM Status Report* (U.S. EPA 1998e). EPA plans to issue status reports on an annual basis while TRIM is under development.

The detailed documentation of TRIM's logic, assumptions, algorithms, equations, and input parameters is provided in comprehensive Technical Support Documents (TSDs) for each of the TRIM modules. The purpose of the TSDs is to provide full documentation of how TRIM works and of the rationale for key development decisions that were made. To date, EPA has issued TSDs for the Environmental Fate, Transport, and Ecological Exposure module (*TRIM.FaTE TSD*, U.S. EPA 1999i and U.S. EPA 1999j, which supersedes an earlier version, U.S. EPA 1998f) and the Exposure-Event module (*TRIM.Expo TSD*, U.S. EPA 1999h). When the Risk Characterization module (TRIM.Risk) is developed, EPA plans to issue a TSD for it. The TSDs will be updated as needed to reflect future changes to the TRIM modules.

In addition to status reports and TSDs, EPA intends to develop detailed user guidance for the TRIM computer system. The purpose of such guidance will be to define appropriate (and inappropriate) uses of TRIM and to assist users in applying TRIM to assess exposures and risks in a variety of air quality situations.

Comments and suggestions are welcomed. The OAQPS TRIM team members, with their individual roles and addresses, are provided below.


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# ACRONYMS

| | |
|---|---|
| APEX | Air Pollutant Exposure Model |
| ATFERM | Agency Task Force on Environmental Regulatory Modeling |
| B(a)P | Benzo(a)pyrene |
| CAA | Clean Air Act |
| CalTOX | California Multimedia Total Exposure Model for Hazardous Waste Sites |
| CART | Classification and regression tree |
| CMAQ | Community Multi-Scale Air Quality |
| CRARM | Presidential/Congressional Commission on Risk Assessment and Risk Management |
| CO | Carbon monoxide |
| $EC_{50}$ | Effective concentration at 50 percent response |
| $EC_{10}$ | Effective concentration at 10 percent response |
| EPA | United States Environmental Protection Agency |
| HAP | Hazardous air pollutant |
| HAPEM4 | Hazardous Air Pollutant Exposure Model Version 4.0 |
| HAPEM-MS | Hazardous Air Pollutant Exposure Model for Mobile Sources |
| HEM | Human Exposure Model |
| HI | Hazard Index |
| HQ | Hazard Quotient |
| GIS | Geographic Information System |
| GUI | Graphical User Interface |
| I/O API | Environmental Decision Support System/Models 3 Input/Output Applications Programming Interface |
| IEM | Indirect Exposure Methodology |
| IEM2M | Indirect Exposure Methodology for Mercury |
| ISCST3 | Industrial Source Complex, Short Term Version 3 |
| IUBK | Intake, Uptake, Biokinetic Model |
| $K_{aw}$ | Air/water partition coefficient |
| $K_{oa}$ | Octanol/air partition coefficient |
| $K_{ow}$ | Octanol/water partition coefficient |
| $LC_{50}$ | Lethal concentration at 50 percent response |
| LOAEC | Lowest observed adverse effect concentration |
| LSODE | Livermore Solver for Ordinary Differential Equations |
| MATC | Maximum acceptable toxicant concentration |
| MPE | Multiple Pathways of Exposure |
| NAAQS | National ambient air quality standard |
| NAS | National Academy of Sciences |
| NATA | National Air Toxics Assessment |
| NOAEC | No observed adverse effect concentration |
| OAQPS | EPA Office of Air Quality Planning and Standards |
| PAH | Polycyclic aromatic hydrocarbon |
| pNEM | Probabilistic NAAQS Exposure Models |
| pNEM/CO | Probabilistic NAAQS Exposure Model for Carbon Monoxide |
| RfC | Reference concentration |
| RfD | Reference dose |

| | |
|---|---|
| RIA | Regulatory impact analysis |
| SAB | Science Advisory Board |
| SETAC | Society of Environmental Toxicology and Chemistry |
| SHEDS | Stochastic Human Exposure and Dose Simulation |
| SRA | Society for Risk Analysis |
| TCCR | Transparency, clarity, consistency, and reasonableness |
| TRIM | Total Risk Integrated Methodology |
| TRIM.Expo | TRIM Exposure-Event module |
| TRIM.FaTE | TRIM Environmental Fate, Transport, and Ecological Exposure module |
| TRIM.Risk | TRIM Risk Characterization module |
| TSD | Technical Support Document |
| URE | Unit risk estimate |
| WASP | Water Quality Analysis Simulation Program |

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# 1. INTRODUCTION

The Office of Air Quality Planning and Standards (OAQPS) of the U.S. Environmental Protection Agency (EPA, or the Agency) has the responsibility for the hazardous and criteria air pollutant programs described by sections 112 and 108 of the Clean Air Act (CAA). Several aspects of these programs require evaluation of the health risks and environmental effects associated with exposure to these pollutants.[1] In response to these risk-related mandates of the CAA, and the scientific recommendations of the National Academy of Sciences (NAS) (NRC 1994), the Presidential/Congressional Commission on Risk Assessment and Risk Management (CRARM) (CRARM 1997), as well as EPA guidelines and policies, OAQPS recognized the need for improved fate and transport, exposure, and risk modeling tools that:

- Have multimedia assessment capabilities;
- Have human health and ecological exposure and risk assessment capabilities;
- Can perform multiple pollutant assessments (*e.g.*, ability to assess mixtures of pollutants, ability to track chemical transformations);
- Can explicitly address uncertainty and variability;
- Have the ability to easily perform analyses iteratively, moving from the use of simpler assumptions and scenarios to more detailed assessments; and
- Are readily available and user-friendly, so that they can be used by EPA, as well as by a variety of Agency stakeholders.

In 1996, OAQPS embarked on a multi-year effort to develop the Total Risk Integrated Methodology (TRIM), a time series modeling system with multimedia capabilities for assessing human health and ecological risks from hazardous and criteria air pollutants.

The main purpose of this Status Report is to summarize the work performed during the second developmental phase of TRIM. The first phase, which included the conceptualization of TRIM and implementation of the TRIM conceptual approach through development of a prototype of the first TRIM module, TRIM.FaTE (U.S. EPA 1998e), was reviewed by EPA's Science Advisory Board (SAB) in May 1998 (U.S. EPA 1998a). The second developmental phase has included refining TRIM.FaTE and developing a model evaluation plan, initiating development of the second module (TRIM.Expo), and conceptualizing the third module (TRIM.Risk). In addition, progress has been made on developing overarching aspects, such as the computer framework and an approach to uncertainty and variability. Consistent with the integral role of peer review in the TRIM development plan, the current Status Report and

[1] Hazardous air pollutants (HAPs) include any air pollutant listed under CAA section 112(b); currently, there are 188 air pollutants designated as HAPs. Criteria air pollutants are air pollutants for which national ambient air quality standards (NAAQS) have been established under the CAA; at present, the six criteria air pollutants are particulate matter, ozone, carbon monoxide, nitrogen oxides, sulfur dioxide, and lead.

Technical Support Documents (TSDs) were subjected to review by representatives from the major program offices at EPA and an EPA Models 2000[2] review team prior to this SAB advisory.

The goals and objectives, design, and development activities for TRIM are summarized in the following sections of Chapter 1, and certain aspects of development are expanded upon in later chapters of the report. Detailed descriptions of the TRIM.FaTE and TRIM.Expo modules are presented in accompanying TSDs (U.S. EPA 1999i, U.S. EPA 1999j, U.S. EPA 1999h).

## 1.1 GOALS AND OBJECTIVES FOR TRIM

The TRIM modeling system is intended to represent the next generation of human and environmental exposure and risk models for OAQPS. For example, TRIM is expected to be a useful tool for performing exposure and/or risk assessments for the following CAA programs: the Residual Risk Program (CAA section 112[f]); the Integrated Urban Air Toxics Strategy (CAA section 112[k]); studies of deposition to water bodies and mercury emissions from utilities (CAA sections 112[m] and 112[n]); petitions to delist individual HAPs and/or source categories (CAA sections 112[b][3] and 112[c][9]); review and setting of the national ambient air quality standards (NAAQS) (CAA section 109); and regulatory impact analyses (RIA).

The goal in developing TRIM is to create a modeling system, and the components of that system, for use in characterizing human health and ecological exposure and risk in support of hazardous and criteria air pollutant programs under the CAA. The goal in designing TRIM is to develop a modeling system that is: (1) scientifically defensible, (2) flexible, and (3) user-friendly.

(1) Characteristics of the TRIM components important to their scientific defensibility include the following.

- **Conservation of pollutant mass.** The modeled pollutant(s)' mass will be conserved within the system being assessed, wherever appropriate and feasible, including during intermedia transfers. For pollutants where transformation is modeled, the mass of the core substance (*e.g.*, mercury for methylmercury as well as divalent mercury) within the modeling simulation will be preserved.

- **Ability to characterize parameter uncertainty and variability.** For critical parameters, the impacts of parameter uncertainty and variability on model outputs will be tracked and, where feasible, differentiated.
- **Capability for multiple pollutant, multiple media, multiple exposure pathway assessment.** The TRIM modeling system is being designed to facilitate assessment of

[2] Following the report of the Agency Task Force on Environmental Regulatory Modeling (U.S. EPA 1994a), the Agency conducted the Models 2000 Conference in December 1997. This conference has led to renewed emphasis on Agency-wide coordination of model development and the proposal for the implementation of a Council on Regulatory Environmental Modeling (CREM) to facilitate and promote scientifically-based, defensible regulatory computer models. The charter for CREM has been reviewed by SAB and is being updated for implementation by the Agency.

risks posed by aggregate exposures to single or multiple chemicals from multiple sources and via multiple exposure pathways.

(2) To ensure flexibility, the features of TRIM include the following.

- **Modular design.** Major components of TRIM will be independent and can be used individually, with outside information or models, or in combination. Only those model components necessary for evaluating the particular pollutants, pathways, and/or effect endpoints of interest need be employed in an assessment.

- **Flexibility in temporal and spatial scale.** Exposure and risk assessments will be possible for a wide range of temporal and spatial scales, including hourly to daily or yearly time steps, and from local (10 kilometers (km) or less) to greater spatial scales (depending on the module).

- **Ability to assess human and ecological endpoints.** Impacts to humans and/or biota can be assessed.

(3) To ensure that TRIM will be user-friendly for a variety of groups, including EPA, state and local agencies, and other stakeholders, TRIM will have the following characteristics.

- **Easily accessible.** The TRIM modeling system will be accessible for use with a personal computer (PC). The system may be available for download from the Internet and accessible through an Agency model system framework (*e.g.*, Models-3 (U.S. EPA 1999g)).

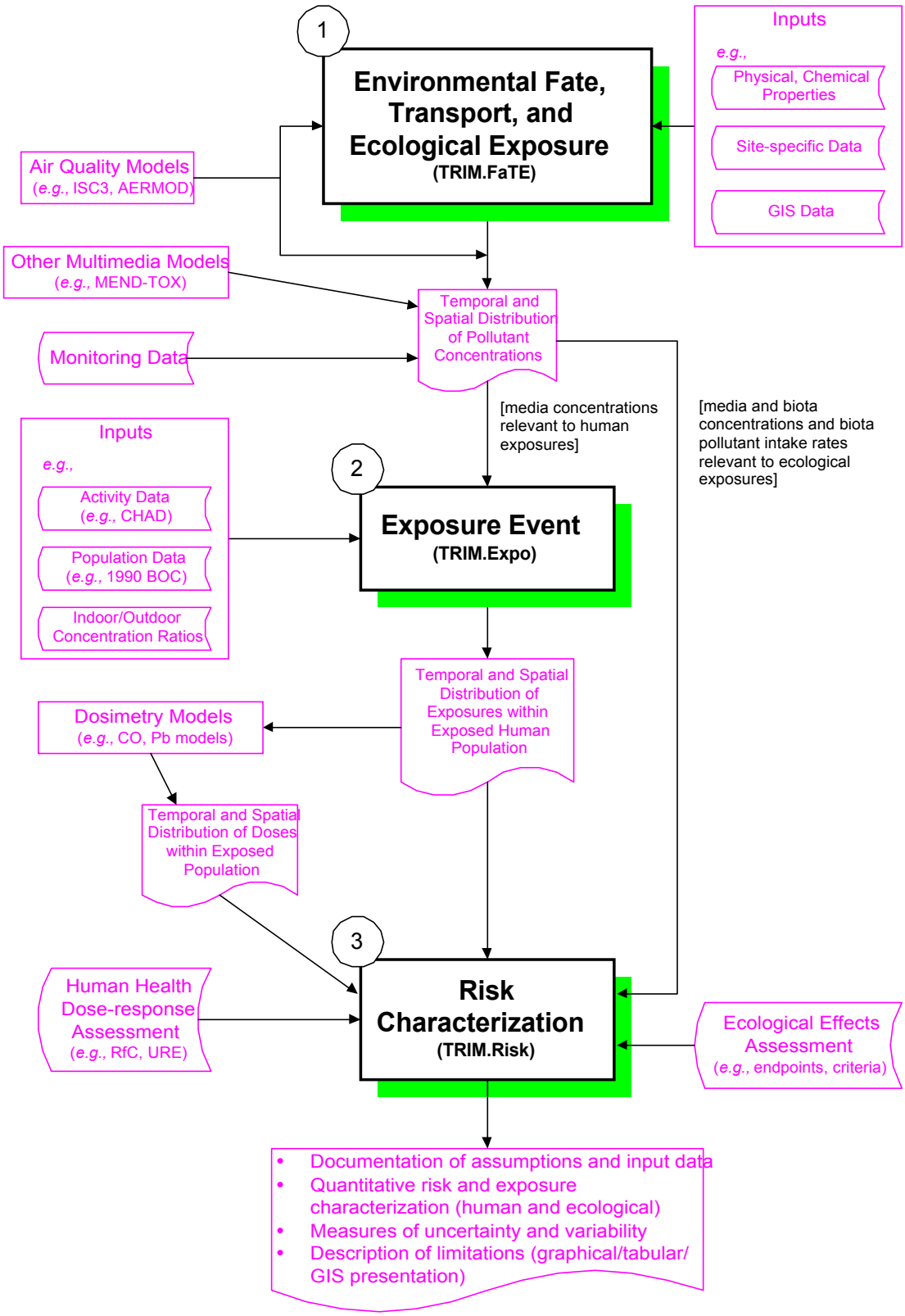
- **Well-documented.** Guidance materials for use of the TRIM modeling system will be provided through a user's guide, with a focus on the modular aspects of the modeling system, limitations of the modeling system, and appropriate uses, user responsibilities, and user options.

- **Clear and transparent.** The graphical user interface of the TRIM computer framework will provide transparency and clarity in the functioning of the TRIM modules, and output from the risk characterization module will document modeling assumptions, limitations, and uncertainties.

## 1.2 TRIM DESIGN

The current TRIM design (Figure 1-1) includes three individual modules. The Environmental Fate, Transport, and Ecological Exposure module, **TRIM.FaTE,** accounts for movement of a chemical through a comprehensive system of discrete compartments (*e.g.*, media, biota) that represent possible locations of the chemical in the physical and biological environments of the modeled ecosystem and provides an inventory, over time, of a chemical

**Figure 1-1**
**Conceptual Design of TRIM**



throughout the entire system. In addition to providing exposure estimates relevant to ecological risk assessment, TRIM.FaTE generates media concentrations relevant to human pollutant exposures that can be used as input to the Exposure-Event module, **TRIM.Expo.** In TRIM.Expo, human exposures are evaluated by tracking population groups referred to as "cohorts" and their inhalation and ingestion through time and space. In the Risk Characterization module, **TRIM.Risk**, estimates of human exposures or doses are characterized with regard to potential risk using the corresponding exposure- or dose-response relationships. The TRIM.Risk module is also being designed to characterize ecological risks from multimedia exposures. The output from TRIM.Risk will include documentation of the input data, assumptions in the analysis, and measures of uncertainty, as well as the results of risk calculations and exposure analysis.

An overarching feature of the TRIM design is the analysis of uncertainty and variability. A two-stage approach for providing this feature to the user has been developed. The first stage includes sensitivity analyses that are useful in identifying critical parameters, while more detailed uncertainty and variability analyses using Monte Carlo methods (*e.g.*, for refined assessment of the impact of the critical parameters) are available in the second stage. The uncertainty and variability feature augments the TRIM capability for performing iterative analyses. For example, the user may perform assessments varying from simple deterministic screening analyses using conservative default parameters to refined and complex risk assessments where the impacts of parameter uncertainty and variability are assessed for critical parameters.

Additionally, the modular design of TRIM allows for flexibility in both its development and application. Modules can be developed in a phased approach, with refinements being made as scientific information and tools become available. Furthermore, the user may select any one or more of these modules for an assessment depending on the user's needs. For example, when performing a human health risk assessment for an air pollutant for which multimedia distribution is not significant, TRIM.Expo may be applied using ambient concentration data or the output from an air quality model external to TRIM; the output from TRIM.Expo may then be used as input to TRIM.Risk to perform the desired risk analyses. In the case of a multimedia air pollutant, such as mercury, the user may choose to run all three TRIM modules to assess both human and ecological risks posed by multipathway exposures from multiple media.

Overview descriptions of the TRIM modules are provided in Sections 1.2.1 through 1.2.3, the status and plans for development are presented in Section 1.3, and plans for application appear in Section 1.4. A summary of the previous SAB comments and OAQPS responses is presented in Chapter 2. The approach for handling uncertainty and variability in TRIM is described in Chapter 3. Certain aspects of the TRIM.FaTE module are addressed in greater detail in Chapters 4 through 7, and additional details on TRIM.Expo and TRIM.Risk are provided in Chapters 8 and 9, respectively. Chapter 10 discusses the computer framework that is being implemented for the TRIM system. In addition, the TRIM.FaTE and TRIM.Expo TSDs provide more detailed explanations of those modules.

### 1.2.1 DESCRIPTION OF TRIM.FaTE

The first TRIM module to be developed, TRIM.FaTE, is a spatial compartmental mass balance model that describes the movement and transformation of pollutants over time, through a user-defined, bounded system that includes both biotic and abiotic components (compartments). The TRIM.FaTE module predicts pollutant concentrations in multiple environmental media and in biota and pollutant intakes for biota, all of which provide both temporal and spatial exposure estimates for ecological receptors (*i.e.*, plants and animals). The output concentrations from TRIM.FaTE also can be used as inputs to a human exposure model, such as TRIM.Expo, to estimate human exposures.

Significant features of TRIM.FaTE include: (1) the implementation of a truly coupled multimedia model; (2) the flexibility to define a variety of scenarios, in terms of the links among compartments as well as the number and types of compartments, as appropriate for the desired spatial and temporal scale of assessment; (3) the use of a transparent approach to chemical mass transfer and transformation based on an algorithm library that allows the user to change how environmental processes are modeled; (4) an accounting for all of the pollutant as it moves among the environmental compartments; (5) an embedded procedure to characterize uncertainty and variability; and (6) the capability to provide exposure estimates for ecological receptors. The TRIM.FaTE module is the most fully developed of the TRIM modules at this time, and this development has produced a library of algorithms that account for transfer of chemical mass throughout an environmental system, a database of the information needed to initialize these algorithms for a test site, and a working computer model.

### 1.2.2 DESCRIPTION OF TRIM.Expo

The TRIM.Expo module, similar to most human exposure assessment models, provides an analysis of the relationships between various chemical concentrations in the environment and exposure levels of humans. Because multiple sources of environmental contamination can lead to multiple contaminated media, including air, water, soil, food, and indoor air, it is useful to focus on the contaminated environmental media with which a human population will come into contact. These media typically include the envelope of air surrounding an individual, the water and food ingested by an individual, and the layer of soil and/or water that contacts the surface of an individual. The magnitude and relative contribution of each exposure pathway must be considered to assess total exposure to a particular chemical. Currently, the focus of TRIM.Expo development is on inhalation and ingestion exposure; however, dermal exposure will be added later.

**TRIM.Expo KEY TERMS**

**Cohort** - A group of people within a population with the same demographic variables who are assumed to have similar exposures.

**Activity pattern** - A series of discrete events of varying time intervals describing information about an individual's lifestyle and routine. The information contained in an activity pattern typically includes the locations that the individual visited (usually described in terms of microenvironments), the amount of time spent in those locations, and a description of what the individual was doing in each location (*e.g.*, sleeping, eating, exercising).

**Microenvironment** - A defined space in which human contact with an environmental pollutant takes place and which can be treated as a well-characterized, relatively homogeneous location with respect to pollutant concentrations for a specified time period.

**Exposure district** - A geographic location within a defined physical or political region where there is potential contact between an organism and a pollutant and for which environmental media concentrations have been estimated either through modeling or measurement.

The exposure analysis process consists of relating chemical concentrations in environmental media (*e.g.*, air, surface soil, root zone soil, surface water) to chemical concentrations in the exposure media with which a human or population has contact (*e.g.*, air, tap water, foods, household dusts, and soils). The initial prototype for TRIM.Expo will predict exposure by tracking the movement of a population cohort through locations where chemical exposure can occur according to a specific activity pattern. In a typical application, TRIM.FaTE could be used to provide an inventory of chemical concentrations across the ecosystem at selected time intervals (*e.g.*, days, hours). For chemicals that are not persistent and/or bioaccumulative, processed air monitoring data or air dispersion modeling results can be substituted for TRIM.FaTE output data. The TRIM.Expo module would then use these chemical concentration data, combined with the activity patterns of the cohorts, to estimate exposures. The movements are defined as an exposure-event sequence that can be related to time periods for which exposure media concentrations are available (*e.g.*, from TRIM.FaTE, ambient data, and/or dispersion modeling results). Each exposure event places the population cohort in contact with one or more environmental media within a specified microenvironment (*e.g.*, inside a home, along a road, inside a vehicle) in an exposure district for a specified time interval. In addition to the location assignments, the exposure event would provide information relating to the potential for pollutant uptake, such as respiration rate and quantity of water consumed. The TRIM.Expo module is intended to contribute to a number of health-related assessments, including risk assessments and status and trends analyses.

### 1.2.3 DESCRIPTION OF TRIM.Risk

Risk characterization is the final step in risk assessment and is primarily used to integrate the information from the other three key steps (*i.e.*, hazard identification, dose-response assessment, exposure assessment). Within the TRIM framework, TRIM.Risk, the risk characterization module, will be used to integrate the information on exposure (human or ecological receptor) with that on dose-response or hazard and for providing quantitative descriptions of risk and some of the attendant uncertainties. The TRIM.Risk module will provide decision-makers and the public with information for use in developing, evaluating, and selecting

appropriate air quality standards and risk management strategies. The purpose of TRIM.Risk is to integrate information from other TRIM modules and to facilitate the preparation of a risk characterization. The TRIM.Risk module will, therefore, be able to summarize or highlight the major points from each of the analyses conducted in the other TRIM modules. Where possible, the TRIM.Risk module will do so in an automated manner. In general, TRIM.Risk will (1) document assumptions and input data, (2) conduct risk calculations and data analysis, and (3) present results and supporting information.

Current and proposed EPA guidance on risk characterization will guide the development of TRIM.Risk. The TRIM.Risk module will be developed in a phased approach similar to other TRIM modules. Ideally, TRIM.Risk will provide all of the information required to prepare a full risk characterization. However, the type and variability of information needed for this purpose are vast. Therefore, the type of information generated by TRIM.Risk will evolve over time as the Agency gains experience and has the resources to implement more flexibility. For example, early versions of TRIM.Risk will be limited to preparing summaries of input data and results, without supporting text. However, as the Agency gains experience, it may be possible to incorporate generic language to more fully describe the information required for a full risk characterization. Many EPA risk assessments will be expected to address or provide descriptions of (1) individual risk,[3] including the central tendency and high-end portions of the risk distribution, (2) population risk, and (3) risk to important subgroups of the population such as highly exposed or highly susceptible groups or individuals, if known. Some form of these three types of descriptors will be developed within TRIM.Risk and presented to support risk characterization. Because people process information differently, it is appropriate to provide more than one format for presenting the same information. Therefore, TRIM.Risk will be designed so that the output can be presented in various ways in an automated manner (*e.g.*, Chart Wizard in Microsoft® Excel), allowing the user to select a preferred format.

## 1.3 TRIM DEVELOPMENT

In the development of TRIM, existing models and tools are being relied upon where possible. Adopting or incorporating existing models or model components into a tool that meets OAQPS' needs is preferable as it is usually the most cost-effective approach. Consequently, review of existing models and consideration of other current modeling efforts is an important part of TRIM development activities. Reviews of relevant models existing at the initiation of development activities for each module are described in the TRIM.FaTE and TRIM.Expo TSDs. Additionally, OAQPS is closely following several current activities as they relate to TRIM.

[3] The phrase individual risk as used here does not refer to a risk estimate developed specifically for a single member of a population. Rather, it refers to the estimate of risk for a subgroup of a population that is presented as an estimate of the risk faced by a person rather than by the population as a whole.

Current Agency model development activities relevant to TRIM development include the recently published updated guidance on assessing health risks associated with indirect exposure to combustor emissions (U.S. EPA 1999d). This guidance, previously referred to as the Indirect Exposure Methodology (IEM), is now called the Multiple Pathways of Exposure (MPE) method. In addition, the multimedia model, FRAMES-HWIR, has recently been developed by the Agency to support a specific risk assessment need regarding hazardous chemicals released from land-based waste management units. The FRAMES-HWIR model has been developed as part of a focused fast-track (two-year) effort to support a risk-based regulation regarding disposal of hazardous waste (HWIR99).[4] Another model of interest for multimedia pollutants is the Stochastic Human Exposure and Dose Simulation (SHEDS) model (*e.g.*, Özkaynak et al. 1999). The OAQPS will be carefully considering the various aspects of MPE, FRAMES-HWIR, and SHEDS with regard to OAQPS needs, as well as compatibility with or future improvements or evaluations of TRIM. As TRIM is intended to be a dynamic method, developmental activities will consider and respond as appropriate to newly available methods and scientific information.

A current major Agency research project involves the design and development of a flexible software system to simplify the development and use of air quality models and other environmental decision support tools. This system, called Models-3, is designed for applications ranging from regulatory and policy analysis to understanding the complex interactions of atmospheric chemistry and physics (U.S. EPA 1999g). The June 1999 release of Models-3 contains a Community Multi-Scale Air Quality (CMAQ) modeling system for urban- to regional-scale air quality simulation of tropospheric ozone, acid deposition, visibility, and fine particles. The long-term goal is to extend the system to handle integrated cross-media assessments and serve as a platform for community development of complex environmental models. In recognition of the availability of Models-3 over the longer term, OAQPS has designed and is developing the TRIM computer framework to be compatible with the Models-3 system.

### 1.3.1 INITIAL DEVELOPMENT ACTIVITIES

The first phase of TRIM development included the conceptualization of TRIM and the implementation of the TRIM conceptual approach through the development of a prototype of the first TRIM module, TRIM.FaTE (U.S. EPA 1998e). The progress on TRIM.FaTE included the development of (1) a conceptual design for the module; (2) a library of algorithms that account for chemical mass transfer throughout the ecosystem; (3) a database to initialize the algorithms for a test site; and (4) a working prototype in spreadsheet format.

Consistent with Agency peer review policy (U.S. EPA 1998b) and the 1994 Agency Task Force on Environmental Regulatory Modeling (U.S. EPA 1994a), internal and external peer review are an integral part of the TRIM development plan. Following the first phase of TRIM development, OAQPS submitted TRIM to SAB under their advisory method of review (U.S. EPA 1998a). In May 1998 in Washington, DC, the Environmental Models Subcommittee (Subcommittee) of the Executive Committee of SAB reviewed the TRIM project. The SAB

[4] The FRAMES-HWIR documentation is scheduled for public release in fall 1999.

Subcommittee was charged with assessing the overall conceptual approach of TRIM and the specific approach of TRIM.FaTE.

The SAB Subcommittee reported that the development of TRIM and the TRIM.FaTE module was conceptually sound and scientifically based (U.S. EPA 1998a). The SAB Subcommittee provided specific recommendations related to six specific charge questions. The SAB recommendations are detailed in Chapter 2 along with brief responses, and changes to TRIM.FaTE based in part on the SAB recommendations are highlighted in Chapter 4 of this report.

### 1.3.2 RECENT ACTIVITIES

During the most recent developmental phase of TRIM, progress has been made in many areas, including a change to the overall modular design of TRIM. As shown in Figure 1-1, the TRIM design now includes three modules: TRIM.FaTE, TRIM.Expo, and TRIM.Risk. The design presented to SAB in May 1998 included three other modules (Pollutant Uptake, Biokinetics, and Dose/Response). In recognition of the flexibility of the TRIM design, which provides an ability to rely on a variety of input data and outside models, OAQPS decided not to include the development of these modules in the TRIM design at this time.

In consideration of SAB comments, TRIM.FaTE was refined, including the development of new and updated capabilities, as well as the development and limited testing of methodologies for model set-up, uncertainty and variability analysis, and evaluation. In addition, OAQPS developed a conceptual plan for TRIM.Expo, initiated work on a prototype of TRIM.Expo (initially focusing on inhalation), and developed a conceptual design for TRIM.Risk. Furthermore, the overall computer framework for TRIM was designed and implemented in a PC-based platform, and substantial progress was made in installing TRIM.FaTE into this framework. Changes and additions to TRIM.FaTE are discussed in more detail in Chapter 4. The development of TRIM.Expo is discussed in Chapter 8, and the conceptual plan for TRIM.Risk is described in Chapter 9. In addition, the TRIM.FaTE and TRIM.Expo TSDs provide more detailed explanations of these modules.

The current TRIM documentation has gone through internal Agency peer review, which involved reviewers across the Agency, including the major program offices, the Office or Research and Development, and staff involved in the Agency's Models 2000 efforts. The current SAB advisory will be the second on TRIM development activities.

### 1.3.3 FUTURE ACTIVITIES

Following the 1999 SAB advisory, improvements will be made to the uncertainty and variability approach, TRIM.Expo prototype, and TRIM.Risk conceptual plan. These revisions are scheduled to be completed in 2000. As needed, refinements will be made to the TRIM.FaTE evaluation plan, and completion of the bulk of those activities are also scheduled for 2000. The Agency has planned for a substantial amount of progress on each of the TRIM modules for 2000 and 2001, as described below.

- **TRIM.FaTE.** Future work on TRIM.FaTE will include model evaluation activities and additional development of the module to accommodate additional chemicals. The TRIM.FaTE module is expected to be available for limited external use late in 2000 and to be publicly released in 2001.

- **TRIM.Expo.** Future work on TRIM.Expo in 2000 will include the further development of ingestion algorithms, incorporation of EPA's Air Pollutant Exposure Model (APEX) coding into the TRIM platform followed by adjustments to APEX to include ingestion algorithms, a test case of the inhalation pathway, and a test case of inhalation and ingestion pathways. Over the longer term, addition of the dermal pathway to the module will be initiated.

- **TRIM.Risk.** Development of TRIM.Risk will begin after SAB comments are received on the conceptual design. Module development will include identification of data needs and formatting of data outputs. Programming for a TRIM.Risk prototype is expected to be completed in 2000.

- **TRIM computer framework.** Further development of the TRIM computer framework, including incorporation of the TRIM.Expo (inhalation) module, will take place during 2000. Features to be refined during this time frame include limited geographic information system (GIS) or mapping capabilities. Additionally, long-range comprehensive GIS planning will occur. Development of user guidance materials is planned for 2000 (see text box).

  In addition to consulting with Agency scientists during future TRIM development (*i.e.*,

**USER GUIDANCE**

Development of the TRIM user's guide is scheduled to begin in 2000, along with a plan for training activities. The OAQPS recognizes the importance of developing detailed user guidance that will assist users in defining, for a particular modeling application, the spatial and temporal resolution, compartments and linkages, and parameters and initial conditions. For example, the TRIM.FaTE guidance will likely emphasize the value of performing several different preliminary simulations in verifying the adequacy of the parcel and compartment specifications for the desired application. Similarly, detailed users guidance will be developed for TRIM.Expo to assist users in defining cohorts, study areas, exposure districts, and microenvironments, as well as various parameters and exposure factors.

It also will be important for the guidance to note the responsibility of the user in defining the simulation as appropriate to the application. For example, in TRIM.FaTE, default values will likely be made available with the model for a variety of parameters ranging from physiological characteristics of various biota to physical characteristics of abiotic media; the user will need to consider appropriateness of these values or others (*e.g.*, site-specific data) for their application. While the TRIM modules are intended to provide valuable tools for risk assessment, and their documentation and guidance will identify, as feasible, uncertainties and limitations associated with their application, the guidance will emphasize that their appropriate use and the characterization of uncertainties and limitations surrounding the results are the responsibility of the user.

peer involvement), in late 2000 or early 2001, OAQPS will seek both internal and external peer review of new aspects following the next phase of TRIM development. In addition to the SAB, which provides the Agency with reviews, advisories, and consultations, other external peer review mechanisms consistent with Agency policy (U.S. EPA 1998b) include the use of a group of independent experts from outside the Agency (*e.g.*, a letter review by outside scientists), an *ad hoc* panel of independent experts, and peer review workshops. The OAQPS intends to seek the peer review mechanism appropriate to the importance, nature, and complexity of the material for review.

## 1.4 PHASING TRIM INTO OAQPS' SET OF MODELING TOOLS

As mentioned earlier, TRIM is intended to support assessment activities for both the criteria and hazardous air pollutant programs of OAQPS. As a result of the greater level of effort expended by the Agency on assessment activities for criteria air pollutants, these activities are generally more widely known. To improve the public understanding of the hazardous air pollutant (or air toxics) program, the Agency published an overview of the air toxics program in July 1999 (U.S. EPA 1999e). Air toxics assessment activities (National Air Toxics Assessment, or NATA) are described as one of the program's key components.[5] The NATA includes both national- and local-scale activities. The TRIM system is intended to provide tools in support of local-scale assessment activities, including multimedia analyses.

One of the Agency's most immediate needs for TRIM comes in the Residual Risk Program, in which there are statutory deadlines within the next two to nine years for risk-based emissions standards decisions. As described in the *Residual Risk Report to Congress* (U.S. EPA 1999f), TRIM is intended to improve upon the Agency's ability to perform multipathway human health risk assessments and ecological risk assessments for HAPs with the potential for multimedia environmental distribution. Another important upcoming use for TRIM is

**EXAMPLES OF TRIM APPLICATIONS**

- A human health or ecological assessment of multimedia, multipathway risks associated with mercury emissions from one or several local sources could be performed using all three modules in the TRIM system.
- An assessment of human health risks associated with air emissions of a criteria air pollutant (*e.g.*, ozone) or one or several volatile HAPs in a metropolitan area could be developed using an external air model or ambient concentration data from fixed-site monitors coupled with TRIM.Expo and TRIM.Risk.

[5] Within the air toxics program, these activities are intended to help EPA identify areas of concern (*e.g.*, pollutants, locations, or sources), characterize risks, and track progress toward meeting the Agency's overall air toxics program goals, as well as the risk-based goals of the various activities and initiatives within the program, such as residual risk assessments and the Integrated Urban Air Toxics Strategy. More specifically, NATA activities include expansion of air toxics monitoring, improvements and periodic updates to emissions inventories, national- and local-scale air quality modeling, multimedia and exposure modeling (including modeling that considers stationary and mobile sources), continued research on health effects of and exposures to both ambient and indoor air, and use and improvement of exposure and assessment tools. These activities are intended to provide the Agency with improved characterizations of air toxics risk and of risk reductions resulting from emissions control standards and initiatives for both stationary and mobile source programs.

in exposure assessment in support of the review of the ozone NAAQS. The TRIM.Expo and TRIM.Risk modules augmented with external air quality monitoring data and models are intended to support this type of criteria pollutant assessment as well as risk assessments for non-multimedia HAPs.

Consistent with the phased plan of TRIM development, the application of TRIM will also be initiated in a phased approach. With the further development of the TRIM modules in 2000 and 2001, EPA will begin to use the modules to contribute to or support CAA exposure and risk assessments. These initial applications also will contribute to model evaluation. The earliest TRIM activities are expected to include the use of TRIM.FaTE side-by-side (at a comparable level of detail) with the existing multimedia methodology[6] in risk assessments of certain multimedia HAPs (*e.g.*, mercury) under the Residual Risk Program. As TRIM.Expo is developed to accommodate inhalation modeling of HAPs and after it has undergone testing, OAQPS plans to initially run it side-by-side (at a comparable level of detail) with EPA's existing inhalation exposure model, HEM (Human Exposure Model (U.S. EPA 1986b)). When TRIM.Risk has been completed, it will be used, as appropriate, in both criteria and hazardous air pollutant risk assessments.

In later years, OAQPS intends to use TRIM and the TRIM modules in a variety of activities including (1) residual risk assessments using TRIM.FaTE, TRIM.Expo, and TRIM.Risk, in combinations appropriate to the environmental distribution characteristics of the HAPs being assessed; (2) urban scale assessments on case study cities as part of the Integrated Urban Air Toxics Strategy; and (3) exposure and risk assessments of criteria air pollutants (*e.g.*, ozone, carbon monoxide) in support of NAAQS reviews.

[6] In support of the *Mercury Report to Congress* (U.S. EPA 1997a) and the *Study of Hazardous Air Pollutant Emissions from Electric Utility Steam Generating Units -- Final Report to Congress* (U.S. EPA 1998d), the Agency relied upon the Indirect Exposure Methodology, which has recently been updated and is now termed the Multiple Pathways of Exposure methodology (U.S. EPA 1999d). This methodology is being used in initial assessment activities for the Residual Risk Program (U.S. EPA 1999f).

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# 2. MAY 1998 SCIENCE ADVISORY BOARD REVIEW AND AGENCY RESPONSES

On May 5 and 6, 1998, the Environmental Models Subcommittee (Subcommittee) of the Executive Committee of EPA's Science Advisory Board (SAB) held a meeting in Washington, DC to perform an early review of TRIM. At the time of the SAB review, only the conceptual approach for TRIM and a prototype of TRIM.FaTE had been developed. The Agency requested an early review of TRIM and the TRIM.FaTE prototype to ensure that the development of TRIM was conceptually sound and scientifically defensible as well as consistent with Agency objectives. Additional reviews of TRIM and its modules will be conducted by SAB over the next few years.

During the May 1998 SAB review, there were six charge questions related to TRIM and TRIM.FaTE.

1. Is the overall conceptual TRIM approach appropriate, given the underlying science, EPA policy, and regulatory needs (*i.e.*, what are the strengths and weaknesses)?

2. The TRIM approach is designed for the explicit treatment of uncertainty and variability, including both model uncertainty and parameter uncertainty. Is the spatial compartmental mass balance approach commensurate with quantifying uncertainty and variability in a scientifically defensible manner?

3. The TRIM.FaTE module is the environmental fate, transport, and exposure component of TRIM. Is the overall conceptual approach represented in the TRIM.FaTE module appropriate, given the underlying science, EPA policy, and regulatory needs (*i.e.*, what are the strengths and weaknesses of the approach)?

4. The TRIM approach is designed to be flexible and to allow for a tiered approach, to function as a hierarchy of models, from simple to complex, as needed.

   (a) As implemented at this time, is the TRIM.FaTE module, with its three-dimensional, spatial compartmental mass conserving approach to predicting the movement of pollutant mass over time, appropriate from a scientific perspective?

   (b) Is the TRIM.FaTE module, as designed, an appropriate tool, when run either at a screening level or for a more refined analysis, for use in providing information for regulatory decision-making? Given the module design (*i.e.*, the potentially large number of model parameters and associated uncertainty and variability), is TRIM.FaTE suitable to support regulatory decisions?

5. Does the TRIM.FaTE module, as it has been conceptualized, address some of the limitations associated with other models (*e.g.*, non-conservation of mass, steady-state approach, inability to quantify uncertainty and variability, limited range of receptors and

processes considered)? Are there other limitations that the TRIM.FaTE module should address?

6. Does the TRIM.FaTE module, as it has been conceptualized and demonstrated to date, facilitate future integration with appropriate data sources (*e.g.*, GIS) and applications (*e.g.*, multipathway exposure assessment for humans)?

The SAB responded to each of these questions and provided EPA with recommendations for improvements in the next versions of TRIM modules and TRIM.FaTE in particular (U.S. EPA 1998a). The SAB comments and Agency responses under each of the six charge questions are summarized below.

Overall, SAB found the development of TRIM and the TRIM.FaTE module to be conceptually sound and scientifically based. The SAB recommended that the TRIM team seek input from users before and after the methodology is developed to maximize its utility; understand the potential uses of TRIM to guard against inappropriate uses; provide documentation of recommended and inappropriate applications; provide training for users; test the model and its subcomponents against current data and models to evaluate its ability to provide realistic results; and apply terminology consistently.

## 2.1 IS THE OVERALL TRIM CONCEPTUAL APPROACH APPROPRIATE?

**COMMENT:** The SAB found the conceptual approach for TRIM to be technically defensible and appropriate for use in regulatory decision-making, but noted that because the system is evolving, it is unclear how the overall methodology will address the spectrum of regulatory questions. The SAB cited the flexibility of TRIM to be a strength, but also recommended that care be exercised to guard against developing unnecessarily complex or inconsistent modeling applications.

**RESPONSE:** The OAQPS agrees with the need to maintain the focus of TRIM uses on practical applications, recognizing that it is not intended to be a research model. The Office intends to provide clear documentation for those applications for which TRIM is an appropriate tool. Preparation of users guidance materials is planned for the next phase of TRIM development.

**COMMENT:** The SAB noted that the largest challenge facing TRIM is the lack of available data for estimating fate, transport, exposure, and risk processes, possibly limiting the ability of TRIM to model many chemicals and hindering model validation efforts. Therefore, SAB recommended identifying and acquiring significant additional field data (*e.g.*, air monitoring data, soil samples) to estimate modeling parameters and to "validate" the model components and other aspects of the modeling system.

**RESPONSE:** The OAQPS developed a strategy for model evaluation for TRIM, and the TRIM.FaTE module specifically, and identified existing data sets for potential use in implementing the approach, as discussed further in Section 4.8 and Chapters 6 and 7. This effort

should facilitate the comparison of model results with "real world" environmental concentration data. Such a comparison is a key element of the TRIM.FaTE mercury case study described in Chapter 7. In addition, OAQPS recognizes the need for evaluation of specific model components and other aspects of the modeling system. Therefore, adjustments to the TRIM.FaTE module were made to increase the transparency of the module and to more readily allow for the testing of individual components within the module.

## 2.2 IS THE SPATIAL COMPARTMENTAL MASS BALANCE APPROACH COMMENSURATE WITH QUANTIFYING UNCERTAINTY AND VARIABILITY IN A SCIENTIFICALLY DEFENSIBLE MANNER?

**COMMENT:** In its review, SAB noted that, at that stage, it was not possible to indicate whether the spatial compartmentalization would be a significant source of uncertainty in generating predictions using TRIM, and added that this issue should be kept in perspective relative to other potential error sources. The SAB recommended that OAQPS conduct a thorough review of the available literature on sensitivity and uncertainty analysis prior to making choices on the specific approaches for incorporating sensitivity and uncertainty analysis into TRIM. Furthermore, SAB recommended that TRIM developers clarify how the analysis of uncertainty and sensitivity will be incorporated into TRIM and how it will be presented as part of the overall assessment. The SAB also stated that the role and limitations of sensitivity and uncertainty analysis be clearly recognized and acknowledged by TRIM developers and users.

**RESPONSE:** As part of the TRIM.FaTE evaluation plan (see Chapter 6), OAQPS is conducting structural evaluations on the effect of spatial configuration on model results. For example, the impact of compartment size, shape, and location on model outputs will be analyzed. These results will be considered along with those of other analyses as part of the TRIM.FaTE evaluation process.

The OAQPS has continued to review the available literature on sensitivity and uncertainty analysis for model parameters (see Appendix B), developed a general approach for uncertainty and variability analysis in TRIM (see Chapter 3), and developed a specific approach for incorporating sensitivity and uncertainty analysis capabilities into the TRIM.FaTE module – recognizing the roles and limitations of sensitivity and uncertainty analysis – as discussed further in Section 4.7 and in Chapter 6 of TRIM.FaTE TSD Volume I. The proposed approach reflects a balance between the additional effort needed in developing the module and the added value to the module. This approach includes adding the capability to present the results of uncertainty and variability analysis as part of an assessment using TRIM.FaTE. Plans for an uncertainty and variability analysis for a simplified environmental scenario are described in Chapter 6 of the TRIM.FaTE TSD Volume I and Chapter 7 of this report.

In the TRIM modeling system, the uncertainty and variability outputs from one module (*e.g.*, TRIM.FaTE) will be carried through to the other modules (*e.g.*, TRIM.Expo, TRIM.Risk). This feature will insure that TRIM outputs include measures of uncertainty and variability, which are important to the characterization of risks for the Agency's decision-making process.

**COMMENT:** The SAB noted that validation of TRIM is a difficult issue because TRIM will never be capable of (in)validation in the classical sense. Rather, the notion of model "validation" should be seen as a matter of designing a tool appropriate for the given (predictive) task. Accordingly, SAB recommended that history matching and qualitative peer review should not be set aside and that the Agency should watch for new methods for quantitatively assuring the quality of models as tools for fulfilling specified predictive tasks.

**RESPONSE:** A model evaluation plan has been developed for TRIM that will use a wide range of model evaluation tools to assess the quality, reliability, and relevance of TRIM and TRIM.FaTE (see Section 4.8 and Chapter 6). This plan includes some reliance on history matching and qualitative peer review. As new methodologies are developed and reviewed within the scientific community, OAQPS will be assessing their acceptance and usefulness for assuring the quality of TRIM and TRIM.FaTE.

## 2.3 IS THE OVERALL CONCEPTUAL APPROACH REPRESENTED IN THE TRIM.FaTE MODULE APPROPRIATE?

**COMMENT:** The SAB found that the TRIM.FaTE module is conceptually sound and aims at an appropriate level of complexity. The Subcommittee noted several strengths of the TRIM.FaTE module, including (1) meeting the requirements of scientific and technical defensibility, (2) flexibility, (3) ability to address exposures relevant to human health and ecological risk assessments, and (4) user friendliness. Limitations that were noted include (1) the use of confusing and contradictory terminology, (2) difficulty in understanding the difference between applications of the module in a screening capacity versus a more in-depth analysis mode, (3) the predisposition toward first-order, linear algorithms representing the fate and transport of chemicals, (4) the emphasis on the steady-state distribution of contaminants, and (5) the constraints and computational overhead associated with the spreadsheet software relied on for Prototype IV of TRIM.FaTE. The SAB also recommended providing examples of applications of the module and developing a user's guide that describes the proper use, strengths, and limitations of the TRIM.FaTE module.

**RESPONSE:** Recognizing the inconsistent and sometimes conflicting terminology used to describe the TRIM.FaTE prototype presented to SAB, OAQPS revised the terminology to be more consistent with other multimedia models. These revisions should help decrease confusion for both experienced and novice fate and exposure modelers. The new set of terms, which is used consistently throughout this report and the TRIM.FaTE TSD, is included in the glossary of each document.

One of the design objectives for the TRIM modeling system has been the ability to use it in performing iterative analyses. That is, the user is able to select the necessary level of analysis, ranging from a simple analysis, for which less site-specific data are required and which will run more quickly, to one needed for a more detailed risk assessment. For example, the more simple analysis, providing a more imprecise, general idea of pollutant distribution, may be sufficient for priority setting or other similar scoping activities (*e.g.*, in a screening analysis for which conservative default input parameters could be used). This allows the Agency to focus a more detailed analysis, where the impacts of parameter uncertainty may be assessed qualitatively for

critical parameters, on situations where a more refined assessment is needed (*e.g.*, human health risk assessments to support environmental regulation).

Although it may appear that there is a predisposition toward using first-order, linear algorithms in TRIM.FaTE because of the use of LSODE (the Livermore Solver for Ordinary Differential Equations, a calculation tools used within TRIM.FaTE), the model is capable of using more complex, non-linear chemical mass transfer algorithms. The application of these higher order algorithms is limited, however, due to a lack of understanding in the scientific community regarding these chemical processes. Furthermore, the use of complex algorithms is sometimes limited because of the need to balance accuracy of outputs with the time needed to run the model.

It is probable that SAB's observation that TRIM.FaTE focuses on steady-state distributions of chemicals is due to the sample results that were presented at the May 1998 SAB meeting, which were virtually all steady-state results. However, the original and current intent of TRIM.FaTE is to develop a model that produces dynamic results. In the past year, the majority of work on TRIM.FaTE focused on presenting dynamic results.

The Agency's development of a computer framework for TRIM is described in Chapter 10. Consistent with the SAB recommendation, Version 1.0 of the framework has been developed primarily, but not entirely, in the Java programming language. Some parts are implemented in Fortran and others in C. The C programming language and Fortran are used in situations where existing code in those languages provides required functionality and where high computational efficiency is needed, such as solving systems of equations. Java provides portability across different hardware and operating systems and offers a good combination of speed of development, robustness, and support for object-oriented designs.

The model evaluation activities described in Chapter 6 and the experience gained through the mercury case study described in Chapter 7 will assist in describing appropriate uses of TRIM.FaTE and in identifying model limitations. The findings from these and other tests will be used to develop guidance for users of TRIM.FaTE, including guidance on the interpretation of results using linear algorithms. In addition, OAQPS is developing plans for providing training on the uses of TRIM and the individual modules.

## 2.4 THE TRIM APPROACH IS DESIGNED TO BE FLEXIBLE AND TO ALLOW FOR A TIERED APPROACH

### 2.4.1 IS THE TRIM.FaTE MODULE APPROPRIATE FROM A SCIENTIFIC PERSPECTIVE?

**COMMENT:** The SAB noted in its review of the prototype of TRIM.FaTE that it had not been checked against a detailed set of observed, spatially varying "real world" environmental concentration data. In addition, SAB stated that because of its highly aggregate representation of environmental compartments, it is unlikely that TRIM.FaTE can be effectively used to address fully variable three-dimensional spatial analyses and cited several other models that may offer greater value for certain applications.

**RESPONSE:** As discussed in Section 2.1, OAQPS developed a model evaluation plan and is conducting a case study using mercury which will include evaluating model results in comparison to monitoring data from a specific site. The TRIM system with its assumption of uniform distribution within a compartment may not effectively address fully variable three-dimensional spatial analyses *within a single compartment*. However, with TRIM's features promoting flexibility, it may be able to represent spatial variability *within a single medium* through the use of multiple compartments. The degree to which the spatial variability within a medium can be captured is dependent on the number of compartments into which that medium can be divided and the number of compartments that can be modeled. Recognizing the importance of this issue, one part of the TRIM.FaTE evaluation effort is to assess, through tests of varying spatial aggregation, the simulation of three-dimensional aspects.

It also should be noted that the Agency does not intend to rely solely on TRIM.FaTE in evaluating the multimedia impacts of air pollutants in support of regulatory and policy decisions. For those pollutants believed to have multimedia impacts, TRIM.FaTE analyses, including analyses of uncertainty and variability, along with other relevant information (including any limitations of the analyses), are intended to be used to inform those decisions. For pollutants for which a particular medium is dominant and for which transport and concentration gradients within that medium dominate the fate and exposure outcome, applicable single media, process-based models may be used to support decision-making.

**COMMENT:** The SAB noted that TRIM.FaTE lacked the ability to handle processes such as diffusive/dispersive transfer perpendicular to the longitudinal direction. Specifically, they cited the omission of dispersion phenomena throughout the module as an important issue that may limit the applicability and credibility of TRIM.FaTE.

**RESPONSE:** The EPA recognizes the need to incorporate such processes into the fate and transport module of TRIM and has conducted additional investigation into how this might be defensibly addressed within the current model architecture. At this time, these investigations have resulted in the inclusion of additional dispersion algorithms in surface water, as well as implementation of methods for including the results of external air models that do consider dispersion processes in TRIM.FaTE. However, due to the coupled relationship between

compartments in TRIM.FaTE and the state of the science in characterizing air dispersion within grid models, dispersion and diffusion algorithms for air transport have not been included.

The structure of the currently implemented air model in TRIM.FaTE is that of a grid model, although it deviates from the traditional grid model used in air simulations for photochemical assessments in that the air compartment volume elements can be unequal in size and extent. Grid models have limitations with respect to characterizing dispersion. The homogeneous assumption used in grid models results in artificial (numerical) dispersion that tends to simulate the dilution of the material in the grid cell. For the typical grid cell on the order of several kilometers in size, it is this "artificial" dilution that is of much larger magnitude than the expected dispersion term. Thus, inclusion of an additional dispersion term may tend to over-dilute the plume. Further, the largest surface impacts can result from nonhomogeneous conditions (*e.g.*, asymmetric vertical mixing in convective conditions).

Due to these limitations, special dispersion characterizations are necessary with grid models, involving parameterizations for subgrid processes such as diffusion. Research indicates that there are few horizontal and vertical dispersion characterizations for grid models currently available. Further, it has been reported that numerical diffusion can dominate the physical diffusion predicted by these characterizations, especially in stable conditions (Nguyen et al. 1997). A method of addressing asymmetric vertical mixing during convective conditions has been explored by Pleim and Chang (1992). This approach will be investigated for inclusion in the TRIM.FaTE algorithm library.

An alternative to incorporating a more sophisticated air model into TRIM.FaTE is to import the results of such a model. The details for how this alternative can be accomplished are described in Appendix B of TRIM.FaTE TSD Volume I. As discussed in Appendix B, this approach has other limitations; notably, either the linkage between the external model and TRIM.FaTE is in one direction only and, hence, conservation of chemical mass is lost, or the external model must be linked with TRIM.FaTE in such a way that chemical transfer can occur in both directions. The difficulty of the latter will depend on the particular external model considered, but it is likely that it would generally require a substantial effort to implement. This is because the user must not only perform the practical tasks associated with computer programming, but also must ensure that no fundamental assumptions or concepts inherent to either model are violated. This could occur, for example, if there is overlap between the models in how they address other processes that are not an explicit component of the model linkage itself (*e.g.*, the external model may be treating deposition using general inputs for vegetative cover, and the user must implement additional checks to ensure that these inputs are consistent with the vegetative compartments used within TRIM.FaTE).

For cases where the lack of air dispersion modeling cannot be accepted, it is suggested that an external air model be used, the results of which would then be used as one of the inputs for TRIM.FaTE. The details of how this can be implemented have been developed (see Section 4.5, and Appendix B of the TRIM.FaTE TSD Volume I) and demonstrated using a common regulatory air model (Industrial Source Complex, Short Term Version 3, or ISCST3) (U.S. EPA

1995c). This approach is not limited to using air models alone, as the same method will work for any compartment type.

**COMMENT:** The SAB recommended that TRIM.FaTE be constructed to permit disaggregation of the component results and that the module be further studied to build confidence in the overall predictive ability of the model.

**RESPONSE:** As noted in Section 2.1, OAQPS recognizes the importance of the evaluation process for specific TRIM.FaTE components and other aspects of the modeling system and, therefore, made adjustments to TRIM.FaTE to allow for easier testing of individual components of the module.

**COMMENT:** The SAB suggested that tracking and accounting within the TRIM.FaTE module is needed to isolate its predictions and to permit benchmark comparison with data sets and other models. The Subcommittee noted that this would permit scrutiny of TRIM.FaTE transformation algorithms and the parameters that are used within this component of the TRIM model.

**RESPONSE:** The accessibility of the algorithm library for TRIM.FaTE permits scrutiny of the transformation and transfer algorithms selected for each modeling simulation. The initial process models and default parameters within TRIM.FaTE have been selected upon consideration of those available in existing models and the current modeling literature. The evaluation strategy proposed for TRIM.FaTE includes mechanistic evaluations to assess the individual process models. For example, OAQPS is performing a comparison of the TRIM.FaTE air transport component to a widely used EPA air dispersion model, ISCST3.

### 2.4.2 IS THE TRIM.FaTE MODULE AN APPROPRIATE TOOL FOR USE IN PROVIDING INFORMATION FOR REGULATORY DECISION-MAKING?

**COMMENT:** The SAB was unable to assess the appropriateness of the module as a decision-making tool because additional testing and evaluation are necessary.

**RESPONSE:** The OAQPS is conducting additional testing and evaluation of the TRIM.FaTE module, including testing against environmental concentration data and comparisons of outputs to other model results (see Chapters 6 and 7), and believes that TRIM.FaTE will be a useful tool that can provide information in support of regulatory decision-making.

## 2.5 DOES THE TRIM.FaTE MODULE, AS IT HAS BEEN CONCEPTUALIZED, ADDRESS SOME OF THE LIMITATIONS ASSOCIATED WITH OTHER MODELS?

**COMMENT:** While TRIM.FaTE includes the mass conserving feature for chemicals undergoing first-order linear mass transfer and transformation processes, SAB found it unclear as to how TRIM.FaTE can be adapted for chemicals that are subject to non-linear higher-order

processes. The SAB recommended that additional methods and guidance be developed to assist users in selecting the appropriate level of spatial and temporal resolution necessary to obtain adequate precision and accuracy in the results.

**RESPONSE:** Thus far in the development of TRIM.FaTE, only first-order linear methods have been implemented for all fate and transport processes. The degree of additional effort required to incorporate non-linear and/or higher-order methods will depend on the types of methods of interest. For example, implementation of the types of equations used to model non-linear kinetics will be straightforward, as the original system of differential equations can be used, after adding the non-linear product terms. More care will be needed for incorporating methods for estimating gradients within what are currently assumed to be homogeneous compartments. The equation solving method used in TRIM.FaTE, LSODE, allows non-linear mass transfers to easily be set up numerically. The primary limitation TRIM.FaTE has for addressing such processes is a result of a lack of appropriate data, not a result of limitations in technical capability.

As part of the TRIM.FaTE mercury case study (see Chapter 7), OAQPS is conducting analyses to examine the level of spatial and temporal resolution necessary to obtain adequate precision and accuracy in the results for various Agency needs. The results of these analyses will assist OAQPS in the development of users guidance for the TRIM.FaTE module that will assist users in selecting an appropriate level of spatial and temporal resolution (see Chapter 5 of TRIM.FaTE TSD Volume I). The results of such testing and initial model applications will inform the guidance development process.

**COMMENT:** The SAB found that the flow model for air transport was highly simplified and recommended further evaluation of available air models and selection of additional process modules or components for incorporation into TRIM.FaTE.

**RESPONSE:** The EPA recognizes the need to incorporate more sophisticated methods for modeling air transport in TRIM.FaTE. Two primary means of doing so have been investigated since the May 1998 SAB review. The first option consists of incorporating algorithms for addressing dispersion/diffusion directly within the TRIM.FaTE algorithm library itself. The second option consists of ensuring that it is possible to use the results of an external air model that addresses these processes. Each of these approaches has drawbacks that limit its applicability within a coupled model such as TRIM.FaTE.

Incorporating horizontal and vertical air dispersion/diffusion algorithms directly within TRIM.FaTE was pursued using a method utilizing both lateral and vertical Pasquill-Gifford plume dispersion coefficients. However, review indicated that such methods are not preferable at this time (see the second response in Section 2.4.1). The alternative (*i.e.*, incorporating the results of an external air model that more appropriately addresses dispersion) has other limitations; notably, either the linkage between the external model and TRIM.FaTE is in one direction only and, hence, conservation of chemical mass is lost, or the external model must be linked with TRIM.FaTE in such a way that chemical transfer can occur in both directions. The difficulty of the latter will depend on the particular external model considered, but it is likely that it would generally require a substantial effort to implement. This is because the user must not

only perform the practical tasks associated with computer programming, but also must ensure that no fundamental assumptions or concepts inherent to either model are violated. This could occur, for example, if there is overlap between the models in how they address other processes that are not an explicit component of the model linkage itself (*e.g.*, the external model may treat deposition using general inputs for vegetative cover, and the user must implement additional checks to ensure that these inputs are consistent with the vegetative compartments used within TRIM.FaTE).

The users guidance materials to be developed in the next TRIM development phase will caution users to carefully consider which external air models should be used as input to TRIM.FaTE. External models for various media can be used in lieu of the TRIM.FaTE algorithms; however, strong caution should be placed on the use of external models that themselves may not conserve mass (*e.g.*, Gaussian plume models), but whose use may be dictated or preferred for regulatory reasons.

**COMMENT:** The SAB noted that the predictive capability of the module is limited because of the gross transfer of mass between sources, receptors, and sinks. Therefore, it recommended comparing results from TRIM.FaTE to results from existing "single-media linked models" to establish the advantages and limitations of TRIM.FaTE.

**RESPONSE:** As part of the evaluation plan described in Chapter 6, OAQPS is testing TRIM.FaTE using monitoring data to compare model results to both "real world" observations and other model outputs, including those from the Agency's Indirect Exposure Methodology (IEM, now termed Multiple Pathways of Exposure or MPE), which is a methodology that relies on a one-way transport process through a series of linked models or algorithms. In addition, outputs from the TRIM.FaTE air modeling component are being compared to outputs from ISCST3. The ISCST3 is the air model relied upon in the MPE methodology.

**COMMENT:** With regard to uncertainty and sensitivity analyses, SAB recommended reviewing the literature on sensitivity and uncertainty analysis (see Section 2.2 for additional details).

**RESPONSE:** As noted in Section 2.2, after reviewing the literature (see Appendix B), OAQPS developed a proposed approach to incorporate sensitivity and uncertainty analysis capabilities into the TRIM computer framework. This approach is described in Chapter 3. In addition, implementation of the approach in the TRIM.FaTE module is summarized in Section 4.7 and described in more detail in Chapter 6 of TRIM.FaTE TSD Volume I.

## 2.6 DOES THE TRIM.FaTE MODULE, AS IT HAS BEEN CONCEPTUALIZED AND DEMONSTRATED TO DATE, FACILITATE FUTURE INTEGRATION WITH APPROPRIATE DATA SOURCES AND APPLICATIONS?

**COMMENT:** The SAB found that TRIM.FaTE could conveniently and effectively be integrated with data sources such as GIS, but that coupling of TRIM.FaTE with other more complex models that generate continuous spatial gradients may be problematic.

The SAB noted that the results from TRIM.FaTE would not be directly usable for human health assessments because TRIM.FaTE does not generate distributions of indoor air pollutants, which are the most important input for TRIM.Expo.

**RESPONSE:** The TRIM.FaTE module was never intended to solely support human health assessments, but only to generate estimates of concentrations in the various environmental and biotic media. The exposure component is critical for any human health assessment. Distributions of indoor air pollutants are not generated in TRIM.FaTE because it was determined that on a total mass basis, the indoor environment represents a negligible reservoir of mass of air pollutants. However, OAQPS recognizes the importance of indoor air pollutant concentrations to human exposure. For that reason, indoor air concentrations will be generated within the TRIM.Expo module by accounting for penetration of pollutants in the ambient air (obtained from output of TRIM.FaTE, from other air models, or from analysis of ambient monitoring data) indoors as well as significant indoor sources. Therefore, distributions of indoor air concentrations and exposures will be generated within the TRIM.Expo module.

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# 3. TREATMENT OF UNCERTAINTY AND VARIABILITY IN TRIM

This chapter summarizes the approach for assessing uncertainty and variability in the TRIM modules. Additional background on how this method was selected is provided in Appendix B of this report. A specific discussion of the approach for TRIM.FaTE is presented in Chapter 6 of TSD Volume I. The following text box presents definitions for the key terms used in this chapter to explain the uncertainty and variability analysis framework for TRIM.

**KEY TERMS FOR UNCERTAINTY AND VARIABILITY ANALYSIS**

**Variability**

Variability represents the diversity or heterogeneity in a population or parameter, and is sometimes referred to as natural variability. An example is the variation in the heights of people. Variability cannot be reduced by using more measurements or measurements with increased precision (taking more precise measurements of people's heights does not reduce the natural variation in heights). However, it can often be reduced by a more detailed model formulation (*e.g.*, modeling people's heights in terms of age will reduce the unexplained variability of heights).

**Uncertainty**

Uncertainty refers to the lack of knowledge regarding the actual values of physical model input variables (parameter uncertainty) and of physical systems (model uncertainty). For example, parameter uncertainty results when non-representative sampling (to measure the distribution of parameter values) gives sampling errors. Model uncertainty results from simplification of complex physical systems. Uncertainty can be reduced through improved measurements and improved model formulation.

**Sensitivity**

Sensitivity refers to the rate of change of the model output with respect to changes in an input parameter.

## 3.1 OBJECTIVES OF THE INTEGRATED UNCERTAINTY ANALYSIS

Development of the TRIM framework involved development of an approach to estimate uncertainty and variability in a manner that allows for integration between the TRIM modules and for tracking the uncertainty and variability through the modules. The TRIM approach for uncertainty and variability analysis is intended to accomplish the following objectives:

- Propagation of variability, uncertainty, and parameter dependencies throughout TRIM in an integrated manner, tracking uncertainty and variability jointly and separately;
- Characterization of uncertainty and variability of model results with respect to parameter distributions and correlations, and calculate summary measures of the uncertainty and variability of model results that clearly convey the important aspects of model uncertainty and variability;

- Identification of critical parameters and correlations through sensitivity analyses;
- Information to guide data improvement efforts (including setting priorities for gathering data to develop distributions of parameters), guide model simplification efforts, and support temporal and spatial aggregation choices;
- Results that can support risk management decision-making; and
- Estimation of uncertainty and variability within a reasonable amount of computer processing time.

## 3.2 GENERAL STEPS IN AN ANALYSIS OF UNCERTAINTY AND VARIABILITY

The analysis of uncertainty and variability in a risk assessment takes place through a series of functional steps. Some steps may be skipped and others may be incorporated in more sophisticated or refined iterations. Underlying the risk assessment is a mechanistic model of the risk process. In the case of the TRIM.FaTE module of TRIM, the model algorithms represent the physical and chemical processes that transfer chemical mass through different compartments of a physical system. As a first step, the mechanistic model can be evaluated in a deterministic manner for its sensitivity to changes in its variable inputs. For example, one very simple sensitivity analysis looks at the percent change in the model output (*e.g.*, risk) given percent changes in model inputs (*e.g.*, emissions, wind velocities, air-to-soil deposition rates, soil density). This technique does not require information about the range of values of the input variables, but requires only a selection of possible single values from which local deviations are calculated. This univariate analysis can be expanded to look at pairs of input variables, thereby taking into account dependencies or interactions between variables. Such simple analyses of model sensitivity are valuable because they can be used quickly and easily to identify the variables that have the greatest potential to "influence" the model results, based on the relationships in the model and the selected set of values.

The second step of the analysis is collecting information about the ranges and likelihoods of the values the variables might take. After the ranges are estimated for the variables, it is possible to conduct a deterministic scenario analysis by selecting a set of values for each variable and using the mechanistic model to calculate risk for each possible combination of the selected values. A probability tree can be created by adding information about the likelihood of each scenario. Either approach can be implemented to identify the most important variables on the basis of the combination of model response sensitivity and indeterminancy (*i.e.*, lack of knowledge of the actual or "true" values) in the variables. A variety of approaches are available to estimate the ranges and likelihoods of the values for the input variables. Examples include direct measurement of the physical system and elicitation of expert judgment. Further processing of the input data may be desirable to fit analytical forms, such as normal or lognormal probability distributions, or to estimate statistics, such as the mean and variance, from the information about the dispersion in the variable values. The bootstrap is a statistical resampling method that can assist with this step (Efron 1980).

The propagation of uncertainty and variability in a very simple mechanistic model may be conducted through combinatorial methods, including the sensitivity analyses described above, discrete probability trees, and analytical approaches such as the method of moments, Taylor series expansions, and differential analysis. An alternative to these approaches is Monte Carlo simulation, using either simple or stratified random samples from the input probability distributions to approximate the output distribution for risk. The Monte Carlo approach was selected for TRIM uncertainty and variability analysis. The selection of the Monte Carlo approach does not exclude the use of the other approaches. In fact, Monte Carlo was selected because it provides flexibility. If input values can be tracked along with the results of each iteration, these data can be used in the other approaches.

If the mechanistic model is very complex, computational resources may be conserved by "modeling the model." One option for this approach is to develop a response surface by simulating a very large number of scenarios, as in the combinatorial approach described above, and fitting a surface to the results using regression techniques. This response surface model can be substituted for the mechanistic model when propagating uncertainty and variability. Alternative methods for "modeling the model" include generalized linear models and other regression models; the class of fuzzy logic, neural networks, and genetic algorithms; and a technique known as classification and regression trees (CART). Any of these approaches can be used to reduce the form of the mechanistic model to dramatically reduce the time required to compute the risk results for large numbers of scenarios or samples in a Monte Carlo application. These approximations to the model are called "reduced form models." Drawbacks to using reduced form models include inaccuracies (because they are only approximations) and the restriction of not extrapolating outside of the scope of the simulations performed to build the reduced form model.

A final step in the analysis of uncertainty and variability is the interpretation of the relationship between the distributions of the results of the model and the distributions of the model inputs. Distributions of model results can be prepared and presented as part of the risk characterization module, TRIM.Risk (see Chapter 9), either directly or interpreted in terms of identifying important assumptions and parameters, which are also presented in TRIM.Risk. Much like the deterministic tests of the sensitivity of the model to local changes in the inputs, tests can be constructed to identify the probabilistic importance of the indeterminate variables. The first step in accomplishing this is to calculate a sensitivity score composed of the elasticity, the coefficient of variation, and the ratio of nominal input and output values. This score considers the range of uncertainty in the variables and the change in output per change in input, and it also identifies variables with both relatively high sensitivity in the model and high dispersion. Additional approaches for calculating and presenting measures of uncertainty include rank correlation, analysis of deviance, confidence intervals, distributions of the model outputs, and joint distributions of the model parameters and outputs.

## 3.3 OVERVIEW OF THE APPROACH SELECTED FOR TRIM

There are numerous expositions in the published literature describing techniques and applications of analysis of uncertainty and variability. Several techniques are used in a wide range of disciplines, including ecological risk assessment, manufacturing, aerospace applications, and nuclear physics. Respected references related to risk analysis include Beck (1987), Cohrssen and Covello (1989), Cullen and Frey (1999), Morgan and Henrion (1990), National Research Council (1994, 1996), and Vose (1996).

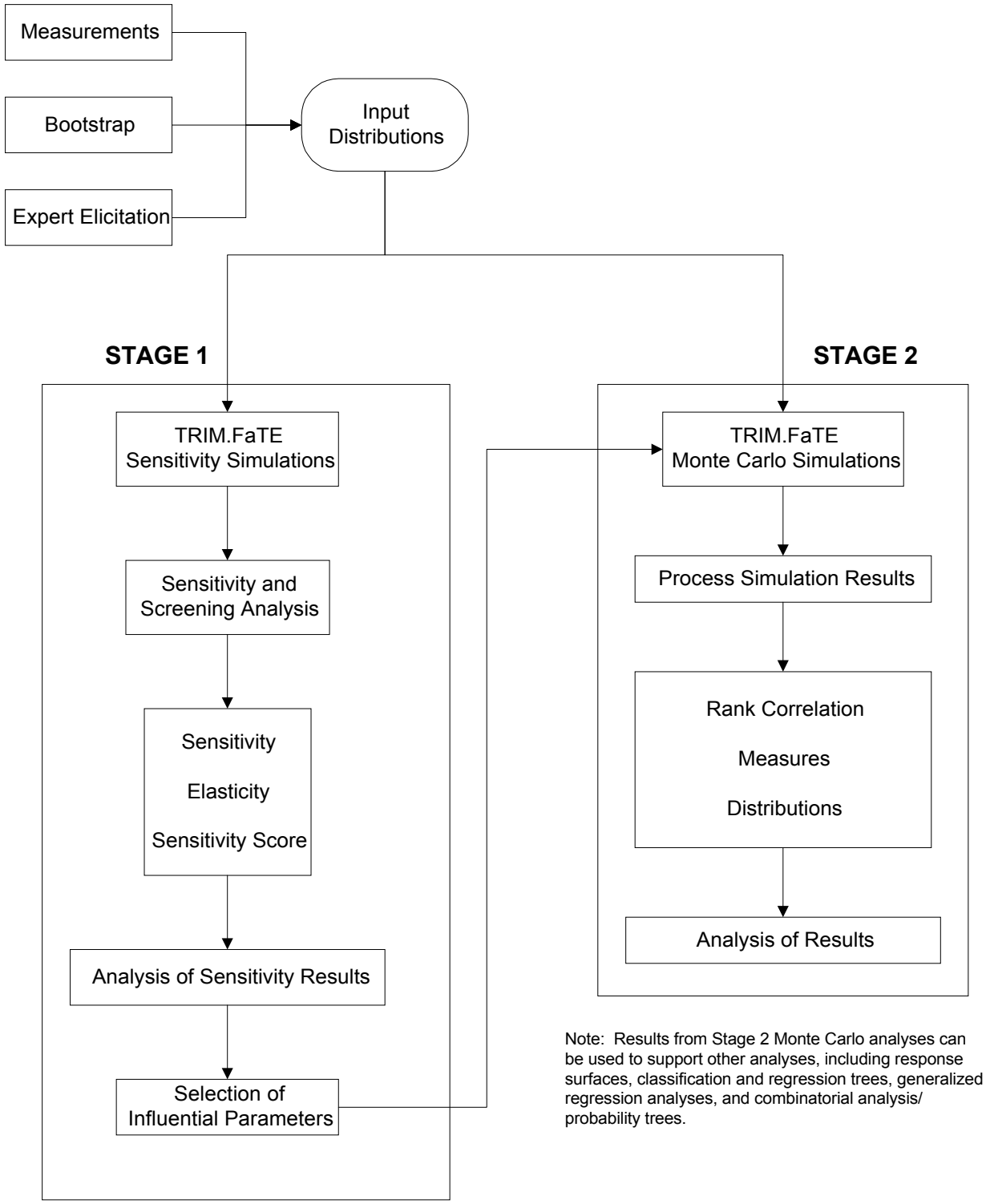
In agreement with EPA guidance on probabilistic assessments, OAQPS chose a staged approach for analysis of uncertainty and variability in TRIM. The use of a staged approach has advantages for models as complex as TRIM. The first stage consists of analyses that are comparatively easy to implement, identifying influential parameters and giving an importance-ranking of parameters, which are useful for narrowing down the number of parameters to be analyzed in the uncertainty and variability analysis. This first stage is considered a sensitivity and screening analysis. The second stage involves uncertainty and variability analyses of increasing detail and complexity. Figure 3-1 illustrates this staged approach and how the functional parts fit together. This approach provides the TRIM user with options to perform a sensitivity analysis or a combined sensitivity and uncertainty/variability analysis, where the sensitivity results guide the selection of parameters for the uncertainty and variability analysis. The user also has the option to perform only the uncertainty and variability analysis, if the user has identified specific parameters to analyze.

The sensitivity and screening analysis calculates the importance of parameters with respect to how the model results change when the parameters vary, varying parameters singly or in pairs. This process provides for a first-order determination of the more influential parameters and allows further analysis to focus on the key parameters.

The screening component of this approach is performed to narrow down the scope of the second-stage detailed analysis, in terms of the number of parameters to be treated, by identifying influential parameters which should be retained for further analyses. This is a critical step toward the goal of producing a economical representation of uncertainty and variability, excluding less influential terms and parameters and still capturing all of the significant features of TRIM uncertainty and variability.

A Monte Carlo approach was selected for the second stage, the detailed uncertainty and variability analyses. Monte Carlo methods for analysis of model uncertainty use statistical sampling techniques to derive statistics that characterize uncertainty. Essentially, a Monte Carlo approach entails performing many model runs with model inputs randomly sampled from specified distributions for the model inputs. Using a two-dimensional Monte Carlo simulation, uncertainty and variability can be modeled separately. These model runs can be set up to characterize the propagation of uncertainty and variability of the model input parameters, taking into account distributions of parameter uncertainty and variability and parameter dependencies. These simulations provide uncertainties of model outputs in terms of distributions of model

**Figure 3-1**
**Uncertainty and Variability Analysis Framework**
**(Illustrated for TRIM.FaTE Module)**



outputs, joint distributions of model inputs and outputs, and summary scalar measures. These are the core data from which information about uncertainty and variability can be extracted.

While the importance of characterizing uncertainty and variability explicitly and separately is well recognized (NRC 1994, CRARM 1997, U.S. EPA 1997c), this does not imply that OAQPS will do so for all cases and all parameters. As stated above and described below, TRIM will have the capability of evaluating and tracking uncertainty and variability separately via two-dimensional Monte Carlo simulation. However, the parameters for which this will be done will be determined on a case-specific basis. The OAQPS intends to characterize uncertainty and variability separately only for critical parameters and where appropriate based on the underlying science and data.

The analysis of uncertainty and variability requires estimates of the distributions of parameters, reflecting both the uncertainty and variability of the parameters in question. In addition, estimates of dependencies (correlations) between parameters would enable a more detailed analysis to be performed. However, typically data are not collected or measured in a way that allows for separating uncertainty and variability for most parameters. When a parameter distribution is available, it is rarely separated into components of uncertainty and variability. For some parameters, such as body weight, the inherent variability within a population has been characterized through the use of large surveys and precise measurement methods. However, emission rates, such as stack gas sampling, have been measured in such a way that separating uncertainty and variability is not supported by the data and would require more of a numeric exercise to tease out variability based on assumptions which may themselves introduce unspecified uncertainty. In some cases, this exercise may result in introducing uncertainty to a greater degree than the variability that is estimated.

This is a current limitation of the Monte Carlo approach which can be addressed over time by developing distributions for parameters to which the model is most sensitive. It should also be noted that OAQPS intends to conduct probabilistic analysis in a tiered approach in accordance with EPA guidance (U.S. EPA 1997b). First, critical parameters are identified through sensitivity analysis, distributions are developed, and correlations are identified only for the more critical parameters. Therefore, distributions are not needed for all parameters for either composite uncertainty or uncertainty and variability separately.

The analysis of the TRIM predictions of risk involves the propagation of uncertainty through the TRIM modules. This can be accomplished by conducting a two-stage analysis of uncertainty and variability sequentially for each of the TRIM modules. The distributions of outputs are passed from one module to the next to propagate distributional information to succeeding modules.

Because the amount of data produced from Monte Carlo simulations is voluminous, the full results will be archived and a reduced set will be retained to feed the next module. The output values from each of the TRIM modules as well as the model inputs (parameter values) for each Monte Carlo simulation will be saved. This large amount of information could be passed along to the next module for subsequent uncertainty analysis, but the amount of data would increase drastically from one module to the next. As illustrated by Figure 3-2, the output data

($B_1|A_1, A_2...A_n|$) from Module I (*i.e.*, TRIM.FaTE) also are part of the input data to Module II (*i.e.*, TRIM.Expo), and a portion of the input data to Module II ($B_1$) is dependent on the input parameters to Module I ($A_i$). The notation $B_1|A_1, A_2...A_n|$ indicates the dependence of the module outputs $B_1$ on the module inputs $A_1$, $A_2$, ...$A_n$. Module II also has input data from different sources, as represented by $B_2$ through $B_n$. Similarly, the output data from Module II ($C_1|B_i|A_i||$) are dependent, in part, on the input parameters to both Module I and Module II. Therefore, it is important to track the input parameters to each TRIM module. However, Figure 3-2 only depicts the information flow for a single simulation, and the actual volume of information would be multiplied by the number of Monte Carlo simulations performed (potentially thousands).

To reduce the size and complexity of the flow of uncertainty and variability information between TRIM modules, these results will be summarized in the form of nonparametric probability distributions that can be passed to the next module, where each distribution to be passed is characterized nonparametrically by its percentiles. Figure 3-3 illustrates how input parameters and output data will be tracked as distributions.

Another way in which the amount of information to be tracked through the modules can be reduced is through the use of the screening and sensitivity stage analysis described above. The simulation could be run with this feature to select the critical parameters in each module to be tracked for the more detailed uncertainty analysis; all other parameters would be set at their central tendency value in the more detailed analysis run. To further reduce the volume of information, after summarizing the results from one module as probability distributions, the transmission of information to the next module is filtered to select the most critical parameters (*e.g.*, those that account for 95 percent of the variance of the uncertainty and variability).

The Agency has begun testing the two-stage approach to uncertainty and variability described in this section as part of the TRIM.FaTE mercury case study (described in Chapter 7). These tests involve the uncertainty analysis for one module and not for a sequence of modules, as depicted by the outlined area in Figure 3-3. When the TRIM modules are linked together, each module after the first will treat its inputs from the previous module in the same way its other inputs are treated, as deterministic values with uncertainty and variability distributions. Therefore, no modification to the approach that OAQPS is testing for TRIM.FaTE is required for the remaining modules, and the extension to other modules will be straightforward.

**Figure 3-2**
**Information Flow for a Single Monte Carlo Simulation of TRIM**

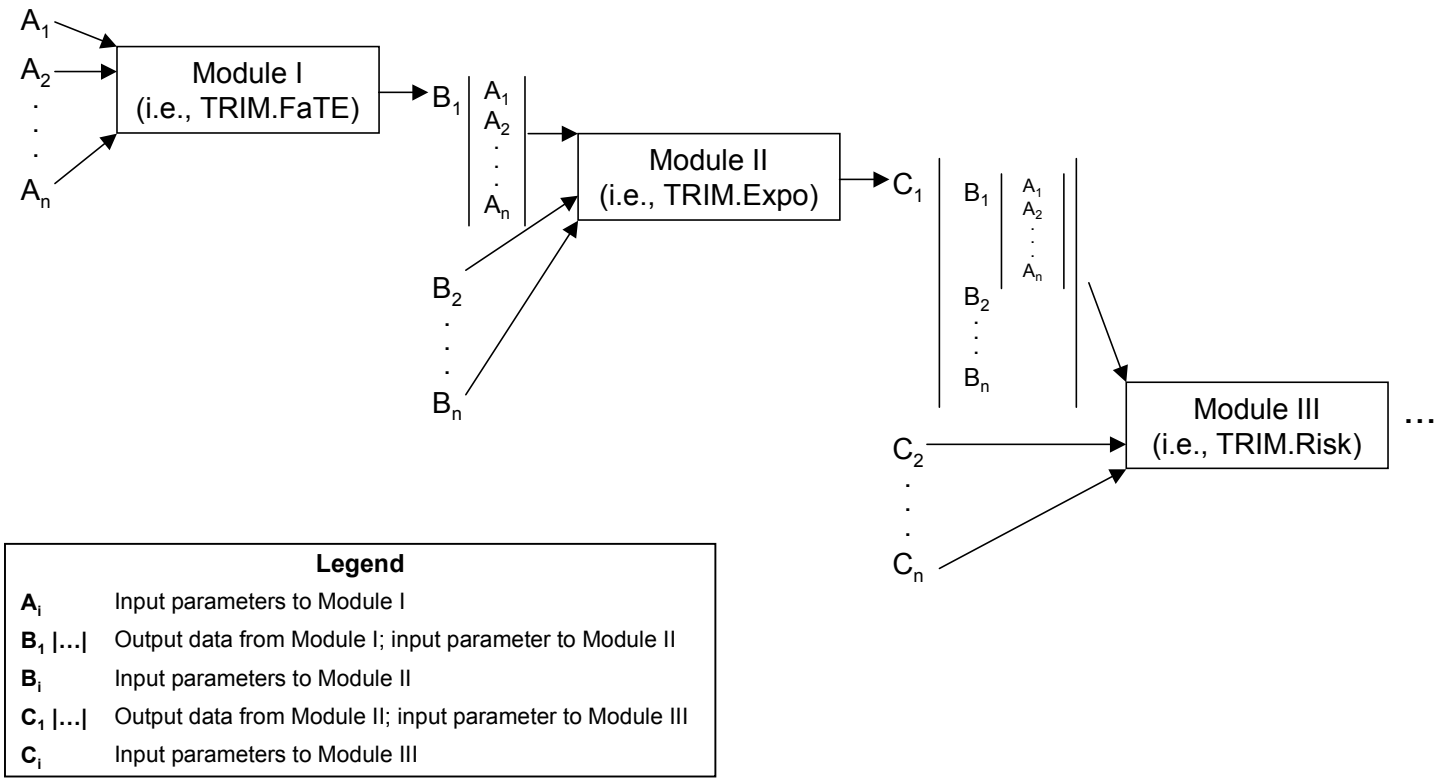
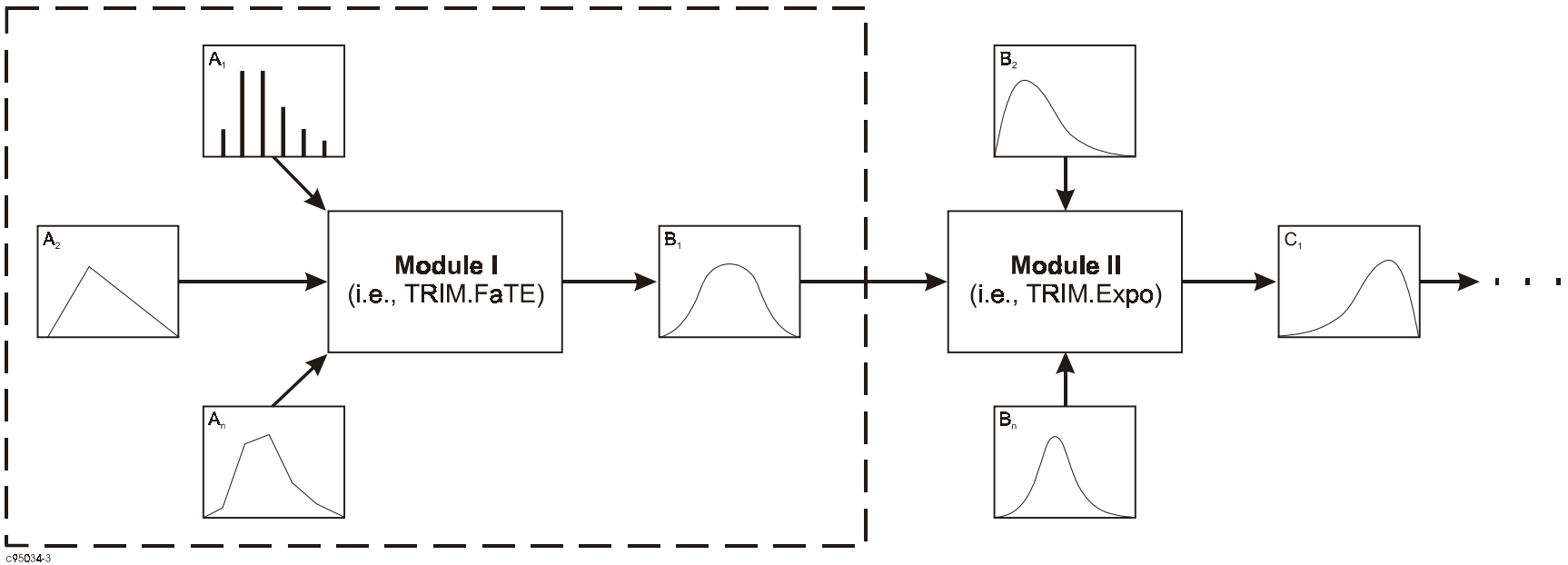


**Figure 3-3**
**Nonparametric Probability Distribution Method for**
**Information Flow in Monte Carlo Simulation**



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# 4. REVISIONS AND ADDITIONS TO TRIM.FaTE

Since May 1998, the Agency has implemented numerous revisions and additions to the TRIM.FaTE module, both in response to SAB comments (see Chapter 2) and as part of the ongoing model development. This chapter summarizes the major revisions and additions, including their basis and current status. As appropriate, revisions and additions to TRIM.FaTE will be assessed in the uncertainty and sensitivity analyses along with the model evaluation activities that are being conducted on this module. Technical terms used in this chapter are defined in the glossary (Appendix A) and in a text box at the beginning of Chapter 5. More detailed information on the aspects of the TRIM.FaTE module that are discussed below is presented in Volume I of the TRIM.FaTE TSD.

## 4.1 ABILITY TO ACCOUNT FOR METALS

Prior to May 1998, the chemical fate and transport algorithms developed for and included in TRIM.FaTE were specific to nonionic organic compounds, with phenanthrene and benzo(a)pyrene as the example chemicals for which all the necessary parameter values were obtained and used in the algorithms. The transfer coefficients used in these algorithms rely upon the concept of fugacity for modeling some types of chemical transfers; however, the concept of fugacity cannot generally be applied to metals and other inorganic compounds. Because addressing the impacts of metals and other inorganic compounds is a priority for OAQPS and to demonstrate that the TRIM.FaTE methodology is not restricted to modeling the fate and transport of organic compounds, algorithms have been added to TRIM.FaTE prototype V that address the fate and transport of inorganic compounds. The new algorithms were developed and included in TRIM.FaTE specifically for mercury and mercury compounds, but many of these algorithms can be used for other metals and inorganic compounds. Thus, TRIM.FaTE now has the flexibility to model fate and transport of organic and inorganic chemicals (assuming the chemical property values required as inputs are available or can be estimated).

## 4.2 ABILITY TO MODEL FATE AND TRANSPORT OF CHEMICAL TRANSFORMATION PRODUCTS

The transformation of chemical substances in the environment can have a profound effect on their potential for dispersion, persistence, accumulation, and exposure. Chemical transformations, which may occur as a result of biotic (*e.g.*, microbial degradation) or abiotic (*e.g.*, oxidation, hydrolysis) processes, can significantly reduce the concentration of a substance or alter its structure in such a way as to enhance or diminish its toxicity. For example, nitrogenous compounds, which are largely represented by aliphatic and aromatic amines, are of particular interest due to their potential genotoxic activities; transformation processes such as photolytic transformation and oxidation and reduction reactions can lead to the interconversion of these compounds between their related condensation products (*e.g.*, azo compounds) and oxidation products (*e.g.*, primary amines). Such transformations may prolong the persistence of these compounds in the environment and determine their genotoxic potencies (Layton et al. 1993).

Prior to May 1998, chemical transformation was represented in the TRIM.FaTE prototypes via the use of reaction sinks, and the fate of the transformed chemical was not tracked. That is, the mass of the chemical being transformed diminished over time, as appropriate, but the fate and transport of the newly created transformation product(s) was not tracked over time. Algorithms have been added to TRIM.FaTE prototype V to model reversible chemical transformation processes (*e.g.*, the transformation of elemental mercury (Hg) to divalent mercury ($Hg^{2+}$) and then back to elemental). These algorithms were developed specifically for three species of mercury (*i.e.*, elemental, divalent, methyl), although the general framework is applicable for any case in which first-order transformation is appropriate. This additional feature provides TRIM.FaTE with the ability to model the fate and transport of chemical transformation products, in addition to the disappearance of the chemical being transformed.

## 4.3 ABILITY TO ACCOUNT FOR SEASONALITY

Although few multimedia fate and transport models include seasonal components, these are desirable for two reasons: (1) for the model to be applicable to regions in the U.S. where below-freezing temperatures occur, and (2) for model runs with durations extending beyond a single growing season. However, model realism gained by accounting for seasonality must be balanced with the burden on the user to collect site-specific data. Therefore, only selected seasonal algorithms have been implemented in TRIM.FaTE at this time.[1]

Since May 1998, two principal seasonal components have been added to TRIM.FaTE: litterfall algorithms and plant uptake of chemicals. The algorithms that have been implemented reflect the seasonality in the following ways:

- During litterfall, which is assumed to be either continuous for one month or one year (depending on the vegetation type), the mass of chemical that is in and on the leaves is transferred to the surface soil compartments; and

- Uptake of chemicals by plants occurs only between the day of last and first frost.

A third seasonal process, harvesting (*i.e.*, removal of pollutant mass from the system), may be easy to implement in TRIM.FaTE; however, the module has not yet been tested in agricultural regions where this process would be relevant.

Additional seasonal processes may be considered in future improvements to TRIM.FaTE. In addition to evaluating the significance of the process to pollutant transfers among media within the modeling system (and the resultant media concentrations), an important part of this consideration will be the extent of modeling revisions needed for implementation in TRIM.FaTE. For example, some seasonal processes would require that the mass and volume of a compartment change during a model run (*e.g.*, growth dilution), and the current implementation of TRIM.FaTE does not include changes to compartment mass or volume with time. Methods may be devised to accommodate this, as in the case of litterfall, which as implemented in TRIM.FaTE does not

[1] Seasonal weather patterns are accounted for in the meteorological data inputs.

involve a change in the mass of the leaves within the compartment. Instead, for litterfall, uptake of the chemical ceases in the winter, and the chemical is transferred from the leaf compartments to the surface soil compartments.

Examples of seasonal processes that may affect pollutant distribution within the modeling system include the following.

- **The dynamics of snow.** The dynamics of snow accumulation and snowmelt and the timing of chemical transfers from snow to water may affect long-term chemical exposure estimates.

- **Growth of organisms.** The dilution of chemical concentrations in an organism because of its growth may affect predicted organism concentrations and dose rates.

- **Litterfall to surface water.** Litterfall to streams and lakes may affect the dynamics of chemical behavior in surface water.

- **Transformation of chemicals in litter.** The transformation of chemicals in leaf litter may occur at a different rate from that in surface and root zone soil; however, little information on these processes is available at this time.

- **Senescence of plant foliage.** Senescence of plant leaves can result in altered gas exchange with leaves, altered rates of chemical transformation in leaves, lowered water content of leaves, and altered uptake rates of chemicals from soil.

- **Blooming of algae.** The timing and rate of growth of algae, not incorporated in the current version of TRIM.FaTE, may affect the assumed exposure of aquatic organisms to chemicals. Furthermore, the sedimentation of algae following a bloom would affect the mass of a chemical in the sediment.

- **Dietary changes of wildlife.** Some wildlife species change diets at different times of the year, affecting chemical exposure estimates.

- **Habitat use.** Some wildlife species hibernate, winter sleep, or migrate from the contaminated region during winter. These seasonal differences in habitat use could decrease exposure to chemical contaminants.

- **Excretion periods.** Excretion of chemical body burdens by egg-laying and lactation occur during spring and summer seasons. These seasonal excretions may affect chemical body burdens and exposure levels of organisms.

# 4.4 OTHER ADDITIONS AND IMPROVEMENTS TO ALGORITHMS

This section highlights major changes and additions to the TRIM.FaTE algorithms. Detailed information on TRIM.FaTE algorithms is presented in Volume II of the TRIM.FaTE TSD.

## 4.4.1 ABIOTIC ALGORITHMS

The TRIM.FaTE module addresses chemical fate and transport within and between seven different abiotic compartment types (see adjacent text box). Many of the current abiotic algorithms were included in an earlier prototype of TRIM.FaTE. Since May 1997, however, several additions and improvements have been made.

**ABIOTIC COMPARTMENT TYPES IN TRIM.FaTE**

| | |
|---|---|
| Air | Surface Water |
| Surface Soil | Sediment |
| Root Zone Soil | Ground Water |
| Vadose Zone Soil | |

### 4.4.1.1 Dispersive Transport Between Surface Water Compartments

The current implementation of the TRIM.FaTE methodology retains the assumption that chemical mass is homogeneous within compartments. However, algorithms have been developed for addressing dispersive transport between surface water compartments (*i.e.*, surface water to surface water). This addresses a limitation of previous TRIM.FaTE prototypes because dispersion may be an important mechanism of transfer of some chemicals. In surface water compartments (see Chapter 4 of the TRIM.FaTE TSD Volume II), the algorithms are based on the methods used in the Water Quality Analysis Simulation Program (WASP) (Ambrose et al. 1995). Thus, TRIM.FaTE can now model the transport of chemicals by both dispersive and advective processes between surface water compartments.

### 4.4.1.2 Diffusion and Advection With Soil Compartments

During the last year, EPA developed a new approach for constructing air-to-soil and soil-to-soil chemical transport algorithms for TRIM.FaTE. This approach provides a simple but reliable method for simulating the transport of chemicals in soil. The new algorithm applies to three soil compartment types: (1) surface soil, (2) root zone soil, and (3) vadose zone soil. These different soils can be represented by two or more soil compartment types for the purpose of assessing chemical mass transfer. Two types of chemical transport are considered by the soil algorithm: (1) diffusion and (2) advection. The top soil layer (*i.e.*, surface soil compartment) exchanges chemical mass with the lowest compartment of the atmosphere (see Section 5.3.1.1) by a combination of diffusion and several advection processes – wet deposition, dry deposition, and resuspension. Each soil layer also can have one or more transformation processes. The specific links for soil compartments for which TRIM.FaTE includes algorithms are discussed in Chapter 5.

Quantifying the exchange of chemical mass between air and soil and among soil layers depends strongly on the concentration gradient within the soil layers. The Agency recognized

that any algorithm that properly addresses chemical mass transfer from air and into soil must account for the concentration gradient. Therefore, EPA developed an exact analytical solution by applying the appropriate boundary conditions to the transport/transformation equations as presented by Jury (1983). The Agency then developed a simplified form of this solution as the basis for an equivalent mass exchange algorithm that is applicable to each soil layer. Differential equations describing the dispersion, diffusion, advection, and transformation of chemicals distributed among air and soil layers were developed and solved analytically in one dimension. An evaluation of the mathematical behavior of the analytical solution resulted in the development of an approximate mathematical form, which uses a series of exponential functions to represent the variation of concentration with depth. Unlike the analytical solution, which requires fixed boundary conditions, these simple forms can be dynamically linked to other compartments in a multimedia fate model. The new algorithm makes it possible to calculate a characteristic soil penetration depth for each chemical based on the chemical's diffusion and degradation rates in various soil types. To confirm the accuracy of the simple model, several chemical property sets were used to compare results of the simple model against the analytical solution. The Agency only needed to conduct testing with a few chemical property sets because the equations are normalized for the chemical-specific soil penetration depth. Therefore, TRIM.FaTE can now be used to assess the penetration of chemicals from air into soil and provide results that are comparable to those obtained from more complex models. The current restriction on this approach is that the chemical concentration in air must be greater than the concentration in the gas phase of the vadose zone soil.

#### 4.4.1.3 Diffusive Transport Between Surface Water and Sediment Compartments

Diffusive transport of chemicals between sediment and surface water compartments in both directions has been addressed in the current TRIM.FaTE prototype using standard methods as discussed in the Water Quality Analysis Simulation Program (WASP) (Ambrose et al. 1995). Inclusion of these algorithms in TRIM.FaTE is important because diffusive exchange of a chemical between surface water and sediment can be a primary means of transport for some chemicals. The methods adopted from WASP allow for the specification of a diffusive water flow velocity, allowing the movement of a chemical between sediment and sediment pore water in the dissolved phase to be simulated. Thus, TRIM.FaTE is capable of modeling the chemical transport between sediment and surface water compartments (in either direction), including sediment pore water.

### 4.4.2 BIOTIC ALGORITHMS

In addition to the abiotic compartment types and algorithms, the TRIM.FaTE module includes numerous biotic compartment types and algorithms related to terrestrial and aquatic plants and animals. The biotic algorithms in TRIM.FaTE represent chemical transfers to and from biotic and abiotic compartments, primarily through diffusion, advection, and dietary uptake processes (see Chapter 5 for additional information on biotic compartment types and algorithms).

Since May 1998, a number of changes and additions to the biotic algorithm library in TRIM.FaTE have been implemented, including the following:

- Several biotic algorithms were added to the library to estimate the accumulation of chemicals by new biotic compartment types, including algae, soil arthropods, plant foliage (as distinct from leaf surface), and plant leaf surfaces (as distinct from plant foliage);

- Minor improvements were made to several existing biotic algorithms, such as diffusion of chemicals into plant foliage, particle washoff from plant leaf surfaces, and litterfall;

- Several alternative biotic algorithms were added to the library to estimate the accumulation of chemicals by various biotic compartment types, including fish, plant roots, and earthworms; and

- An algorithm was added to the library to represent the link between plant stems and leaves.

### 4.4.3 CHEMICAL- OR CHEMICAL CLASS-SPECIFIC ALGORITHMS

Chemical- or chemical class-specific algorithms are included in TRIM.FaTE to model chemical fate and transport processes that are specific to a particular chemical or chemical class and that cannot be as accurately represented in the more generic abiotic or biotic algorithms. Because of the specificity of chemical- and chemical class-specific algorithms, the TRIM.FaTE module will be most useful and cost-effective if only a small number of chemical-specific algorithms are included (*i.e.*, if the algorithms included are applicable to a broad range of chemicals so new algorithms do not often have to be developed for new applications). At this time, a few chemical-specific biotic algorithms are necessary because certain chemical parameters (*e.g.*, rate constants, partition coefficients) are only applicable to certain chemicals and chemical classes. For example, biotic uptake of a specific chemical may be dependent on particular environmental parameters. The goal, however, is to implement generic algorithms for all important transport and transformation processes, supplemented by class-specific algorithms (*e.g.*, for metals) as needed, and to minimize the use of chemical-specific algorithms to chemicals and processes where a real benefit can be realized. In the current version of TRIM.FaTE, algorithms are included that (1) are applicable to high priority chemicals, such as mercury and polycyclic aromatic hydrocarbons (PAHs), (2) pose issues in multiple environmental media, and (3) are not addressed by other EPA models.

The previous prototype of TRIM.FaTE included some chemical class-specific algorithms for PAHs in support of the TRIM.FaTE test case. To test the ability of TRIM.FaTE to model metals, the Agency added some chemical-specific algorithms for mercury. For example, TRIM.FaTE now includes an algorithm to model the transformation of methylmercury to divalent mercury in plant leaves and stems. More detailed information on the mercury-specific algorithms included in the current prototype is presented in Appendix A of Volume II of the TRIM.FaTE TSD.

## 4.5 INTERFACE WITH EXTERNAL MODELS

Over the past year, the Agency developed and implemented methods for incorporating the results from an external fate and transport model (*e.g.*, an air model, such as ISCST3) within the current TRIM.FaTE framework. This provides additional flexibility because, for example, external model data can be used in place of certain TRIM.FaTE algorithms during a simulation. These methods are described in detail in Appendix B of the TRIM.FaTE TSD Volume I. These methods have been implemented in prototype V of TRIM.FaTE in two ways: (1) the results of an external air model (*e.g.*, ISCST3) can be used as input data, and (2) the concentration can be fixed in specified compartments during a simulation. In either case, certain TRIM.FaTE algorithms are bypassed and essentially "replaced" by model results or fixed concentrations.

As discussed in Appendix B of TRIM.FaTE TSD Volume I, there are limitations with this approach. Either the linkage between the model and TRIM.FaTE is in one direction only and, hence, conservation of chemical mass is lost, or the external model must be linked with TRIM.FaTE in such a way so that chemical transfer can occur in both directions. The difficulty of the latter option will depend on the particular external model considered, but it is likely that it would generally require a substantial effort to implement. This is because the user must not only perform the practical tasks associated with computer programming, but also must ensure that no fundamental assumptions or concepts inherent to either model are violated. Such a violation could occur, for example, if there is overlap between the models in how they address other processes that are not an explicit component of the model linkage itself (*e.g.*, the external model may be treating deposition using general inputs for vegetative cover, and the user must implement additional checks to ensure that these inputs are consistent with the vegetative compartments used within TRIM.FaTE).

The user guidance materials to be developed in the next TRIM development phase will caution users to carefully consider which external air models should be used as input to TRIM.FaTE. External models for various media can be used in lieu of the TRIM.FaTE algorithms; however, strong caution should be placed on the use of external models that themselves may not conserve mass (*e.g.*, Gaussian plume models), but whose use may be dictated or preferred for regulatory reasons.

## 4.6 METHODOLOGY FOR DETERMINING PARAMETERS OF THE MODELING ENVIRONMENT

While previous prototypes of TRIM.FaTE allowed for specification of the parameters of the modeling environment (*e.g.*, scale and spatial resolution, and selection of parcels, volume elements, and compartments), it did not provide a structured process for the user to follow. As a first step in designing this feature, the Agency has developed a consistent general stepwise procedure for setting up a simulation using TRIM.FaTE. These general steps are described in detail in Chapter 5 of TRIM.FaTE TSD Volume I and summarized below. Appendix C of TRIM.FaTE TSD Volume I provides, as an example, more detailed discussion for one step: defining the parcels used in setting up the spatial configuration of a model application.

1. **Define the analysis objective.** As part of the problem definition phase (*i.e.*, the first step in developing a TRIM.FaTE simulation), the user defines the objective of the analysis, including the chemical(s) of concern, the potentially exposed population(s), and the health and/or ecological effects endpoint(s) to be assessed.

2. **Define parcels.** The user considers factors including the likely pattern of transport and transformation of each chemical of concern (*i.e.*, where significant concentration gradients are likely to occur), the location of natural boundaries, and locations of key receptors to help determine the appropriate level of complexity (*e.g.*, size of modeling region, location, size, and number of parcels) for the simulation. The TRIM.FaTE module is intended for local-scale assessments of multimedia pollutant distribution.

> A **parcel** is a planar (*i.e.*, two-dimensional) geographical area used to subdivide a modeling region. Parcels, which can be virtually any size or shape, are the basis for defining volume elements. There can be air, land, and surface water parcels.

3. **Designate volume elements and compartments.** After parcels have been defined and boundaries established, the user designates volume elements and then defines abiotic and biotic compartments. Abiotic compartments include air, surface soil, root zone soil, vadose zone soil, surface water, sediment, and ground water. The depths of each abiotic compartment can be based on generic values, chemical-specific values (*e.g.*, whether a chemical is likely to penetrate deeply into the soil), or site-specific values (*e.g.*, the average depth of a modeled pond). The landscape property values assigned to compartments (*e.g.*, fraction organic carbon, amount of particles in the air) can be based on generic values or site-specific values. Biotic compartments include terrestrial and aquatic organisms; only plant compartments are required to be included in a simulation. A user can perform an assessment for an entire trophic group or for a particular animal species of concern.

4. **Select links and algorithms.** Following the establishment of TRIM.FaTE compartments for a given simulation, the appropriate links and algorithms are selected to model mass transfer and transformation. This step may include specifying the data or data source and the algorithms to use or may in some cases require a user to add algorithms to the algorithm library.

5. **Determine specifications for the simulation.** The last step of TRIM.FaTE setup is preparing the simulation, which involves specifying the simulation time-step, the chemical properties of each modeled chemical, the initial distribution of the chemical mass in the compartments, the data for each modeled source, all site data needed by the selected algorithms, and the output time period(s) of interest.

The steps above describe the general process for setting up a simulation using TRIM.FaTE. The flexible, user-friendly design of TRIM.FaTE provides the user with the ability to perform simulations in an iterative fashion. That is, the user is able to select the necessary level of analysis, ranging from a simple analysis, for which less site-specific data are required and which will run more quickly, to one needed for a more detailed risk assessment. For

example, the more simple analysis, providing a more imprecise, general idea of pollutant distribution, may be sufficient for setting priorities or other similar scoping activities (*e.g.*, in a screening analysis for which conservative default input parameters could be used). This allows the user to focus a more detailed analysis, where the impacts of parameter uncertainty may be assessed for critical parameters, on situations where a more refined assessment is needed (*e.g.*, human health risk assessments to support environmental regulation or other environmental control actions).

## 4.7 OVERVIEW OF THE UNCERTAINTY AND VARIABILITY ANALYSIS APPROACH SELECTED FOR TRIM

In accordance with National Academy of Sciences guidance (NRC 1994), current EPA risk characterization guidance (U.S. EPA 1995a, U.S. EPA 1995b), and updated guidance being developed (*e.g.*, U.S. EPA 1998c), EPA is developing TRIM to allow for stochastic modeling so that uncertainty and variability can be explicitly characterized. This involves the development of an approach to estimate uncertainty and variability within TRIM in a manner that allows for integration between the TRIM modules and for tracking the uncertainty and variability through the modules. At this time, an overall uncertainty and variability analysis approach has been developed for TRIM, as described in Chapter 3 of this report. Chapter 6 of TRIM.FaTE TSD Volume I describes the specific approach being implemented for TRIM.FaTE.

Following a review of current peer reviewed literature and assessment of the available options for uncertainty and variability analyses (see Appendix B), the Agency selected a staged approach for analysis of uncertainty and variability in TRIM, which has advantages for models as complex as TRIM. This approach provides the user with the option to include one of two stages of uncertainty and variability analyses in the simulation. The first stage, consisting of analyses that are comparatively easy to implement, identifies influential parameters and gives an importance-ranking of parameters. This information is useful for narrowing down the number of parameters to be analyzed in a more complex uncertainty and variability analysis. This first stage can be considered a sensitivity and screening analysis. The second stage involves uncertainty and variability analyses of increasing detail and complexity. For TRIM, a Monte Carlo approach was selected for this stage. This approach entails performing numerous model runs with model inputs randomly sampled from specified distributions for the model inputs. Figure 3-1 illustrates this staged approach for TRIM.FaTE.

As work on TRIM.FaTE and the other TRIM modules progresses, EPA plans to continue to evaluate new uncertainty analysis techniques for applicability to improving the current methodology. For example, methods using Fourier transforms, such as the Fourier Amplitude Sensitivity Test (Saltelli et al. 1999), will be evaluated in this context.

## 4.8 MODEL EVALUATION

In its May 1998 review, SAB recognized the challenge in developing a methodological framework for evaluating a model such as TRIM.FaTE. In developing the evaluation plan for TRIM.FaTE, the Agency has attempted to design an approach that contains the essential ingredients for judging the acceptability of TRIM.FaTE for its intended uses, while allowing enough flexibility to accommodate new methods that become available or changes in direction indicated by knowledge gained through the evaluation process. Chapter 6 presents a detailed description of the model evaluation plan designed for TRIM.FaTE.

The evaluation plan for TRIM.FaTE includes four types of model evaluation activities, described below.

- **Conceptual model evaluation** activities focus on whether the model is conceptually sound. This type of evaluation begins in the early stages of model development.

- **Mechanistic and data quality evaluation** activities focus on the algorithms and assumptions used in the model. They determine whether the individual process models and input data used are scientifically sound, and if they properly "fit together."

- **Structural evaluation** activities focus on how changes in modeling complexity affect model performance. They address, for example, the effects of varying the level of both temporal and spatial resolution.

- **Performance evaluation** activities focus on whether the output of the full model is relevant, reliable, and useful. They involve comparing modeling results to some type of benchmark (*e.g.*, monitoring data, other model results, expert judgment).

The first three types of evaluation focus primarily on model inputs (*e.g.*, theory and data) and processing (*e.g.*, process models, assumptions and algorithms, model setup), while the fourth focuses mainly on the information that comes out of the model (*e.g.*, comparing overall model outputs to environmental monitoring data).

The model evaluation plan designed for TRIM.FaTE must be flexible. Results from initial evaluation efforts are posing new questions and leading to additional review, analysis, and testing. A number of evaluation activities have been completed or are underway (*e.g.*, code verification, model documentation, peer review, case studies, sensitivity analysis), while others are still in the conceptual or planning stages.

# 5. CURRENT STATUS OF TRIM.FaTE

As discussed in Chapter 4, EPA has implemented many changes and additions to TRIM.FaTE since May 1998. This chapter summarizes the current status of the TRIM.FaTE module, including the compartment types that are addressed and the links and processes that are represented by the algorithms included in Prototype V.

**TRIM.FaTE HISTORY**

**Prototype I** was designed in 1997 to test the mass transfer methodology and the Livermore Solver for Ordinary Differential Equations (LSODE) utility. Air, soil, ground water, surface water, and fish compartment types were included. Chemical reaction was not simulated. The runs produced estimates of benzene mass throughout the system.

**Prototype II**, also developed in 1997, included more spatial detail in the types and number of compartments. It included multiple volume elements for soil and air compartment types and included plant and sediment compartments. Prototype II was developed using benzo(a)pyrene (B(a)P) as an example chemical. The links between compartments had multiple-phase (*i.e.*, gas, liquid, solid) mass transfers.

**Prototype III**, developed later in 1997 using B(a)P as an example chemical and greater complexity than previous prototypes, included a focus on code and input data structure refinements. This prototype was primarily developed to incorporate lessons learned from earlier prototypes, including a refined set of algorithms, and to set up the module for a case study model run using Prototype IV.

**Prototype IV**, developed in 1998 using B(a)P as an example chemical, was designed to be applied to an actual site rather than for evaluation simulations with generic inputs like the earlier prototypes. Prototype IV was used to evaluate the likely limits of TRIM.FaTE with respect to the number of land parcels and the length of time steps used.

**Prototype V**, the current prototype, addresses the issues identified by the SAB in their May 1998 advisory and includes additional and revised fate and transport algorithms. This prototype was designed to be applied to an actual site for a metal contaminant (*i.e.*, mercury) rather than an organic contaminant, as was the case for Prototype IV.

**Version 1.0** is a computer framework that is intended to support all of TRIM, although only TRIM.FaTE is currently implemented. While the prototype versions of TRIM.FaTE were developed using Microsoft Visual Basic™, Fortran, and Microsoft Excel™ software, Version 1.0 was developed using Java, C, and Fortran in a manner that allows it to run on multiple operating systems, including Windows and UNIX. Version 1.0 also provides improved management of multiple modeling scenarios and is more user-friendly and reliable. Version 1.0 is designed for assessments of any chemical, although it includes some specific algorithms for B(a)P and mercury.

## 5.1 COMPARTMENT TYPES

The TRIM.FaTE module includes both abiotic and biotic compartment types. The seven abiotic compartment types that are included in Prototype V of TRIM.FaTE are air, surface soil, root zone soil, vadose zone soil, surface water, sediment, and ground water. Biotic

compartment types are generally defined by trophic group. Terrestrial plant compartment types include leaves, stems, leaf surfaces, and roots. Table 5-1 lists the 24 biotic compartment types that currently are included in TRIM.FaTE.

## 5.2 LINKS AND ALGORITHMS

Algorithms are used to model the transport of chemicals from one compartment to another (*i.e.*, through links) and the transformation of chemicals from one form to another within a compartment. Prototype V of TRIM.FaTE includes abiotic, biotic, and chemical- and chemical class-specific algorithms. Many algorithms are currently included in the algorithm library of TRIM.FaTE, and users can add algorithms to the library as needed.

### 5.2.1 ABIOTIC LINKS AND ALGORITHMS

Abiotic algorithms in TRIM.FaTE represent the transfer of chemicals from one abiotic compartment to other compartments of the same or different compartment type. The links between abiotic compartment types and the processes modeled by abiotic algorithms are provided in Table 5-2. The major changes and additions to abiotic algorithms since May 1998 are discussed in Chapter 4, and detailed information on abiotic algorithms is provided in Chapters 3 through 7 of the TRIM.FaTE TSD Volume II.

**KEY TERMS**

A **chemical** is a unit whose mass is being modeled. A chemical can be any element or compound, or even group of compounds, assuming the necessary parameters (*e.g.*, molecular weight, diffusion coefficient in air) are defined.

A **compartment** is a homogeneous unit of space characterized by its physical composition and within which it is assumed, for modeling purposes, that all chemical mass is in equilibrium.

A **compartment type** is a specific kind of compartment, such as an air compartment type or a mule deer compartment type. Compartment types are distinguished from each other by the way they exchange chemical mass with other compartment types.

An **abiotic compartment type** is one consisting primarily of a non-living environmental medium (*e.g.*, air, soil) for which TRIM.FaTE calculates chemical masses and concentrations; it may also contain biota, such as the microorganisms responsible for chemical transformation.

A **biotic compartment type** is one consisting of a population or community of living organisms (*e.g.*, bald eagle, benthic invertebrate), or in the case of terrestrial plants, portions of living organisms (*e.g.*, stems, leaves), for which TRIM.FaTE calculates chemical masses and concentrations.

A **volume element** is a bounded three-dimensional space that defines the location of one or more compartments. This term is introduced to provide a consistent method for organizing objects that have a natural spatial relationship.

A **link** is a connection that allows the transfer of chemical mass between any two compartments. Each link is implemented by an algorithm or algorithms that mathematically represent the mass transfer.

A **source** is an external component that introduces chemical mass directly into a compartment.

**Table 5-1**
**Compartment Types in TRIM.FaTE**

| Abiotic Compartment Types | Biotic Compartment Types |
|---|---|
| Air | Leaf |
| Surface soil | Leaf surface |
| Root zone soil | Stem |
| Vadose zone soil | Root |
| Surface water | Algae |
| Sediment | Macrophyte |
| Ground water | Water column herbivore |
| | Water column omnivore |
| | Water column carnivore |
| | Benthic invertebrate |
| | Benthic omnivore |
| | Benthic carnivore |
| | Terrestrial omnivore |
| | Semiaquatic piscivore |
| | Terrestrial herbivore |
| | Semiaquatic predator/scavenger |
| | Terrestrial insectivore |
| | Semiaquatic herbivore |
| | Terrestrial predator/scavenger [a] |
| | Semiaquatic insectivore |
| | Semiaquatic omnivore |
| | Terrestrial ground-invertebrate feeder |
| | Flying insect |
| | Soil detritivore |

[a] Includes terrestrial carnivores (*e.g.*, hawks).

### 5.2.2 BIOTIC LINKS AND ALGORITHMS

Biotic compartments in TRIM.FaTE are linked, using biotic algorithms, to abiotic compartments through two principal chemical processes: diffusion and advection. For example, in the process of ingestion, chemicals are advected in the air or diet to a mammal or bird. Active uptake of chemicals that mimic nutrients is possible but not represented mechanistically in TRIM.FaTE.

Examples of links between biotic compartment types and between abiotic and biotic compartment types in TRIM.FaTE are shown in Figure 4-1 in the TRIM.FaTE TSD Volume I. Many of these links also are summarized below in Table 5-3, which shows the links between biotic compartment types and between abiotic and biotic compartment types and the processes that are modeled by biotic algorithms.

## Table 5-2
## Links and Processes Addressed for Abiotic Compartment Types

| Links Between Compartment Types | | Processes Addressed |
|---|---|---|
| **Receiving** | **Sending** | |
| Air | Air | Bulk Advection |
| | Surface Soil | Diffusion<br>Resuspension |
| | Surface Water | Diffusion |
| Surface Soil | Surface Soil | Diffusion<br>Erosion<br>Runoff |
| | Root Zone Soil | Diffusion |
| | Air | Diffusion<br>Dry Deposition<br>Wet Deposition |
| Root Zone Soil | Root Zone Soil | Diffusion<br>Percolation |
| | Surface Soil | Diffusion<br>Percolation |
| | Vadose Zone Soil | Diffusion |
| Vadose Zone Soil | Vadose Zone Soil | Diffusion<br>Percolation |
| | Root Zone Soil | Diffusion<br>Percolation |
| Surface Water | Surface Water | Bulk Advection<br>Dispersion |
| | Surface Soil | Erosion<br>Runoff |
| | Air | Dry Deposition<br>Wet Deposition<br>Diffusion |
| | Sediment | Resuspension<br>Pore Water Diffusion |
| Sediment | Surface Water | Abiotic Solids Settling<br>Pore Water Diffusion |
| Ground Water | Surface Water | Recharge |
| | Vadose Zone Soil | Percolation |
| Air Advection Sink | Air | Bulk Advection Beyond System Boundary |
| Surface Water Advection Sink | Surface Water | Bulk Advection Beyond System Boundary |
| Sediment Burial Sink | Sediment | Solids Advection Beyond System Boundary |

## Table 5-3
## Links and Processes Addressed For Biotic Compartment Types

| Links Between Compartment Types | | Processes Addressed |
|---|---|---|
| **Receiving** | **Sending** | |
| Leaf Surface | Air (Particulates) | Dry Deposition [b] |
| | Air (Rain Water) | Wet Deposition [b] |
| | Leaf | Diffusion/Advection |
| Surface Soil | Leaf Surface | Particle Washoff [b]<br>Litterfall [b] |
| | Leaf | Litterfall [b] |
| | Terrestrial Ground-Invertebrate Feeder | Excretion [a] |
| | Terrestrial Herbivore | |
| | Terrestrial Omnivore | |
| | Terrestrial Insectivore | |
| | Semiaquatic Omnivore | |
| | Predator/Scavenger | |
| | Semiaquatic Insectivore | |
| | Semiaquatic Herbivore | |
| | Semiaquatic Piscivore | |
| Leaf | Leaf Surface<br>Air<br>Stem | Uptake [a] |
| Air<br>Stem | Leaf | Diffusion/Advection |
| Root | Root Zone Soil | Uptake [a] |
| Stem | Root Zone Soil (Water Phase)<br>Leaf | Uptake [a] |
| Soil Detritivore | Root Zone Soil | Uptake [a] |
| Root Zone Soil | Root | Equilibrium Partitioning |
| | Soil Detritivore | |
| Flying Insect | Sediment | Uptake [a] |
| Terrestrial Ground-Invertebrate Feeder | Soil Detritivore<br>Surface Soil | Diet [b] |
| | Air | Inhalation [b] |

| Links Between Compartment Types | | Processes Addressed |
|---|---|---|
| **Receiving** | **Sending** | |
| Terrestrial Herbivore | Leaf<br>Leaf Surface<br>Surface Soil | Diet [b] |
| | Air | Inhalation [b] |
| Terrestrial Omnivore | Leaf<br>Leaf Surface<br>Soil Detritivore<br>Surface Soil | Diet [b] |
| | Air | Inhalation [b] |
| Terrestrial Insectivore | Soil Detritivore | Diet [b] |
| | Air | Inhalation [b] |
| Semiaquatic Omnivore | Benthic Invertebrate<br>Soil Detritivore<br>Herbivorous Fish<br>Omnivorous Fish<br>Carnivorous Fish<br>Surface Soil | Diet [b] |
| | Air | Inhalation [b] |
| Predator/Scavenger | Terrestrial Herbivore<br>Terrestrial Omnivore<br>Terrestrial Insectivore<br>Soil Detritivore<br>Benthic Invertebrate (Insect) | Diet [b] |
| Semiaquatic Insectivore | Benthic Invertebrate (Insect) | Diet [b] |
| Semiaquatic Herbivore | Benthic Invertebrate<br>Leaf | Diet [b] |
| Semiaquatic Piscivore | Terrestrial Omnivore<br>Terrestrial Herbivore<br>Terrestrial Insectivore<br>Herbivorous Fish<br>Omnivorous Fish<br>Carnivorous Fish | Diet [b] |
| Surface Water | Semiaquatic Omnivore | Excretion |
| | Semiaquatic Insectivore | |
| | Semiaquatic Herbivore | |
| | Semiaquatic Piscivore | |
| | Algae | Equilibrium Partitioning [a] |
| | Macrophyte | |
| | Water Column Herbivorous Fish | Equilibrium Partitioning [ac] |
| | | Elimination [bd] |

| | | |
|---|---|---|
| Surface Water (continued) | Water Column Omnivorous Fish | Equilibrium Partitioning [ac] |
| | | Elimination [bd] |
| | Water Column Carnivorous Fish | Equilibrium Partitioning [ac] |
| | | Elimination [bd] |
| | Benthic Omnivorous Fish | Equilibrium Partitioning [ac] |
| | | Elimination [bd] |
| | Benthic Carnivorous Fish | Equilibrium Partitioning [ac] |
| | | Elimination [bd] |
| Algae | Surface Water | Uptake [a] |
| Macrophyte | Surface Water | Uptake [a] |
| Benthic Invertebrate | Sediment | Uptake [a] |
| Sediment | Benthic Invertebrate | Equilibrium Partitioning [a] |
| Water Column Herbivorous Fish [c] | Algae | Diet [b] |
| Water Column Herbivorous Fish [d] | Algae | Diet [b] |
| | Surface Water | Gill filtration [a] |
| Water Column Omnivorous Fish [c] | Herbivorous Fish | Diet [b] |
| Water Column Omnivorous Fish [d] | Herbivorous Fish | Diet [b] |
| | Surface Water | Gill filtration [a] |
| Water Column Carnivorous Fish [c] | Water Column Omnivorous Fish | Diet [b] |
| Water Column Carnivorous Fish [d] | Water Column Omnivorous Fish | Diet [b] |
| | Surface Water | Gill filtration [a] |
| Benthic Omnivorous Fish [c] | Benthic Invertebrate | Diet [b] |
| Benthic Omnivorous Fish [d] | Benthic Invertebrate | Diet [b] |
| | Surface Water | Gill filtration [a] |
| Benthic Carnivorous Fish [c] | Benthic Omnivorous Fish | Diet [b] |
| Benthic Carnivorous Fish [d] | Benthic Omnivorous Fish | Diet [b] |
| | Surface Water | Gill filtration [a] |

[a] Uptake, filtration, or partitioning which includes diffusion, advection, and/or active accumulation by organism.
[b] Advection processes.
[c] Equilibrium model for bioaccumulation by fish.
[d] Bioenergetic model for bioaccumulation by fish.

An alternative way to describe the chemical transfer processes and types of links handled by TRIM.FaTE is as follows:

- Diffusion of gaseous forms of elements into and out of plants following the concepts of conductance and resistance;

- Deposition of particles to the leaf surface;

- Equilibrium partitioning of chemicals from one environmental medium to another, using the time-to-equilibrium (*e.g.*, plant roots, soil detritivores, benthic invertebrates, algae, macrophytes, herbivorous fish, omnivorous fish, carnivorous fish); and

- Ingestion, inhalation, and excretion by terrestrial and semiaquatic wildlife.

All biotic transfer algorithms in TRIM.FaTE represent first-order chemical transfers between compartments. As for the abiotic compartments, there is no gradient of mass within a single compartment. For example, all of the plant leaves or benthic invertebrates within a single volume element have a homogeneous chemical concentration at any simulation time step. In addition, EPA developed mechanisms in TRIM.FaTE that allow the user to turn off or on particular algorithms at certain times (*e.g.*, at night, on a certain date such as the date of first or last frost).

### 5.2.3 CHEMICAL-SPECIFIC ALGORITHMS

As discussed in Chapter 4, TRIM.FaTE Prototype V includes some chemical- and chemical class-specific fate and transport algorithms for processes that are specific to particular chemicals and chemical classes. For such chemical classes, TRIM.FaTE can substitute the specific algorithms for certain of the more generic abiotic or biotic algorithms. Currently, TRIM.FaTE includes chemical-specific algorithms for three forms of mercury (elemental, divalent, methyl). Appendix A of the TRIM.FaTE TSD Volume II provides detailed information on these algorithms. In addition, TRIM.FaTE is designed to allow users to add chemical- and chemical class-specific algorithms to the algorithm library, as necessary.

Chemical-specific algorithms can also represent the transformation of chemicals from one form to another within a compartment. At this time, these algorithms consist of using input transformation rates.

# 6. EVALUATION PLAN FOR TRIM.FaTE

TRIM.FaTE is a predictive environmental fate and transport model designed to support decisions on programmatic policy and regulation for multimedia air pollutants. These decisions can have far reaching human health, environmental, and economic implications. It is important that an assessment of how well the model is expected to perform the tasks for which it was designed is incorporated within the model development process. In other words, the trustworthiness of models used to determine policy or to attest to public safety should be ascertained (Oreskes et al. 1994). This chapter describes the role of model evaluation in developing an assessment of model quality and acceptability in support of regulatory decisions. The chapter provides background on the evolution of model validation terminology and concepts as well as previous Agency efforts (Section 6.1). The chapter then provides an introduction to model evaluation (Section 6.2) and presents an evaluation plan for TRIM.FaTE using four basic components (Sections 6.3 through 6.6). Finally, the Agency's progress in implementing the plan to date is described (Section 6.7).

## 6.1 BACKGROUND

Most of the early efforts to establish the quality of models used in supporting policy decisions focused on model validation. The term *validation* does not necessarily denote an establishment of truth, but rather the establishment of legitimacy (Oreskes et al. 1994). However, common practice has been not consistent with this restricted sense of the term, and the term validation has been commonly used in at least two ways: (1) to indicate that model predictions are consistent with observational data, and (2) to indicate that the model is an accurate representation of physical reality (Konikow and Bredehoeft 1992). The ideal of achieving – or even approximating – truth in predicting the behavior of natural systems is unattainable (Beck et al. 1997). As a result, the scientific community no longer accepts that models can be validated using ASTM standard E 978-84 (*i.e.*, comparison of model results with numerical data independently derived from experience or observation of the environment) and, therefore, be considered to be "true" (U.S. EPA 1998g). It is unreasonable to equate model validity with its ability to correctly predict the future (unknowable) true behavior of the system. A judgment about the validity of a model is a judgment on whether the model can perform its designated task reliably (*i.e.*, minimize the risk of an undesirable outcome (Beck et al. 1997)).

The current approach used by the Agency is to replace model *validation*, as though it were an endpoint that a model could achieve, with model *evaluation*, a process that examines each of the different elements of theory, mathematical construction, software construction, calibration, and testing with data (U.S. EPA 1998g). Therefore, the term *evaluation* will be used throughout this report to describe the broad range of review, analysis, and testing activities designed to examine and build consensus about a model's performance.

Over the last 10 years, the Agency has been considering model acceptance or model use acceptability criteria for selection of environmental models for regulatory activities. The Agency's efforts in this area are a result of SAB recommendations in 1989 that "EPA establish a general model validation protocol and provide sufficient resources to test and confirm models with appropriate field and laboratory data" and that "an Agency-wide task group to assess and

guide model use by EPA should be formed" (U.S. EPA 1989). In response, EPA formed the Agency Task Force on Environmental Regulatory Modeling (ATFERM). This cross-agency task force was charged to make "a recommendation to the Agency on specific actions that should be taken to satisfy the needs for improvement in the way that models are developed and used in policy and regulatory assessment and decision-making" (Habicht 1992). In its March 1994 report, ATFERM recommended the development of "a comprehensive set of criteria for model selection (that) could reduce inconsistency in model selection and ease the burden on the regions and states applying the models in their programs," and they drafted a set of "model use acceptability criteria" (U.S. EPA 1994a).

More recently, an Agency white paper work group was formed to re-evaluate the recommendations in the 1994 ATFERM report. As a result, in 1998, EPA drafted the *White Paper on the Nature and Scope of Issues on Adoption of Model Use Acceptability Guidance* (U.S. EPA 1998g), which recommends the use of updated general guidelines on model acceptance criteria (to maintain consistency across the Agency) and the incorporation of the criteria into an Agency-wide strategy for model evaluation that can accommodate differences between model types and their uses. The work group also recommended the initial use of a protocol developed by the Agency's Risk Assessment Forum to provide a consistent basis for evaluation of a model's ability to perform its designated task reliably. The *White Paper* was reviewed by SAB in February 1999, and it is currently being revised in respond to SAB comments. The proposed approach for evaluation of TRIM.FaTE, as described in the evaluation plan presented here, is intended to be consistent with the Agency's current thinking on approaches for gaining model acceptability.

In its May 1998 review of TRIM.FaTE, SAB recognized the challenge in developing a methodological framework for evaluating a model such as TRIM.FaTE. Further, SAB suggested that "novel methodologies may become available for quantitatively assuring the quality of models as tools for fulfilling specified predictive tasks" (U.S. EPA 1998a). In developing the evaluation plan for TRIM.FaTE, the Agency has attempted to incorporate the essential ingredients for judging the acceptability of TRIM.FaTE for its intended uses, while retaining the flexibility to accommodate new methods that become available or changes in direction indicated by knowledge gained through the evaluation process.

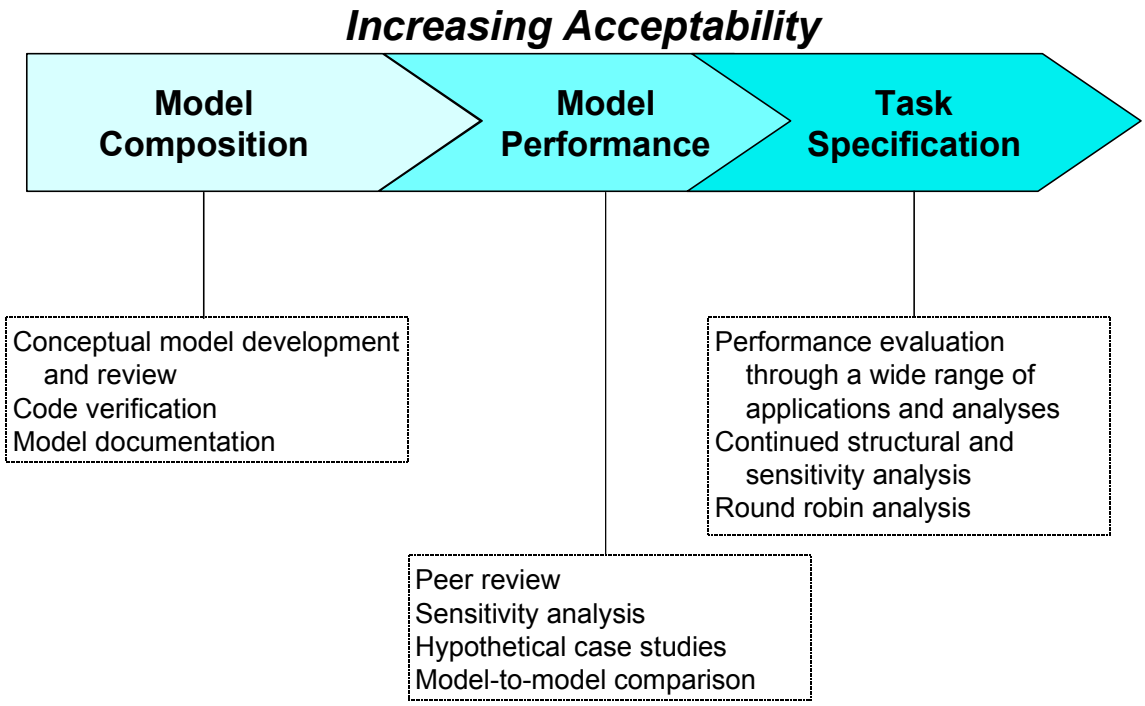
## 6.2 MODEL EVALUATION

Model evaluation is necessary to increase the acceptance of a model. It is not a one-time exercise but a continuing and critical part of model development and application. Several model evaluation methods have emerged in recent years (Dennis et al. 1990, Hodges and Dewar 1992, U.S. EPA 1994b, Cohn and Dennis 1994, Eisenberg et al. 1995, Spear 1997, Schatzmann et al. 1997, Beck and Chen 1999, Arnold et al. 1998, Chen and Beck 1998). All of these methods can be placed into one of two basic categories: (1) those that focus on the performance or output from the model, and (2) those that test the internal consistency (Beck et al. 1997, Beck and Chen 1999) or scientific credibility (Eisenberg et al. 1995) of the model. These methods range from objectively matching model output with monitoring data to more subjective and abstract quality measures (*e.g.*, expert judgment, peer review). The focus of model evaluation activities will change during the life of a model. As a model matures, less emphasis will be placed on peer

review and internal consistency checks and more resources will be directed toward evaluating how well the model satisfies both its original design objective and the specific modeling objectives of individual users.

Model evaluation can be viewed as a consensus building process (Figure 6-1) including three aspects as identified by Beck et al. (1997) – (1) model composition, (2) model performance, and (3) task specification – and recognized in the Agency's December 1998 *White Paper* (U.S. EPA 1998g).

**Figure 6-1**
**Conceptual Representation of the Model Evaluation Process**




The evaluation plan for TRIM.FaTE is presented in the following four sections of this chapter, which correspond to different (but overlapping) types of model evaluation activities:

- Conceptual model evaluation;
- Mechanistic and data quality evaluation;
- Structural evaluation; and
- Performance evaluation.

The first three primarily focus on the information that goes into the model (*e.g.*, theory and data); how this information is synthesized (*e.g.*, process models, assumptions, and algorithms); and how the finished model is set up (*e.g.*, relevant level of complexity). The fourth focuses mainly on the information that comes out of the model (*e.g.*, comparing overall model outputs to various kinds of benchmarks).

The model evaluation plan designed for TRIM.FaTE must be flexible. Results from initial TRIM.FaTE evaluation efforts are posing new questions and leading to additional review, analysis, and testing. The various evaluation activities performed on TRIM.FaTE increase the experience and understanding that will ultimately lead to a judgment about its quality, reliability, relevance, and acceptability. The activities that are currently part of the consensus building process for TRIM.FaTE are described in the following sections. A number of these activities have been completed or are underway (*e.g.*, code verification, model documentation, peer review, case studies, sensitivity analysis), while others are still in the conceptual or planning stages.

**EVALUATION THROUGHOUT MODEL DEVELOPMENT**

As noted in the text, model evaluation is being performed in conjunction with model development. The evaluation activities performed to date have used the most current Prototype (*i.e.*, I through V) of TRIM.FaTE available at the time. Activities since the May 1998 SAB meeting have focused on Prototype V. These evaluation activities are fully applicable to TRIM.FaTE Version 1.0, which is being built from the same simulation algorithms and data as Prototype V. After verification that Version 1.0 produces identical results to Prototype V, Version 1.0 will become the focus of future model evaluation activities.

## 6.3 CONCEPTUAL MODEL EVALUATION

### 6.3.1 DEFINITION AND GENERAL APPROACH

**Conceptual model evaluation activities** focus on the theory and assumptions underlying the model. These activities seek to determine if the model is conceptually sound.

Conceptual model evaluation is initiated in the early stages of model development. During the process of framing the problem and designing the conceptual model, the appropriate level of modeling complexity (*e.g.*, what to include and what to exclude), the availability and quality of information that will be used to run the model (*i.e.*, input data), and the theoretical basis for the model should be evaluated. A literature review should be undertaken to identify and evaluate the state-of-the-science for processes to be included in the model, as well as to compile and document the initial set of values that will be used as model inputs.

Examples of conceptual model evaluation activities include:

- Literature review;
- Model documentation; and
- Peer review of problem definition and modeling concepts and approaches.

### 6.3.2 TRIM.FaTE-SPECIFIC ACTIVITIES

Considerable progress has been made in developing, documenting, evaluating, and refining TRIM.FaTE, including the following.

- An initial literature review identifying the state-of-the-science and the rationale for development of TRIM.FaTE has been completed (U.S. EPA 1997b, U.S. EPA 1997c), and the problem and design objective have been clearly defined (U.S. EPA 1998e).

- Model documentation has been extensive. TRIM Status Reports have been published in 1998 (US EPA 1998e) and 1999 (this document), and presentations have been made at scientific meetings including the Society of Environmental Toxicology and Chemistry (SETAC) annual meetings in 1997 (McKone et al. 1997a, Zimmer et al. 1997, Efroymson et al. 1997) and 1998 (Vasu et al. 1998) and the Society for Risk Analysis (SRA) in 1997 (Vasu et al. 1997, Guha et al. 1997, Lyon et al. 1997, Bennett et al. 1997, McKone et al. 1997b, Johnson et al. 1997). A detailed Technical Support Document for TRIM.FaTE is available (U.S. EPA 1999i, U.S. EPA 1999j), updated from a previous version (U.S. EPA 1998f).

- A May 1998 review by the SAB has been published (U.S. EPA 1998a). Additional evaluations of the conceptual model will continue to be reported in peer reviewed journals and will be subject to additional SAB consultation and review.

As refinements to TRIM.FaTE are made and as new applications are performed, conceptual model evaluation will continue.

## 6.4 MECHANISTIC AND DATA QUALITY EVALUATION

### 6.4.1 DEFINITION AND GENERAL APPROACH

**Mechanistic and data quality evaluation activities** focus on the specific algorithms and assumptions used in the model. These activities seek to determine if the individual process models and input data used in the model are scientifically sound, and if they properly "fit together."

Multimedia fate models are built around a series of process models (*i.e.*, algorithms or groups of algorithms) that make up the mechanics of the model. Many individual process models are taken directly from the literature and have been tested previously for performance and peer reviewed. The prior testing and review provides a degree of confidence that the process model correctly captures the behavior of the processes it is intended to model. New process models and assumptions are often introduced during model development; these new components need to be evaluated individually to ensure that they are working properly.

Mechanistic and data quality evaluations help to elucidate the internal workings of the model and, when necessary, provide a basis to refine process models and assumptions that play a critical role in the calculations. Sensitivity analysis methods are used to identify important model inputs during mechanistic evaluations and to identify the process models having the greatest influence on the model output. For example, alternative algorithms for the same process can be modeled and the results compared. Similarly, each time the model is used for a new kind of application, a sensitivity analysis may be appropriate to identify inputs, algorithms, and assumptions that have the greatest influence on the model outcome in that application. The quality and reliability of these influential factors directly affect the quality and reliability of the outcome from the analysis (Maddalena et al. 1999, Taylor 1993). When feasible, these influential factors should be refined to provide the best inputs to the analysis or, at the very least, identified as a potential source of uncertainty in the outcome.

Some mechanistic and data quality evaluation activities consider the model in its entirety. Process models are typically developed and tested in controlled or simplified systems. Therefore, how well these individual process models will perform in a fully coupled system is unknown. Mechanistic and data quality evaluations are designed and used to measure certain bounded indices of performance (*e.g.*, mass balance, appropriate and realistic mass transfer rates, relative concentrations within reasonable bounds). In addition, algorithms or routines that are used in a model to manipulate the data or to solve a system of equations (*e.g.*, LSODE, the differential equation solver used in TRIM.FaTE) need to be tested during the mechanistic evaluation to ensure proper performance.

Examples of mechanistic and data quality evaluation activities include:

- Computer code verification;
- Verification of generic algorithms adapted for and used within a model;
- Literature review to determine the extent of prior process model testing;
- Peer review of model components;
- Sensitivity analysis to identify important process models;
- Mass or molar balance checks;
- Performance evaluation of new and existing individual process models and of multiple process models in a linked system (*e.g.*, compare with existing models or with measurements, when available);
- Comparison of alternative process models (*e.g.*, equilibrium versus bioenergetic model for fish bioaccumulation of mercury);
- Data acquisition and evaluation (*e.g.*, data quality or reliability relative to the other inputs and assumptions), and development and documentation of default input data;

- Distribution development for input data to support probabilistic analysis; and

- Generic sensitivity analysis to help identify parameters that are most influential on model results, as well as potential data limitations (*i.e.*, model inputs that need further refinement or that are potential sources of uncertainty in the analysis).

### 6.4.2 TRIM.FaTE-SPECIFIC ACTIVITIES

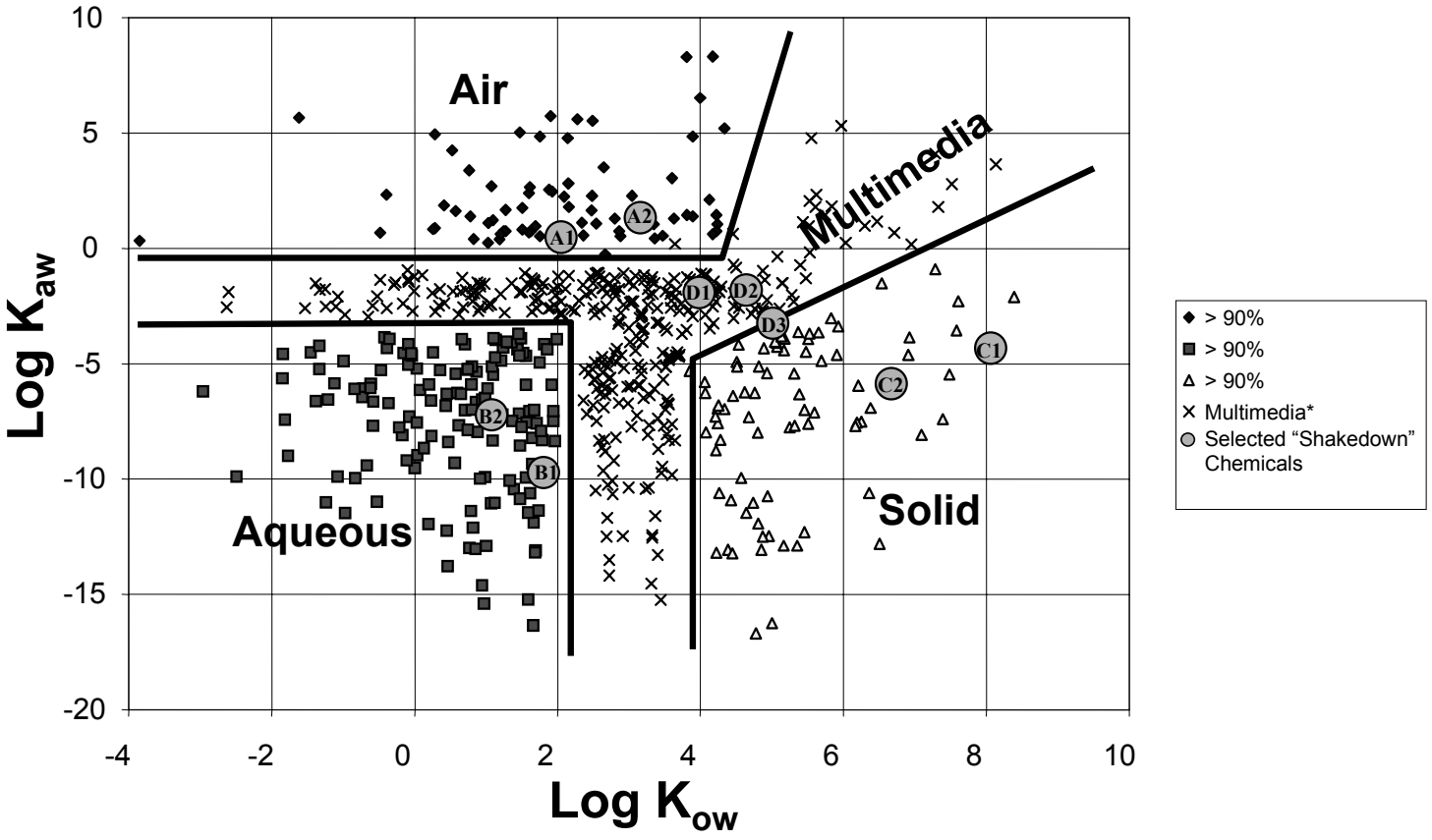
Prototype V (*i.e.*, spreadsheet-based model) is the current working version of TRIM.FaTE, and Version 1.0 (*i.e.*, Java-based platform) is under development (see Chapter 10). One of the features of TRIM.FaTE Prototype V that aids in mechanistic and data quality evaluation is its web-based output functions. There is an option to create a "full-recursive output," which documents the mass flow, as well as the associated transfer factors, to and from each compartment. The equation for each transfer factor can be viewed on a separate web page, and any calculated quantities used in that equation can then be viewed on additional pages. In this manner, checks can be made to ensure that the equations are input properly, and that the computer code is correctly calculating intermediate values. Analyses have been conducted on various parts of the code using this function.

In addition to the standard computer code verification efforts, performance of the generic code used to solve the differential equations in TRIM.FaTE (*i.e.*, LSODE) has been reviewed. Mass and molar balance checks are incorporated in the model for non-transforming organic compounds and mercury to allow for the quick assessment of model performance under a range of conditions.

Prior to conducting detailed evaluations of TRIM.FaTE's process models, numerous model runs were performed. It was determined that there was too much information in a complete run to evaluate whether the model was producing results that are logical, internally consistent, and reasonable. Thus, a "shakedown" phase of the model evaluation was begun using a set of hypothetical chemicals with a broad range of chemical properties. These hypothetical chemicals were designed to systematically probe the model across the broadest range of fate scenarios. The environment in its simplest form can divided into three major phases (*i.e.*, solid, aqueous, and gaseous). The relative solubility of a chemical in each of these phases indicates much about where and how the chemical will partition when released to the environment. These three solubilities can be represented by two fundamental partition coefficients, $K_{ow}$ (*i.e.*, octanol/water partition coefficient) and $K_{aw}$ (*i.e.*, non-dimensionalized Henry's Law constant, air/water partition coefficient).

A simple, level three (steady-state) mass balance model was used to identify the environmental phases for a randomly generated set of 500 "pseudochemicals" plotted in Figure 6-2. From this plot, the regions of parameter space that result in predominantly (>90 percent) single medium pollutants or multimedia pollutants can be identified. Two chemicals from each

**Figure 6-2**
**Single Medium and Multimedia Chemical Regions for 500 "Pseudochemicals"**




* Multimedia defined as not more than 80% of total mass in any single medium. Chemicals between 80% and 90% of total mass in any single medium were excluded from selection as "shakedown" chemicals.

single medium pollutant class and three from the multimedia pollutant class were selected for use as the initial shakedown evaluation set. This approach is particularly useful when performing diagnostic evaluations because the set of pseudochemicals provides insight into possible reasons for unexpected model outcomes. For example, if the model predicts an unusually high concentration in plants for the gas phase chemicals while the aqueous, solid, and multimedia phase chemicals seem reasonable, a problem in one of the diffusion algorithms would be suspected. Often, the model is run with only a subset of the available compartment types to focus on a particular algorithm or set of algorithms. To date, this group of shakedown chemicals has been used to evaluate and debug the soil algorithms, the plant algorithms, and the general biotic algorithms. These pseudochemicals will continue to be used to further evaluate the process models in TRIM.FaTE and the model as a whole.

Tests are being performed or designed to evaluate process models that, according to the literature review, have not been thoroughly tested, as well as for approaches and algorithms developed specifically for TRIM.FaTE. Examples of process models that have been identified for evaluation include the particle/plant leaf algorithms, the soil flux model, and the air transport algorithms. Approaches and algorithms that are related to seasonality (*e.g.*, snow, plant growth, senescence) will be evaluated so that they can be incorporated into TRIM.FaTE, if appropriate.

When different models are available for the same process (*e.g.*, bioaccumulation in fish), model-to-model evaluations may be performed at a process model level to test the overall performance of TRIM.FaTE using different input algorithms. As one example of this, EPA is comparing the air transport component of TRIM.FaTE to a widely used EPA air dispersion model, ISCST3 (U.S. EPA 1995c). In addition, measured concentrations that are available for a single medium or multiple adjacent media (*e.g.*, water and sediment, or water and fish) will be used, where available, to test single or multiple process models.

Data acquisition and the careful evaluation of model inputs are ongoing. To date, the majority of effort has focused on compiling an initial set of model inputs for a small set of test chemicals (*i.e.*, phenanthrene, benzo(a)pyrene, mercury) and environmental settings (U.S. EPA 1998f; also Chapter 7 and Appendix C of this document).

In addition, sensitivity analysis techniques are being used to provide a first-order determination of the most influential parameters in TRIM.FaTE. The sensitivity of model outputs to changes in individual parameters is assessed by performing a series of simulations where each parameter is varied with the other parameters held constant. This does not take into account parameter dependencies or synergistic effects, but is an efficient way to perform an initial assessment of the relative influence of the parameters. This information supports model evaluation by providing a prioritized list of parameters on which to focus the evaluation efforts.

To take full advantage of the probabilistic capabilities of TRIM, some inputs will need to be described using probability distributions that separate uncertainty and variability. The uncertainty and variability analysis methodology that has been developed for TRIM.FaTE is further described in Section 4.7 and in TRIM.FaTE TSD Volume I, Chapter 6. Following the implementation of this methodology, sensitivity analyses are being performed to help identify potential influential factors and data limitations. One of the key functions of the uncertainty

analysis methodology is to evaluate the importance, in terms of both uncertainty and variability, of specific model inputs and of model components in relation to other inputs and components. This gives insight into priorities for reducing uncertainty and for focusing efforts on the improved representation of model inputs. The ability to rank input parameters in order of their influence on the uncertainty and variability of the model results is an important component of establishing such priorities.

As refinements to TRIM.FaTE are made and as new applications are performed, data quality evaluation will continue to be revisited. Sensitivity analysis can be used to identify inputs, algorithms, and assumptions that have the greatest influence on the model outcome in specific applications. When feasible, influential factors may be refined to provide the best inputs to the analysis or identified as a potential source of uncertainty in the outcome.

## 6.5 STRUCTURAL EVALUATION

### 6.5.1 DEFINITION AND GENERAL APPROACH

**Structural evaluation activities** focus on how changes in modeling complexity affect model performance. These activities seek to determine how the model will respond to being set up differently for different applications.

Judging the reliability of a model requires an understanding of how the model responds to changes in complexity (*i.e.*, changes in the modeling structure). Both temporal and spatial changes can be made to the model structure. Structural evaluation addresses these kinds of changes and provides valuable information about the performance and behavior of the model under a range of conditions, improving the ability to judge the model's quality and reliability. Ideally, these evaluations can help determine the optimal model structure to balance the level of complexity needed to create reliable outputs with the simplifications that can make the model easier and more practical to use. If the model is less complex, it is easier to perform additional analysis, such as uncertainty and sensitivity analysis, and is more practical to apply to specific sites and situations. Structural evaluation can provide insight and guidance for future model applications, and it is a very useful input to developing user guidance.

A large number of well designed runs is necessary to evaluate the way a model performs under different conditions. These structural evaluations combine sensitivity analysis methodology with model-to-model comparisons. For a structural evaluation, the model is set up for an application, using either real or hypothetical data. Changes are then made to the structure (*e.g.*, spatial elements are split or recombined; time steps are changed; compartment shapes, sizes, and locations are altered), and the model outcomes are compared (*i.e.*, the model is compared to itself under various set-up conditions).

Structural evaluations encompass a series of comparisons designed to measure the model's response to various changes, which can include:

- Different run duration and/or time step values;

- Varying spatial configurations;
- Changes in initial and boundary chemical concentrations;
- Changes in the source and/or target locations; and
- Other changes in complexity (*e.g.*, including/excluding biota, using average precipitation versus discrete rain events).

### 6.5.2 TRIM.FaTE-SPECIFIC ACTIVITIES

TRIM.FaTE is intended to be used in a wide range of modeling applications (*e.g.*, various chemicals, environmental settings, exposure conditions). Because TRIM.FaTE can be used at various levels of complexity, it is important to understand the level of complexity needed for a particular analysis and the stability of model output when the system structure is changed. Given the complexity of the "real world" and the large number of inputs used in TRIM.FaTE, a complete set of structural evaluations cannot be identified and performed. The focus of structural evaluation activities for TRIM.FaTE will be responsiveness to changes in model complexity with respect to both temporal and spatial scales and the types of compartments included.

Several structural evaluation activities have been identified for TRIM.FaTE, including the following.

- **Response of abiotic compartments to the exclusion/inclusion of biota.** It has typically been assumed that the mass of a chemical in biota compared to the mass in abiotic compartments (*e.g.*, soil, water, air) is not large enough to influence the overall chemical mass balance. However, if both the flux into the biotic compartment and the reaction rates within the compartment are rapid enough, the biota can potentially influence the mass balance even when a relatively small volume of biota is present (Maddalena 1998). Testing will be done to measure the model response to biota inclusion to determine when and to what extent biota need to be included in mass balance calculations.

- **Response to temporal scales of analysis and to aggregate inputs.** Detailed meteorological data are available and will be used in a simplified scenario, as part of the mercury case study (see Chapter 7), to test the model's response to aggregation of input data over various time periods. By running the model with varying degrees of input aggregation, the level of input detail required to achieve a specified level of detail in the output can be determined.

- **Response to changes in the size, shape, and location of compartments.** As part of the mercury case study (see Chapter 7), EPA plans to examine the effect of varying spatial configurations on TRIM.FaTE results. This will include changing the size of compartments in multiple dimensions to determine the most appropriate way to grid the

model, as well as adding compartments at the edges of the model region to examine the boundary effects around the model system (*i.e.*, flux of chemical mass into or out of the system).

Results from initial structural evaluation analyses would likely lead to further testing (*i.e.*, diagnostic evaluations). Different tests could be designed and executed until a clear understanding of the behavior of TRIM.FaTE at different levels of complexity emerges. This understanding will ultimately be incorporated into a user's manual to provide guidance on setting up the model at an appropriate level of complexity for a given application. For practical reasons, it is important to limit the complexity of model setup to that which is needed to produce acceptable modeling results.

## 6.6 OVERALL PERFORMANCE EVALUATION

### 6.6.1 DEFINITION AND GENERAL APPROACH

**Performance evaluation activities** focus on the output of the full model. These activities seek to determine if the output is relevant, reliable, and useful.

Unlike the other types of model evaluation discussed above, which focus on specific aspects of the model (*e.g.*, inputs, process models), performance evaluation focuses on the model as a whole. Performance evaluation compares modeling results to some type of benchmark (*e.g.*, monitoring data, other modeling results). Generally, various performance evaluation analyses are conducted in a similar manner, with only the source of the comparison data changing. The optimized model, as modified based on all prior evaluations, is used for performance evaluation.

Matching model output to monitoring data is often considered the most desirable form of performance evaluation. Although comparing model output to measured values provides useful information on the model, history matching experiments provide only part of the overall picture of the model's quality, reliability, and relevance (Beck et al. 1997). Several other forms of performance evaluation exist. In addition to monitoring data, output of another model and expert opinion and judgment about how output should look can be used as comparison benchmarks in performance evaluation.

Moreover, each evaluation provides an opportunity to use the model. In addition to the ultimate findings of the performance evaluation itself, the experience gained through these exercises contributes to an overall understanding of the model, which ultimately enables both model developers and users to judge the quality of the model.

A different form of performance evaluation is the "round-robin" experiment (Cowan et al. 1995), in which several different users independently set up the model and generate output using the same data for a particular case study (*e.g.*, site description, chemical properties). Model outputs are then compared, and the users' experiences are reviewed to identify weaknesses and ambiguities in the program's user interface and other user guidance that could lead to errors inapplying the model. The lessons learned can then be incorporated into user guidance to help prevent user errors and inappropriate model applications.

Examples of performance evaluation activities include:

- Comparison of model output to monitoring data (*e.g.*, concentrations in environmental media and biota, exposure markers);
- Model-to-model comparison;
- Round-robin experiments; and
- Some forms of regional sensitivity analysis (*i.e.*, output is tested against knowledge about a plausible bound).

### 6.6.2 TRIM.FaTE-SPECIFIC ACTIVITIES

An extensive review of the literature was undertaken following SAB's initial comments on the importance of model evaluation for the TRIM project (U.S. EPA 1998a). The review focused on identifying potential data sets for use in evaluating the performance of TRIM.FaTE. The usefulness of some of the reported environmental measurements was limited because in many cases the source of the chemical contamination was not well characterized. Several studies were identified that report chemical measurements in multiple environmental media (Table 6-1). The majority of these studies focus on measuring the current chemical concentrations in the environment with little emphasis on temporal variability or trends. Several of the studies were designed to assess multimedia partitioning (*e.g.*, atmospheric partitioning among the gas, aerosol, and water phases) or to investigate specific environmental processes such as the transfer rate across an environmental interface. Although historical emission patterns can potentially be reconstructed for certain chemicals using sediment chronology (Cowan et al. 1995), little effort has gone into matching historical emissions to multimedia environmental concentrations.

None of the studies identified during EPA's literature review provides complete and concurrent information on chemical concentrations in the five major environmental media (*i.e.*, air, water, sediment, soil, biota) along with the associated source term(s) and environmental characteristics (*e.g.*, meteorology, hydrology, landscape properties). Although some of these studies can and will be used to evaluate certain aspects of the model, it is important not to overvalue these results when judging the overall quality of the model.

As noted above, comparisons of TRIM.FaTE outputs to monitoring data are difficult because complete multimedia data sets from well-characterized systems (*e.g.*, known source, meteorology, and landscape) to use in a performance evaluation are not currently available. However, limited data sets are becoming available through the literature (see Table 6-1) and through unpublished sources (*e.g.*, multimedia monitoring by state or local agencies). These smaller data sets will allow TRIM.FaTE's output to be evaluated and compared with measurements, at least to some degree.

## Table 6-1
## Multiple Environmental Media Studies

| Chemical | Speciation? | Source | Location | Media Measured | Sampling Frequency | Study |
|---|---|---|---|---|---|---|
| Benzo(a)pyrene, other PAHs | NA | Urban | Florence, Italy | • Air particulate<br>• Plant | Once | Ignesti et al. (1992) |
| Benzo(a)pyrene, PAHs (4), PCBs | NA | Petrochemical factories | Stenungsund, Sweden | • Plant<br>• Soil | Once | Thomas et al. (1984) |
| Chlorpyrifos | NA | Not specified | Chesapeake Bay | • Air<br>• Water | 1993 (four times per year from eight stations) | McConnell et al. (1997) |
| Dioxins | NA | Urban | Bolsover, Derbyshire, England | • Air (including deposition rate)<br>• Plant | Once | Jones and Duarte-Davidson (1997), Duarte-Davidson et al. (1997) |
| Mercury | In mammals and earthworms only | Chloralkali plant | Great Britain | • Air<br>• Earthworm<br>• Grass<br>• Soil<br>• Wood mouse and vole organs | Once | Bull et al. (1977) |
| | None | Lithium separation facility | Oak Ridge, TN | • Earthworm<br>• Grass<br>• Mouse<br>• Shrew<br>• Soil | Once | Talmage and Walton (1993) |
| | None | Chloralkali plant | India | • Goat<br>• Some plant species parts<br>• Sheep<br>• Soil | Once | Shaw and Panigrahi (1986) |
| | None | Chloralkali plant | India | • Aquatic plant<br>• Crop plant<br>• Soil<br>• Sediment<br>• Water | Once | Lenka et al. (1992) |

| Chemical | Speciation? | Source | Location | Media Measured | Sampling Frequency | Study |
|---|---|---|---|---|---|---|
| Mercury (continued) | None | Chloralkali plant | Italy | • Air<br>• Soil<br>• Plant | Once | Maserti and Ferrara (1991) |
| | None | Cinnabar, mining | Italy | • Air<br>• Rain water<br>• Plant<br>• Soil<br>• Surface water sediment | Once | Ferrara et al. (1991) |
| | Some methylmercury | Chloralkali plant | Saltmarsh ecosystem near Brunswick, GA | • Birds<br>• Fish<br>• Invertebrates<br>• Mammals<br>• Plant Parts<br>• Sediment | Once | Gardner et al. (1978) |
| | Total, methyl, dissolved gaseous | Urban/runoff | Chesapeake Bay and streams | • Precipitation<br>• Sediment<br>• Water | Several single event measurements (1995 through 1997) | Mason et al. (1999, 1997a,b) |
| Metals, pesticides, PAHs | NA | Not specified | Two different regions in US | • Air (indoor and outdoor)<br>• Biologic fluid<br>• Food (market basket)<br>• Soil | Single measurements per household (early 1990s) | U.S. EPA (1999a), Sexton et al. (1995) |
| | NA | Not specified | Northeastern US | • Air (indoor and outdoor)<br>• Biologic fluid<br>• Food (market basket)<br>• Soil | Longitudinal study of several households (early 1990s) | U.S. EPA (1999a), Sexton et al. (1995) |
| MTBE | NA | Multiple estimated | California | • Air<br>• Ground water<br>• Surface water | 1997-98 and prior | University of California (1998) |
| Organochlorines | NA | Not specified | Lake Baikal, Russia | • Fish<br>• Seal<br>• Water (dissolved and particulate)<br>• Zooplankton | 1993 (August - September) | Kucklick et al. (1996) |

| Chemical | Speciation? | Source | Location | Media Measured | Sampling Frequency | Study |
|---|---|---|---|---|---|---|
| Organochlorines (continued) | NA | Not specified | Lake Superior | • Aquatic biota (19, from amphipod to lake trout) | Summer 1994 (at multiple sites) | Kucklick and Baker (1998) |
| | NA | Urban | Lake Michigan | • Precipitation | Summer 1994 (at multiple sites) | Offenberg and Baker (1997) |
| Organochlorines, PAHs | NA | Not specified | Chesapeake Bay and streams | • Air (vapor and aerosol)<br>• Atmospheric deposition<br>• Diffusive exchange<br>• Water (dissolved and suspended particles)<br>• Plankton<br>• Wet deposition | October 1990 - August 1992 (at multiple sites over, in, and adjacent to lake) | Ko and Baker (1995), Leister and Baker (1994) |
| PAHs (10) | NA | Urban | Indiana | • Air (particulate)<br>• Gas<br>• Plant | Every 20-30 days for several months | Simonich and Hites (1994) |
| Total PAH | NA | Road | Australia | • Air (particulate)<br>• Grass<br>• Soil | Once | Yang et al. (1991) |

An important aspect of the plan for performance evaluation of TRIM.FaTE is a detailed case study of a mercury-emitting industrial facility, which was chosen in part because of the availability of multimedia monitoring data and concurrent emission estimates from a local source. The mercury case study site also is playing a critical role in the mechanistic and data quality, and structural evaluations being done, as well as serving as the basis for a variety of sensitivity analyses. Chapter 7 describes the mercury case study, including the available environmental and biotic measurement data, in more detail.

The previous prototype of TRIM.FaTE was compared with two similar models, CalTOX (McKone 1993a, McKone 1993b, McKone 1993c) and SimpleBox (van de Meent 1993, Brandes et al. 1997). The pollutants modeled for this comparison were PAHs (U.S. EPA 1998f). More recently, outputs from TRIM.FaTE are being compared to outputs from the EPA's ISCST3 and IEM2M models, as part of the mercury test case (see Chapter 7). ISCST3 will be used to generate air deposition and concentration data that will be used in IEM2M to estimate multimedia concentrations of mercury. These concentrations will be compared to TRIM.FaTE outputs that will be modeled using consistent inputs, as well as to TRIM.FaTE outputs from an analysis where the air depositions and concentrations from ISCST3 are incorporated into TRIM.FaTE (in essence, substituting for TRIM.FaTE's air transport component). As part of the mercury test case, TRIM.FaTE outputs (*e.g.*, ranges of predicted environmental media and biotic concentrations of mercury) will also be compared to the available measurement data for mercury in environmental media and biota. The predicted ranges of model results used for these comparisons will be based on the results of TRIM.FaTE uncertainty and variability analyses, as described in Chapter 6 of TRIM.FaTE TSD Volume I.

Although most model-to-model comparisons are performed on a scenario-specific basis, a more informative approach may be to compare models across a range of conditions using multiple regression or data mining software (Helton et al. 1989, Spear et al. 1994). In the future, more robust forms of model-to-model comparison may be considered for TRIM.FaTE.

Sensitivity analyses are often used in performance evaluations to identify the part of the model that is actually being tested. Given the large number of inputs used in multimedia models such as TRIM.FaTE, it is not always obvious which processes and algorithms are participating in the calculation. TRIM features for uncertainty and variability analysis (see Chapter 3), standard sensitivity analysis methods, and regional sensitivity or parameter space analysis methods (Beck and Chen 1999, Spear 1997) may be used to understand and communicate the results from performance evaluations and to improve the ability to assimilate the results from all the evaluation efforts.

## 6.7 SUMMARY OF TRIM.FaTE EVALUATION ACTIVITIES

The TRIM.FaTE evaluation plan, as described in this chapter, includes a variety of activities designed to build consensus about the model's performance and increase acceptance of the model for its intended applications. A few of these activities have been completed, many are in progress, and several others are in the planning stages. Table 6-2 summarizes key elements of the evaluation plan by providing examples of TRIM.FaTE evaluation activities to date as well as examples of planned future activities.

## Table 6-2
## Summary of TRIM.FaTE Evaluation Activities

| Type of Evaluation | Evaluation Activity | Examples of Progress to Date | Examples of Future Plans |
|---|---|---|---|
| Conceptual Model Evaluation | Literature review | Extensive during model conceptualization and early development | Perform targeted reviews when adding or refining algorithms |
| | Model documentation | Status Reports and comprehensive TSDs in 1998 and 1999, presentations at scientific meetings | Update and expand documentation throughout development; develop user guidance |
| | Peer review of modeling concepts and approaches | Reviewed by SAB in 1998; full internal EPA review and SAB advisory in 1999 | Periodic internal and external peer review |
| Mechanistic and Data Quality Evaluation | Computer code verification | Extensive during development for Prototypes I to V and Version 1.0; performed review of LSODE; compared Prototype V and Version 1.0 results for some test cases; developed automated tests of internal functions for Version 1.0 | Complete comparisons between Prototype V and Version 1.0 results and reconcile any differences; develop and evaluate additional Version 1.0 internal tests |
| | Performance evaluation of process models that are components of TRIM.FaTE | Compared TRIM.FaTE to CalTOX output for nine "pseudochemicals" (*i.e.*, varying $K_{ow}/K_{aw}$) in a simple scenario (*i.e.*, air, water, soil); compared TRIM.FaTE to ISCST3 for air transport of mercury | Continue performance evaluation for process models (*e.g.*, particle/plant leaf algorithm, soil flux model) |
| | Comparison of alternative process models | Compared chemical flux across soil/air interface with results from Jury model; comparing chemical transfer from soil to root with physically based model | Compare $K_{oa}$ (*i.e.*, octanol/air partition coefficient) aerosol model with the Junge model; perform model-to-model evaluations for bioaccumulation in fish models |
| | Data acquisition and evaluation/ development and documentation of default input data | Compiled an initial set of data for test chemicals (phenanthrene, benzo(a)pyrene, mercury) and environmental settings | Continue data acquisition and evaluation (*e.g.*, other chemicals and environmental settings) |
| | Generic sensitivity analysis of input parameters | Some analyses of Prototypes I to IV; initial analyses to determine elasticities of >100 parameters for Prototype V using mercury case study | Assess the most influential input parameters as part of future evaluations and applications |

| Type of Evaluation | Evaluation Activity | Examples of Progress to Date | Examples of Future Plans |
|---|---|---|---|
| Structural Evaluation | Analysis of time step resolution and other time-related aspects of modeling as part of case study | Very limited analysis | Perform detailed analyses; characterize variance due to temporal resolution changes in inputs; ensure that time-averaged output sufficiently maps the temporally resolved output |
| | Analysis of varying spatial configurations as part of case study | Limited analysis for air component only | Perform detailed analyses to characterize how robust the model is to spatial configuration changes |
| | Analysis of changes in complexity | Compared TRIM.FaTE for a simplified mercury case study scenario with and without biota | Identify issues to be addressed when setting up the model for an application |
| Overall Performance Evaluation | Regional sensitivity analysis | None to date | Identify regions of parameter space that are critical to certain model outcomes as part of future evaluations and applications |
| | Model-to-model comparison | Compared early prototypes to CalTOX and SimpleBox; have begun comparisons with ISCST3/IEM2M for mercury case study | Complete ISCST3/IEM2M for mercury case study comparisons |
| | Comparison to monitoring data | Have begun multimedia comparisons for mercury case study | Complete mercury case study; identify other test chemicals and sites, as needed |

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# 7. TRIM.FaTE MERCURY CASE STUDY

As discussed in Chapter 6, systematic model evaluation is an important step in determining if a model performs as expected. Model evaluation activities have been undertaken for the TRIM.FaTE module starting with the early model prototypes and have included case studies with organic chemicals. Consistent with SAB recommendations, OAQPS has continued its model evaluation activities for TRIM.FaTE Prototype V. As described in Chapter 6, OAQPS is performing a variety of evaluation activities, including a case study for mercury at a chlor-alkali plant in the U.S. This case study, currently in progress, will begin with data quality, mechanistic, and structural evaluations, which will improve understanding of the most important model processes and inputs and of the effects of varying the model's spatial and temporal resolution. After gaining an understanding of and confidence in the model's structure and performance, the case study will proceed to compare TRIM.FaTE outputs with environmental and biotic measurement data for the selected site as well as with outputs from other models. The case study site and conditions also serve as the basis for extensive testing, troubleshooting, and sensitivity analysis of TRIM.FaTE. This chapter provides summary information on the mercury case study, including the study objectives, information on selection of the study chemical and test site, and an overview of the evaluation activities. In the future, EPA may perform additional case studies and apply TRIM.FaTE to other chemicals (*e.g.*, dioxins) and other locations.

## 7.1 OBJECTIVES

The specific objectives of the TRIM.FaTE mercury case study are three-fold:

1. Demonstrate that TRIM.FaTE can be used effectively for metals and other inorganic chemicals;

2. Demonstrate that TRIM.FaTE can account for reversible transformation of chemicals and can track the environmental fate of transformation products; and

3. Test TRIM.FaTE and compare the results with measured data, as well as against modeled results from IEM2M (EPA's Indirect Exposure Methodology, as modified for mercury and applied in the *Mercury Study Report to Congress* (U.S. EPA 1997a)).

**MERCURY**

Mercury is one of the 188 HAPs listed under section 112(b) of the CAA, is one of 33 HAPs being addressed by the Integrated Urban Air Toxics Strategy under section 112(k) (U.S. EPA 1999e), is a pollutant of concern under the section 112(m) Great Waters program (U.S. EPA 1999b), and is one of the seven specific pollutants listed for source identification under section 112(c)(6). In addition, the findings of the *Mercury Study Report to Congress* (U.S. EPA 1997a) indicate that mercury air emissions may be deposited to water bodies, resulting in mercury uptake by fish. According to that report, ingestion of mercury-containing fish is a critical environmental pathway of concern for mercury-related health effects in humans, particularly developmental effects in children.

## 7.2 CASE STUDY CHEMICAL SELECTION

As part of the evaluation process for TRIM, EPA must test TRIM.FaTE with both organic and inorganic pollutants because of their distinctly different multimedia fate and transport properties. The EPA selected PAHs for an organic chemical test case, and the methodology and results of that testing were reported in the *1998 TRIM Status Report* (U.S. EPA 1998e). The Agency selected mercury as an inorganic chemical for testing TRIM.FaTE because of its fate and transport properties (*e.g.*, transformation to multiple chemical species), the concern for multipathway exposure (particularly through ingestion of fish), and the potential health effects associated with exposure.

## 7.3 CASE STUDY SITE SELECTION

After selecting mercury for this case study, the Agency evaluated different stationary sources of mercury that are significant on a national basis. The four types of stationary sources with the highest total national air emissions of mercury, based on the findings of the *Mercury Study Report to Congress* (U.S. EPA 1997a), are – in order of highest to lowest mercury emissions – electric utility plants, municipal waste combustors, medical waste incinerators, and chlor-alkali plants. Electric utility plants, which are addressed in section 112(n) of the CAA, are still undergoing evaluation by EPA for possible regulation of mercury air emissions. For municipal waste combustors and medical waste incinerators, national air emission standards have been promulgated under section 129 of the CAA, and these standards are expected to result in large reductions of mercury air emissions.

Chlor-alkali plants were selected for further assessment in the TRIM.FaTE case study because they are a large source of mercury air emissions and are not yet regulated for HAP emissions. In addition, these plants are more likely than other major mercury emission sources to pose localized health concerns as a result of their lower stack heights and relatively high estimated level of fugitive emissions.

The Agency selected a single chlor-alkali plant for the mercury case study after evaluating data availability for several sites. At the time of the site selection, 14 chlor-alkali plants were in operation in the United States. Mercury air emission estimates were available for all 14 plants; however, data on mercury levels in environmental media and biota were available for only two of the plants. Fish tissue, water quality, and air quality data had been collected for one of the two plants, but ultra-clean techniques were not used for collecting and analyzing the water samples. For the second plant, air quality, soil, fish tissue, sediment, and additional biotic data had been collected and analyzed. In addition, accumulation of mercury in environmental media and biota near the second plant was possible because the plant has been in operation since 1967. Because the data set for the second plant was more complete, of higher quality, and readily available for use, that chlor-alkali plant was selected for the mercury case study. A simplified map of the site area showing delineation of the parcels used for the case study is provided in Figure 7-1 (for a

general discussion of the process of defining parcels, volume elements, and compartments for a TRIM.FaTE application, see Chapter 5 of TRIM.FaTE TSD Volume I).[1]

## 7.4 CASE STUDY EVALUATION ACTIVITIES

As part of the TRIM.FaTE mercury case study, several different types of analyses are being performed that correspond with the types of evaluations (i.e., mechanistic and data quality, structural, performance) described in Chapter 6. These analyses are described below. The model input values being developed for the TRIM.FaTE mercury study are documented in Appendix C. Some of these values will likely be revised over the course of the case study as better information is acquired.

### 7.4.1 MECHANISTIC AND DATA QUALITY, AND STRUCTURAL EVALUATIONS

Evaluating the quality of the input data for a given model application is an iterative process. A literature search is completed to determine the value and identify any available information on the predicted uncertainty or variability associated with that value. The current values resulting from our search are listed in Appendix C. Then, a sensitivity analysis will be performed for all of the parameters to evaluate how the uncertainty in an input value influences the model output. If a model input is very uncertain and this uncertainty significantly influences the model output, more research may be completed to refine that input value. Additionally, the stage 2 Monte Carlo analysis (described in Chapter 3 of this report and Chapter 6 of TRIM.FaTE TSD Volume I) will be performed on these critical input parameters.

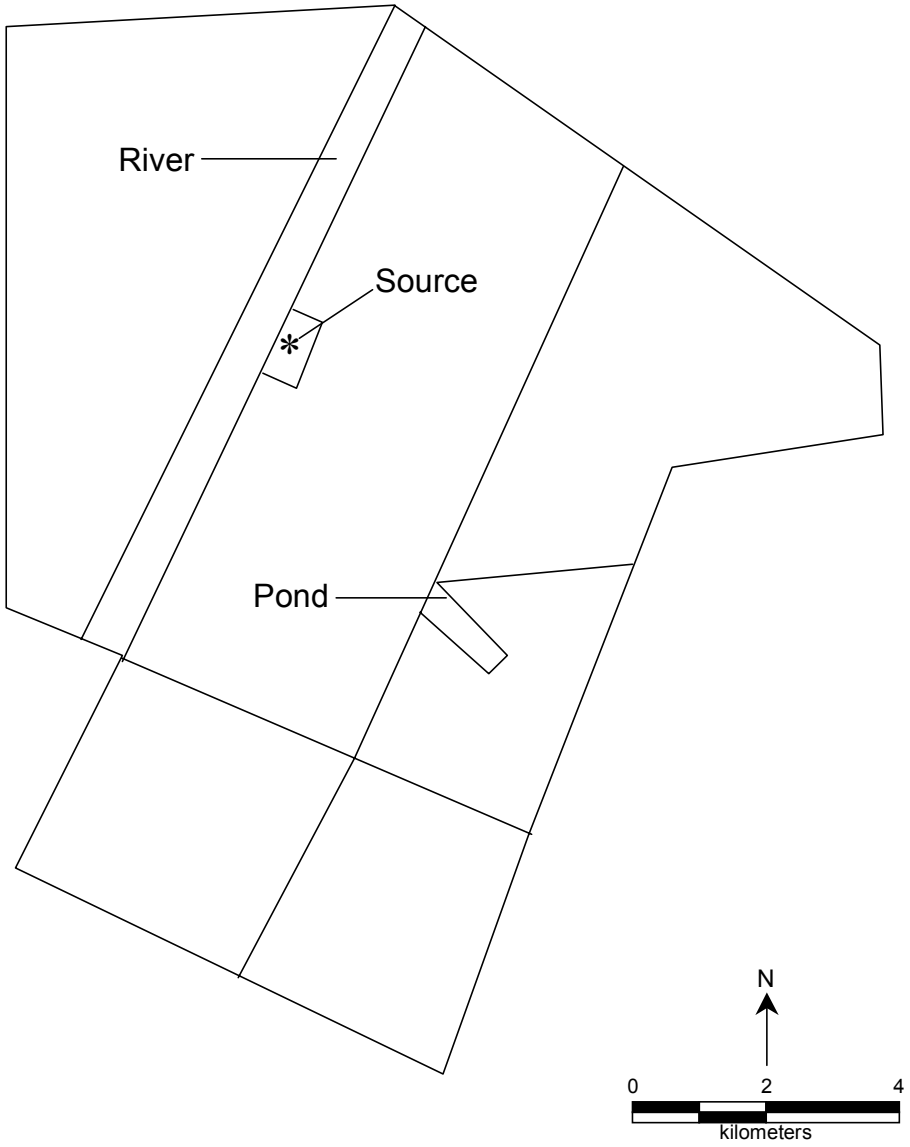
Evaluating the model's internal mechanisms (*i.e.*, mechanistic evaluation) involves assessing selected chemical fate and transport algorithms used in the model. In addition to assessing selected components of the model, intermediate processes, such as flows between compartments, will be assessed to ensure that the model accurately represents the current understanding of physical and chemical processes. It also must be confirmed that the algorithms work effectively together within the model. Because of the number of compartment types and links included in TRIM.FaTE, this will be a complex process.

One mechanistic evaluation being performed is a comparison of the TRIM.FaTE air component with a commonly used EPA air dispersion model, ISCST3 (U.S. EPA 1995c). Specifically, the concentration and deposition results from ISCST3 are being compared to the concentrations and total deposition fluxes estimated for the air compartments in TRIM.FaTE to provide insight into how the methodology for modeling transport and fate in TRIM.FaTE compares to the conventional Gaussian plume methodology used in ISCST3.

Another type of evaluation being performed in the TRIM.FaTE mercury case study is an assessment of the influence of the structural representation of the system being modeled. Some of the key assumptions in any TRIM.FaTE application, including this case study, involve

[1] While the case study site is a real facility and site-specific data are being used to the extent available, the name and location of the site are being kept confidential.

**Figure 7-1**
**Simplified Parcel Layout for TRIM.FaTE Mercury Case Study**[2]




[2] This diagram shows the initial set of surface water (*i.e.*, river, pond) and soil (*i.e.*, all other) parcels for the TRIM.FaTE mercury case study; the air parcels are slightly different. The Agency also plans to use more complex parcel layouts as the case study progresses.

determination of the simulation time step, the background and boundary concentrations, the spatial representation of the modeled system, and the compartment types selected for modeling. Examples of structural evaluation include the following:

- **Understanding the effect of temporal variability,** by assessing the impact of the temporal resolution of the meteorological and source emissions data on model outputs;

- **Understanding the effect of spatial configuration,** by comparing results obtained using a variety of spatial layouts; and

- **Determining the effect of external boundaries on internal compartments,** by assessing, for example, whether wind direction changes result in elevated concentrations in the air advected back into the system.

After the mechanistic and data quality, and structural evaluations are performed for the case study site, and greater understanding of and confidence in the model has been gained, the performance evaluation will begin.

### 7.4.2 PERFORMANCE EVALUATION

Model performance evaluation, as described in Chapter 6, can include comparisons of model outputs to outputs from other models and to available measurement data for a specific site. Both types of performance evaluations will be performed as part of the TRIM.FaTE mercury case study.

#### 7.4.2.1 Comparison with Other Models

The objective of this part of the case study is to model environmental media and biota concentrations of mercury using ISCST3 and IEM2M for comparison to the fate and transport results from the TRIM.FaTE simulations. These models were selected as comparison benchmarks because they (or in case of IEM2M, the core model from which it was derived, IEM; see Section 2.1 of TRIM.FaTE TSD Volume I for more discussion of IEM) have been extensively reviewed and widely used by EPA to estimate air and multimedia fate and transport of air toxics for regulatory applications. Furthermore, IEM2M was applied previously by OAQPS in the *Mercury Study Report to Congress* (U.S. EPA 1997a). When possible, the inputs used for ISCST3/IEM2M will be identical to the TRIM.FaTE inputs in order to provide results that are most appropriate for comparison. In some cases, such as the spatial representation of the modeled system, this will not be possible because of fundamental differences in modeling approaches, and assumptions will be necessary to maximize the similarities between the models as applied.

Annual average air concentrations and deposition rates predicted by ISCST3 will be used as the chemical source inputs to the IEM2M fate and transport algorithms. Environmental media and biota concentrations predicted by IEM2M will be used for comparison to the corresponding TRIM.FaTE outputs. They also will be compared to a second set of TRIM.FaTE outputs generated using ISCST3 results as inputs instead of the built-in TRIM.FaTE air component. The

fate and transport of three forms of mercury (*i.e.*, elemental, divalent, and methylmercury) will be tracked and compared. Because mercury speciation affects its fate and transport properties and because the speciation of the chlor-alkali source emissions is not known with certainty, two sets of simulations will be performed: (1) assuming that source emissions are composed of 100 percent elemental mercury (in gaseous form), and (2) assuming that source emissions are composed of 70 percent elemental mercury (in gaseous form) and 30 percent divalent mercury (in particulate form).

#### 7.4.2.2 Comparison with Measurement Data

The objective of this part of the case study is to model environmental media and biota concentrations of mercury for the test site and compare the modeled outputs to the available monitoring data. Comparisons of multimedia model results to monitoring data are challenging because it is difficult to match modeling conditions to site conditions. However, these comparisons are useful analyses in the early stages of model evaluation and may lead to diagnostic assessments.

The parcels being modeled for the test site were constructed, in part, based on the available monitoring data so that data comparisons would be most relevant and meaningful. The results (*i.e.*, concentrations in environmental media and biota) from the TRIM.FaTE simulations will be compared to available measurement data for the chlor-alkali plant vicinity. Appendix D provides details on the abiotic and biotic monitoring data sets that are available for use in the TRIM.FaTE mercury case study. For each data set, Appendix D includes the following information: environmental medium, number of data points (including the number of duplicates and measurements below the detection limit), measurement endpoint(s) and units, sampling date(s), sample location(s), purpose of monitoring, range of values, mean and standard deviation of values, and other information (if relevant).

Some of the monitoring data sets are from on-site sampling that was conducted as part of site investigations in 1995 and 1997. In many cases, the on-site data sets also include at least one measurement from an off-site reference location. Most of the sample collection and analysis for the site investigations was performed by a contractor or by the facility. Several of the on-site sediment and surface water data sets that were available are not summarized in Appendix D because the data appear to represent mercury concentrations in waste streams, rather than mercury in the environment as a result of air emissions. There are also data sets from off-site locations, including additional data collected during the site investigations and data collected by independent researchers during monitoring efforts not related to the facility. Most of the available measurement data, however, are for total mercury, rather than being speciated into the various forms, which will limit direct comparisons to the speciated mercury results from TRIM.FaTE.

The abiotic environmental media data sets include both on-site and off-site monitoring data sets. The on-site monitoring data sets include five data sets for surface and subsurface soil measurements from various locations. The off-site monitoring data sets include ambient air mercury concentration measurements from three monitors within 7,000 feet of the facility;

surface water measurements from the adjacent river both downstream and upstream of the facility; and sediment measurements from four nearby ponds and lakes.

The biotic data sets also include on-site and off-site monitoring data sets. Deer mouse and earthworm tissue measurements from a variety of locations comprise the on-site data. Off-site data sets include various mercury concentration measurements in loons, including local level (*e.g.*, juvenile blood concentrations, adult male blood concentrations, egg concentrations from nearby ponds) and state level (*e.g.*, state average and individual site-specific juvenile, male adult, and female adult blood concentrations; state average egg concentrations) data. The off-site data sets also include measurements of mercury concentrations in skinless fillets of white perch from nearby ponds; mercury concentrations in short-tailed shrew tissues; mercury concentrations in eel tissues from the adjacent river; and a single measurement of the mercury concentration in a river minnow from the adjacent river. For full details on each of these on-site and off-site data sets, refer to Appendix D.

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# 8. DEVELOPMENT OF TRIM.Expo

The TRIM.Expo module of TRIM is an exposure-event model that is being developed to assist in assessing health risks related to chemical exposures. The exposure assessment process consists of relating chemical concentrations in environmental media (*e.g.*, air, surface soil, root zone soil, surface water) to chemical concentrations in the exposure media with which a human population has contact. This model uses concentrations of chemicals in different environmental media over time to provide information such as the number of individuals in a population that are exposed to various levels of chemicals over various time periods of interest. The TRIM.Expo module can function as an integral part of TRIM, using the output data from TRIM.FaTE as input data, or it can function independently of TRIM, using other environmental fate models or monitoring data as input data.

## 8.1 PURPOSE OF DEVELOPING TRIM.Expo

The TRIM.Expo module is intended to contribute to a number of health-related assessments, including risk assessments and status and trends analyses. The TRIM.Expo module, like most exposure models, provides a key step in the analysis of the link between various chemical sources and potential human health risks. Multiple sources of environmental contamination lead to multiple contaminated media, including air, water, soil, food, and dust. When considering human exposure, it is necessary to focus on the more immediate contact or exposure media, which include the envelope of air surrounding a human receptor, the water and food ingested, and the layer of soil and/or water that contacts the skin surface. The magnitude and relative contribution of each exposure pathway must be considered to assess the total exposure of a particular chemical to humans.

**EXPOSURE**

Exposure is the contact between a target organism and a pollutant at the outer boundary of the organism, quantified as the amount of pollutant available at the boundary of the receptor organism per specified time period. As an example, inhalation exposure over a period of time may be represented by a time-dependent profile of the exposure concentrations.

Human exposures to air pollutants can result from contact with contaminated air, water, soil, and food. Such exposures may be dominated by contact with a single environmental medium or may reflect concurrent or successive contacts with multiple media. The nature and extent of such exposures depend largely on two elements: (1) human factors and (2) the concentrations of a chemical in the exposure 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 include contact rates with food, air, water, and soil. Activity patterns, which are defined by an individual's or a group of people's allocation of time spent participating in different activities at various locations, are also significant because they directly affect the magnitude of exposures to substances present in different indoor and outdoor environments. The information on activity patterns is taken from measured data collected during field surveys of individuals' daily activities, the amount of time

spent engaged in those activities, and the locations where the activities occur. Therefore, from an exposure assessment standpoint, the principal goal is to estimate or measure an individual's or group's exposure as a function of relevant human factors and the measured and/or estimated chemical concentrations in the contact or exposure media. This is a challenge due to the paucity of information regarding many of the human factors that affect exposure. Therefore, a tiered approach is being used for the initial development of TRIM.Expo. Specifically, model development is being focused on applications where the input parameters are most critical and where input data exist.

With respect to population groups, the exposure-event module within TRIM.Expo uses the concept of a cohort. Cohorts are subsets of a population grouped so that the variation of exposure within a cohort is much lower than the variation between or among cohorts. This approach is used because available data are not adequate to estimate the exposure of each individual in a population; therefore, information about people who are expected to have similar exposures is aggregated together to make more efficient use of the limited data. The cohorts are assumed to include individuals with exposures that can be characterized by the same probability distribution for key characteristics. The demographic variables used to describe a cohort are selected to minimize the differences between individuals within the cohort. The model selects an individual from the appropriate cohort and uses that individual's activity pattern data to create an exposure-event sequence for that day. Currently, TRIM.Expo accounts for variability within a cohort through multiple runs of the model for the exposure duration under study. As new statistical techniques are developed, future versions of TRIM.Expo will be modified to use the best available approaches for characterizing time/activity pattern data. At the present time, however, the current method of using cohorts is a useful technique for modeling the exposures of a large population in the absence of adequate time/activity pattern data (see the TRIM.Expo TSD for a more detailed discussion on cohorts).

The TRIM.Expo module was designed to allow flexibility in the user's ability to select a cohort's characteristics. The demographic variables (*e.g.*, age, gender, work status) that characterize a cohort can be modified by a user of TRIM.Expo providing that there are data available. Hence, the cohorts' characteristics can be chosen for individualized studies on a site-specific or case-specific basis.

Using exposure modeling approaches instead of exposure monitoring studies has several advantages: (1) direct monitoring of the exposure of humans to chemicals (*i.e.*, personal exposure monitoring) is expensive, and (2) direct monitoring of exposures resulting from large numbers of pollutants can present large logistical and analytical difficulties. Therefore, OAQPS has determined that exposure modeling, such as using TRIM.Expo, is useful for estimating exposures to air pollutants and may be used in conjunction with limited personal exposure monitoring data.

## 8.2 OVERVIEW OF TRIM.Expo

Emissions of chemicals to air can (depending on the characteristics of an individual chemical) lead to contamination of multiple environmental media, including ambient outdoor air, indoor air, surface and ground water, soil, food, and dust. The more immediate contact or exposure media, which include the envelope of air surrounding a receptor, the water and food

ingested, and the layer of soil and/or water that contacts the skin surface, should be the main focus of an exposure assessment. Furthermore, the magnitude, duration, and frequency of exposures via each exposure route (inhalation, ingestion, or dermal contact) must be considered to assess the aggregate exposure to a particular chemical.

As shown in Figure 8-1, the TRIM exposure assessment process consists of relating chemical concentrations in environmental media (*e.g.*, air, surface soil, root zone soil, surface water, vegetation, ground water) to chemical concentrations in the immediate exposure/contact media with which a human population has direct contact (*e.g.*, personal air, tap water, foods, house dust, soil). The TRIM.Expo module simulates the movement of an individual and/or a subset of the human population (*i.e.*, a cohort) according to activity patterns, through locations (*i.e.*, microenvironments) of varying chemical concentrations, thus allowing the estimation of exposures to the various cohorts within the population.

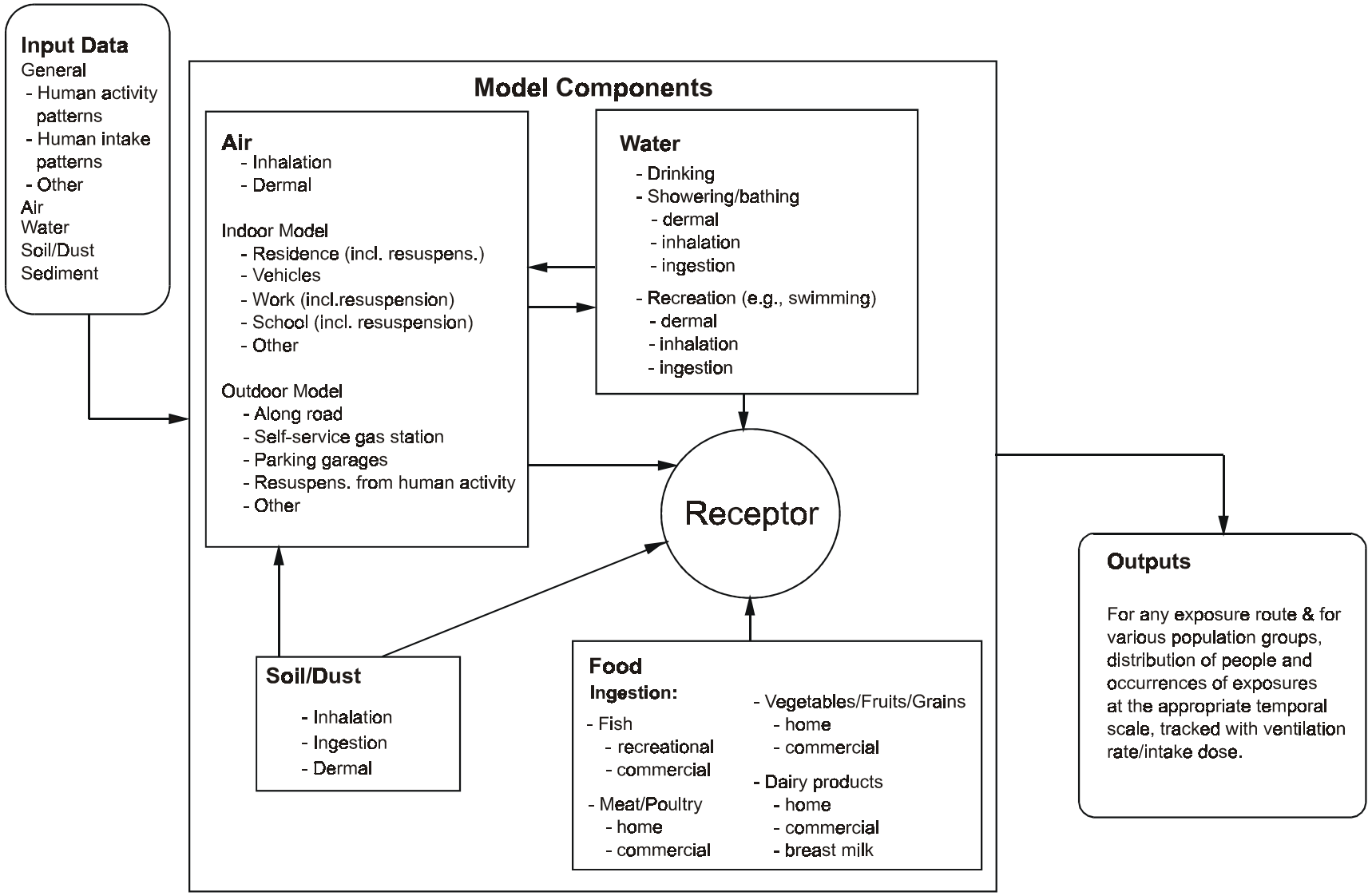
In a typical TRIM application, TRIM.FaTE data may be used to provide an inventory of chemical mass across an ecosystem for selected time steps (*e.g.*, hours, days, years), or monitoring data may be substituted for TRIM.FaTE data. Alternatively, concentration estimates from an air dispersion model may be used if inhalation is the only exposure route of interest and either (1) the chemical is not persistent, or (2) the impacts of only current emissions are of interest. The TRIM.Expo module uses these data, combined with the characteristics and movements of individuals and/or cohorts, to estimate exposures. The movements are defined through a sequence of exposure events that corresponds to the time steps modeled by TRIM.FaTE. Each exposure event places the individual or cohort in contact with one or more of the exposure media for a specified time. Besides the individual's or cohort's sequence of locations, other characteristics that relate to exposure and uptake, such as the respiration rate or the water consumption rate, are also tracked over time.

Current development of TRIM.Expo includes incorporation of the Probabilistic National Ambient Air Quality Standards Exposure Models (pNEM) (Johnson et al. 1992, Johnson et al. 1999) and Hazardous Air Pollutant Exposure Model (HAPEM4)[1] into the TRIM.Expo platform for short-term and long-term inhalation exposures, respectively; incorporation of ingestion algorithms based on the EPA Indirect Exposure Methodology (IEM)[2] (U.S. EPA 1999d) and the California Total Exposure Model for Hazardous Waste Sites (CalTOX) (McKone 1993a, McKone 1993b, McKone 1993c); and the performance of test cases for inhalation and ingestion pathways. These test cases will undergo an SAB review.

[1] The development and testing of HAPEM4 were recently completed. The developers are in the process of producing a report and accompanying Programmer and User Guides.

[2] The EPA now refers to this as Multiple Pathways of Exposure (MPE) methodology.

**Figure 8-1**
**Conceptual Diagram of TRIM.Expo**



## 8.3 CONCEPTUALIZATION OF TRIM.Expo

The TRIM.Expo module is built around the concept of simulating a series of exposure events. Exposure events are human activities that bring individuals in contact with a contaminated exposure medium within a specified microenvironment at a given geographic location. In TRIM.Expo, exposure of each individual or cohort is determined by a sequence of exposure events specific to the individual or cohort. The exposure-event sequence is a chronologically-ordered series of events that identifies the locations and amount of time spent in those locations. Each exposure-event sequence consists of a series of events with durations ranging from one to 60 minutes. Each exposure event assigns the cohort to a particular combination of exposure district, microenvironment, and activity (*e.g.*, cooking, playing, resting). An exposure district is a geographic location within a defined physical or political region, where there is potential contact between an organism and a pollutant, and for which environmental media concentrations have been estimated either though modeling or measurement. A microenvironment is a location defined by a specific chemical concentration where exposure may occur. The following important attributes of an exposure event are used to estimate the corresponding exposure concentrations and potential doses:

- Chemical concentration in an environmental medium (*e.g.*, ambient outdoor air, surface water, soil);
- Any significant intermedia transfer to the exposure medium (*e.g.*, from soil to house dust to air in an indoor microenvironment);
- Chemical concentration in an exposure medium (*e.g.*, personal air, tap water);
- Duration of contact with the exposure medium;
- Number of contacts with the exposure medium; and
- Time scale of interest.

The TRIM.Expo algorithms will use this information to estimate the exposure concentration at each time step to create an exposure time series or profile. By combining the exposure concentration and the breathing rate at each time step, TRIM.Expo will also create a potential dose profile. Depending upon the health effects associated with the chemical of interest, the exposure and potential dose profile may be used to derive several metrics, such as the number of person-hours of exposure to concentrations above a threshold value, the sum of the concentrations that exceed a threshold value, the average of concentrations that exceed a threshold value, or the maximum concentration corresponding to an averaging time of interest for the simulation period.

## 8.4 FUNCTIONAL ATTRIBUTES OF TRIM.Expo

The goal of the TRIM project is to develop a framework that is scientifically defensible, flexible, and user-friendly; that can address the broad range of risk assessments required under the various CAA programs/provisions; and that supports the regulatory decision-making process for these programs. TRIM is intended to be part of a new generation of environmental risk and exposure models for OAQPS. It will eventually be a predictive environmental model of chemical transfers to human health endpoints that is flexible and applicable to both criteria pollutants and HAPs, while incorporating multimedia, multipathway estimates of exposure and dose. To be successful, TRIM must address the wide range of spatial and temporal scales, endpoints, and pathways of interest to specific CAA programs. To meet these goals, TRIM.Expo will include the following functional attributes:

- Indoor and outdoor environments;
- Indoor and outdoor sources;
- Portable, modular, and flexible algorithms;
- Explicit treatment of uncertainty; and
- Explicit treatment of variability.

### 8.4.1 DIMENSIONS OF THE EXPOSURE ASSESSMENT PROBLEM

Three important dimensions of the exposure assessment problem are considered: (1) the route of exposure, (2) the time scale of an exposure event relevant to the pollutant's associated effects, and (3) dependence of exposure on the location of the exposed subject (*i.e.*, how strongly or weakly dependent is exposure on the location of the exposure subject?). Addressing these three issues has the greatest impact on the structure of the exposure model (*e.g.*, on the exposure media included, the degree of spatial resolution, and the level of temporal and spatial aggregation). For example, consider a model used to assess inhalation exposures to chemicals with health effects that depend on the number and duration of contacts above a threshold concentration. This model requires a compilation of short-term exposure events and must provide relatively detailed information on the location of the exposed individual. In contrast, an exposure model used to assess ingestion contact with a chemical that has health effects that depend primarily on the lifetime cumulative intake of that chemical would require much different temporal and spatial detail about the exposed individuals. In this case, rather than tracking the detailed time/location profile of the exposed cohort, it is more important to know the location of the exposed cohort's food or water supply and the cumulative intake of food or water from a specific supply.

The primary routes of exposure to environmental chemicals are inhalation, ingestion, and dermal contact. The primary time scales for exposure assessment models vary from short-term resolution (*e.g.*, minutes to hours and days) to long-term resolution (*e.g.*, days to months and years). Short-term resolution allows for the assessment of both cumulative intake and the number and duration of peak exposure events. Long-term resolution allows primarily for the assessment of cumulative intake. The quantitative distinction between short-term and long-term depends to some extent on the pharmacokinetics (*i.e.*, uptake and distribution) and toxicokinetics of the chemical substance. Location dependence specifies the level of detail required for the

time-activity budget of an exposed individual. For example, to address inhalation exposures where chemical concentration varies significantly from among several districts in which the exposed cohort lives and differs strongly between indoor and outdoor microenvironments, location dependence is high. But, if the properties of the chemical are such that concentrations are similar in almost all microenvironments, location dependence is lower. For ingestion exposures to a chemical in ground water that is distributed throughout a region, the location of the exposed cohort is much less important than the source of the cohort's drinking water.

Three primary attributes are used to describe an exposure problem using TRIM.Expo: (1) exposure route, (2) exposure time scale, and (3) the degree of location dependence. This set of attributes gives rise to a broad set of exposure problems, such as short-term inhalation exposure with strong location dependence, long-term ingestion exposure with weak location dependence, and short-term dermal contact exposure. The general exposure-event function used in TRIM.Expo has a form that can be adapted across the broad range of problems defined by these attributes. In some situations, aggregating among two or more sets of exposure model attributes may be necessary (*i.e.*, combining long-term ingestion exposures that are weakly location dependent with short-term inhalation exposures that are strongly location dependent). The TRIM.Expo module is designed to make such aggregation possible.

### 8.4.2 DESIGN FEATURES OF TRIM.Expo

Although exposures to some types of exposure media, such as commercial foodstuffs, are not location or time dependent, most of the chemical exposures addressed by TRIM.Expo are associated with particular locations. Also, because of spatial and temporal differences in contamination of exposure media, tracking the locations and activities of individuals or cohorts through time and space to estimate their exposure is important. This requires methods for logging both time-activity-specific locations of individuals or cohorts and the time-specific concentrations of chemicals in relevant exposure media. The process of combining these three different types of information (*i.e.*, location, activity, and concentration) is the *exposure characterization process*. The exposure characterization process can be short-term (*i.e.*, over hours or days) or long-term (*i.e.*, over months or years). The critical issue of the exposure characterization process is to identify appropriate and transparent methods to combine concentration information with activity tracking (*i.e.*, tracking locations and activities at different times) to assess short- and long-term exposures. To develop the exposure characterization process for TRIM.Expo, the following attributes that define an exposure event were identified and ranked:

- Route of exposure;
- Time/space scale of the chemical concentration;
- Time scale of the health effects;
- Duration of the exposure event;
- Contributing environmental medium;
- Exposure medium; and
- Demographic characteristics of the exposed individual (*e.g.*, age, gender).

The route of exposure refers to the way the chemical can enter the receptor during the exposure event (*i.e.*, by inhalation, ingestion, or dermal uptake). The route of potential uptake (*i.e.*, absorption into the body) is a very important attribute of an exposure event. The health effects of an exposure may vary significantly among these three routes. Both the exposure medium and exposure-related activity are often strongly associated with a particular intake route. For example, air is associated with the inhalation route, and the inhalation rate varies significantly with activity location. Water, food, and soil are associated with the ingestion route and with eating and hand-to-mouth activities.

The time scale and spatial scale of the chemical concentration variation provide critical insight on time and space resolution needed in constructing an exposure event. If a chemical shows little spatial variation in concentration over a large region, even if the concentrations vary with time, there is little need for large numbers of geographic regions in an assessment. Similarly, for a chemical whose concentrations do not vary significantly in time, even if they show large spatial variation, using longer time steps may be possible than that needed for a chemical whose concentrations vary more quickly in time. However, the time scale of exposure associated with health effects for a particular pollutant also strongly effects the temporal resolution required of the exposure-event model. Some chemicals, such as most of the criteria air pollutants, require the estimation of the number and duration of peak exposure events. For hazardous air pollutants with acute health effects, exposures may need to be aggregated over periods as short as one hour or less. For many hazardous air pollutants, only long-term cumulative exposure may need to be characterized.

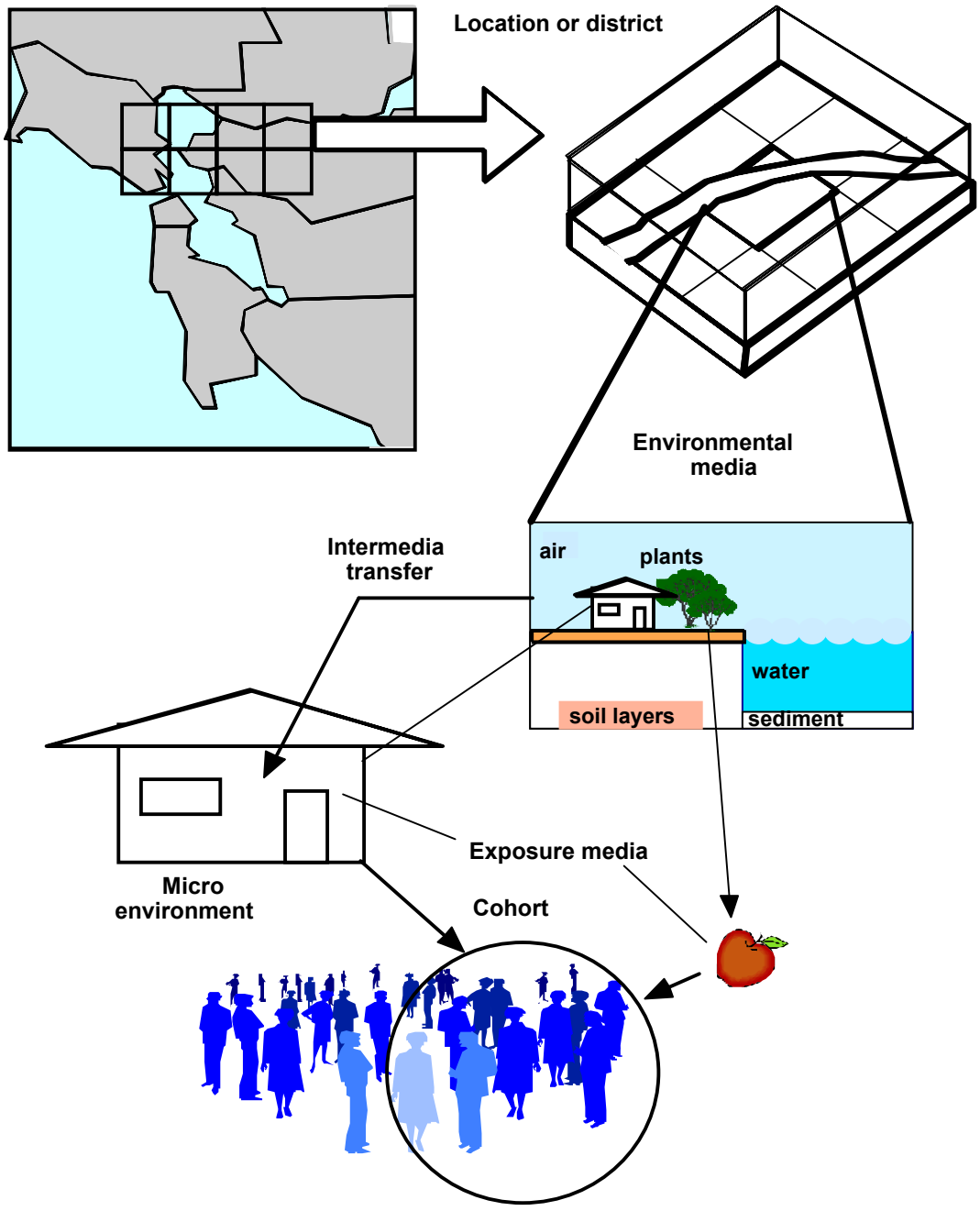
The durations of the exposure events and human activities are important considerations in the structure of the exposure-event model. Other factors that affect the structure of the exposure-event model are the demographic characteristics of an exposed individual or population group, such as age or gender, that may influence both their activity pattern and their health response to exposure. Other characteristics, such as proximity to particular emission sources or health status, also may be important. The interconnected nature of the relationships among the locations, microenvironments, environmental media, intermedia transfers, exposure media, and cohorts within TRIM.Expo is illustrated in Figure 8-2.

## 8.5 APPROACH USED IN DEVELOPING TRIM.Expo

The TRIM.Expo module will model exposures from the inhalation, ingestion, and dermal contact routes. For the first prototype, however, the exposure routes are limited to inhalation and ingestion. Dermal contact will be addressed as a longer-term goal of TRIM.Expo.

The TRIM.Expo TSD includes a comprehensive discussion of currently available exposure models. These models were reviewed to determine whether they would be suitable for the exposure modeling needs of OAQPS. Although no single model or set of models has been identified that meets all the requirements for the exposure modeling needs of OAQPS, many of the concepts and components developed for existing models have been used in TRIM.Expo. For the inhalation pathway, the structure from EPA's pNEM/CO (probabilistic NAAQS Exposure Model for Carbon Monoxide) and HAPEM4 models

**Figure 8-2**
**Relationships Among Locations, Microenvironments, Environmental Media, Intermedia Transfers, Exposure Media, and Cohorts**



have been adopted for short-term and long-term exposures, respectively. These constructs use activity patterns to track population groups/cohorts as they move among exposure media. The pNEM/CO model also includes a mass balance treatment of the relationship between the environmental medium (*i.e.*, outdoor air) and the exposure medium (*i.e.*, indoor air), as well as the characterization of uncertainty and variability. For the ingestion pathway, algorithms from EPA's IEM and CalTOX have been adopted. The CalTOX model can model multimedia transport and transformation of chemicals, and multipathway exposure for humans. The IEM incorporates current EPA guidance for addressing exposures via inhalation, ingestion, and dermal contact.

## 8.6 SUMMARY REVIEW OF EXISTING EXPOSURE MODELS AND THE UNIQUENESS OF TRIM.Expo

This section provides a brief review of currently available and emerging exposure modeling approaches. The Agency critically evaluated each of the exposure models described in this section, assessing their strengths and limitations. Based on this review, none of the models adequately meets the modeling needs of OAQPS (see Chapter 1 for a discussion of OAQPS' needs). The review in this section, however, highlights the unique features of these models that can be included in TRIM.Expo to meet the modeling needs.

### 8.6.1 OVERVIEW OF CURRENT MODELS

In general, the models that most closely meet the design goals for TRIM.Expo development are the focus of this section. These include models that can calculate short-term exposures (*i.e.*, one hour or shorter) and that can be adapted to evaluate long-term exposures as well. The models should also be able to explicitly treat variability and uncertainty. Other desirable model attributes meeting OAQPS' needs are the inclusion of multiple media, the use of a mass balance approach for estimating indoor air concentrations, and the ability to track exertion rates concurrent with exposure. For inhalation, this means providing estimates of the respiration rate (also called the ventilation or breathing rate) for various activities. Additional useful features include accounting for indoor air emission sources and the ability to include geographic mobility (*e.g.*, commuting) in the exposure simulation.

The development of TRIM is designed to focus on the processes that have the greatest impact on chemical fate and transport and on human exposure. To have the same scientific basis as the rest of the TRIM system, TRIM.Expo needs to incorporate the same attributes, including (1) mass conservation; (2) the ability to characterize uncertainty and variability; (3) the capability to assess multiple chemicals, multiple media, and multiple exposure pathways; and (4) the ability to perform iterative analyses at varying levels of complexity. Hence, these four design attributes are the basis for critically comparing the strengths and limitations of current exposure models and for determining the features that will be used in TRIM.Expo development.

No single model exists that can meet all of the needs of OAQPS for a multimedia, multichemical exposure model. However, several models use methodologies that can be adopted in the development of TRIM.Expo. One model that has many of the desirable attributes is the pNEM/CO (Johnson et al. 1992, Johnson et al. 1999). Although this model is for a single

medium only (*i.e.*, air), it incorporates many of the features needed for the inhalation component of TRIM.Expo. The pNEM/CO benefits from having most of its input variables chosen stochastically. This stochastic approach allows both variability and uncertainty to be incorporated into the model operation. The pNEM/CO treats human exposure as a time series of the convergence of human activities occurring in a particular microenvironment and air quality in those microenvironments. The model also is designed to provide estimates of the intake dose associated with exposures. In addition to the other criteria listed above, pNEM/CO is well documented and is already being used by OAQPS as an input to regulatory decision-making. Furthermore, the pNEM/CO has undergone review.

The disadvantages of the pNEM/CO model in its current form are that it is difficult to execute and cannot be readily updated and calibrated as more data becomes available. Furthermore, the pNEM/CO model, as with all of the pNEM models, is a single pollutant, single media model.

For modeling the non-inhalation routes of exposure, the CalTOX model, developed at the Lawrence Berkeley National Laboratory, includes many features needed for estimating indirect routes of exposure (McKone 1993a, McKone 1993b, McKone 1993c). The CalTOX model can calculate multipathway exposures for organic chemicals and some metals. In addition, the model is stochastic and can quantify the variability and uncertainty in the exposure calculations. The CalTOX model consists of two main components: (1) a multimedia transport and transformation model and (2) a multipathway human exposure model. The CalTOX model has 23 exposure pathways encompassing all three routes of human exposure, which are used to estimate average daily doses within a human population near a hazardous air pollutant release site. The exposure assessment process consists of relating contaminant concentrations in the multimedia model compartments to pollutant concentrations in the media with which a human population has contact (*e.g.*, personal air, tap water, foods, house dust). This provides explicit treatment of the differentiating environmental media pollutant concentrations and the pollutant concentrations to which humans are exposed. In addition, all input variables are taken from distributions that are provided with the model.

The CalTOX model is limited in the extent of the environmental settings for which it can be applied. For example, it has limited effectiveness for settings where there is a large ratio of surface water area to land area. In addition, it was developed for a limited range of pollutants (*i.e.*, only organic chemicals). As a result, CalTOX does not provide adequate flexibility in the environmental settings nor the chemical classes it models. Also, CalTOX does not allow spatial tracking of a pollutant, hence it is not directly applicable to the TRIM approach.

The Hazardous Air Pollutant Exposure Model (previously called the Hazardous Air Pollutant Exposure Model for Mobile Sources, or HAPEM-MS) has undergone many enhancements in recent years (Johnson et al. 1993, Palma et al. 1996). The latest version of the HAPEM is designated HAPEM4. It allows exposure to population cohorts to be simulated at the census tract level. This is a much finer spatial resolution than was previously possible with the model. It also means that calculation of population exposures no longer needs to rely solely on

data from fixed-site monitors. This is an important step in being able to estimate exposures to HAPs because widespread monitoring networks for these chemicals are not available.

The HAPEM4 calculates long-term average exposure concentrations in order to address exposures to pollutants with carcinogenic and other long-term effects. Thus, HAPEM4 does not preserve the time-sequence of exposure events when sampling from the time/activity database. This means that information to evaluate possible correlations in exposures to different pollutants due to activities that are related in time is not preserved. Also, the model does not include any measures of the ventilation rate associated with an activity, so that there is no ability to calculate the potential dose received when engaging in various activities.

The IEM includes fate and transport algorithms, exposure pathways, and exposure algorithms. It focuses on procedures for estimating the indirect (*i.e.*, non-inhalation) human exposures and health risks that can result from the transfer of chemicals from air to soil, vegetation, and water bodies. The IEM addresses exposures via inhalation, ingestion of food, water, and soil, and dermal contact. The methodology has undergone extensive scientific peer review.

The IEM has limitations, however, related to the design goals for TRIM. The methodology can be applied only to pollutants that are emitted to air. Another important limitation of IEM is that it does not provide a detailed time-series estimation of media concentrations and resultant exposures. Also, the methodology does not provide for the flexibility needed by OAQPS in site-specific applications or in estimating population exposures. Significant site-specific adjustments must be made to allow for spatially tracking the relationship between concentrations and exposures. Much of the focus of the methodology is on evaluating specific receptor scenarios (*e.g.*, recreational or subsistence fisher) that may be indicative of high-end or average exposures, but it does not readily allow for modeling the distribution of exposures within a population.

The models summarized in this section provide background information for some of the most commonly used exposure models currently available. More detailed information about these and the other exposure models that were evaluated can be found in the TRIM.Expo TSD.

### 8.6.2 RATIONALE AND NEED FOR DEVELOPING TRIM.Expo

The TRIM.Expo module is intended to contribute to a number of health-related assessments, including risk assessments and status and trends analyses. The TRIM.Expo module provides a key step in the analysis of the potential for various pollutant sources to contribute to human and ecological health risks. Multiple sources of environmental contamination can lead to multiple contaminated environmental media, including air, water, soil, food, and dust. When considering human exposure, it is necessary to focus on the more immediate contact or exposure media, which include(s) the envelope of air surrounding a human receptor, the water and food ingested, and the layer of soil and/or water that contacts the skin surface. The magnitude and relative contribution of each exposure pathway must be considered to assess the total exposure of a particular pollutant to humans.

The TRIM development is designed to focus on the processes that have the greatest impact on chemical fate and transport and on human exposure. Besides the four design attributes for TRIM.Expo (see Section 8.6.1), OAQPS determined that the model must also (1) address varying time steps (one hour or greater) and provide sufficient spatial detail at varying scales, (2) have the "transparency" needed to be practical to a large and diverse group of users, (3) be modular in design, and (4) be easily accessible.

The summary review of multimedia models presented here, and described in more detail in Chapter 3 and Appendix B of the TRIM.Expo TSD, showed that none of the currently available models offers all of the design features needed by OAQPS for multimedia exposure assessments. Although some models incorporate individual features, none of these, separately or in combination with other models, can function to provide an integrated system that meets the modeling requirements previously described. In addition, most models are limited in the type of media and environmental processes addressed. No model currently exists that addresses the broad range of chemicals and environmental fate and transport processes that are anticipated to be encountered by OAQPS and other stakeholders when evaluating the risks from the multitude of hazardous air pollutants and criteria air pollutants. Therefore, the developers of TRIM have constructed a new model framework that is distinct from the other multimedia models and unique among the current suite of EPA exposure models.

Another reason for developing TRIM.Expo is that none of the currently available exposure models that OAQPS investigated is a sufficiently integrated multimedia model that accounts for inherent "feedback" loops in the exposure continuum and that provides the temporal and spatial resolution needed for estimating human exposures. It is not known to what extent modeled exposure estimates would differ between the currently available models and a truly integrated multimedia exposure model. However, models that are not fully coupled have long been considered to lack scientific credibility. Therefore, OAQPS has determined that it is necessary to undertake efforts to develop a truly coupled multimedia exposure model.

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# 9. GENERAL DESCRIPTION AND CONCEPTUAL DESIGN OF TRIM.Risk

The National Academy of Sciences (NAS) has defined risk characterization as a description of the nature and magnitude of human or ecological risk and the attendant uncertainties (NRC 1983). Risk characterization is the final step in risk assessment and is primarily used to integrate the information from the other three key steps (*i.e.*, hazard identification, dose-response assessment, exposure assessment). Within the TRIM framework, the risk characterization module (TRIM.Risk) will be used to integrate the information on exposure (to human and ecological receptors) with that on dose-response or hazard and to provide quantitative descriptions of risk and the attendant uncertainties. The TRIM.Risk module will provide decision-makers and the public with information for use in developing, evaluating, and selecting appropriate air quality standards and risk management strategies. The sources of input data for TRIM.Risk can be other TRIM modules, including model assumptions, inputs, and results, or outside information sources or models.

## 9.1 BACKGROUND ON RISK CHARACTERIZATION

In general, the Agency's risk characterization guidance described below addresses two essential elements of a full characterization of risk. First, the characterization should address qualitative and quantitative features of the assessment. That is, in addition to quantitative estimates of risk, a full risk characterization should clearly describe (1) the hazard information and associated relevant issues, (2) the dose-response relationship used, and (3) what is known about the principal paths, patterns, and magnitudes of exposure. Furthermore, for each of these three items, the characterization should describe any assumptions, the rationale behind these assumptions, and the effect of reasonable alternative assumptions on the conclusions and estimates. The second essential element of a full risk characterization is the identification and discussion of any important uncertainties. As noted by the Agency's Deputy Administrator in issuing the Agency's initial risk characterization policy memo "... scientific uncertainty is a fact of life (and) ... a balanced discussion of reliable conclusions and related uncertainties enhances, rather than detracts, from the overall credibility of each assessment..." The uncertainty discussion is important for several reasons (Habicht 1992):

- Information from different sources carries different kinds of uncertainty, and knowledge of these differences is important when uncertainties are combined for characterizing risk, allowing for decisions to be made about expending resources to acquire additional information to reduce the uncertainties; and

- Uncertainty analysis provides the decision-maker and the public with clear and explicit statements of the implications and limitations of a risk assessment and of the related uncertainties.

Each step of the analysis phase of risk assessment (*i.e.*, hazard identification, dose-response assessment, exposure assessment) should include its own summary characterization section. Because every risk assessment has many uncertainties and involves many assumptions,

the challenge in characterizing risk for decision-makers, whose time is limited and who may not be risk experts, is to convey that small subset of *key* strengths and limitations that are crucial to the assessment outcome. When integrated, they identify the fundamental, irreducible set of key points that must be communicated to characterize adequately any risk assessment. Therefore, the risk characterization should provide the following:

- A clear description of the key strengths and weaknesses;
- A brief "bottom-line" statement about the risks, including the assessor's confidence in any estimate(s) of risk and in the conclusions; and
- Information that allows the reader to grasp easily what is known about the nature, likelihood, and magnitude of any risk.

For each step of the analysis phase of risk assessment, the assessor should identify the following items:

- Available studies and their robustness (*e.g.*, have the findings been repeated in an independent laboratory?);
- Assumptions and extrapolations used and the residual uncertainties;
- Use of defaults, policy choices, and any risk management decisions;
- Quality of the data used for the risk assessment (*e.g.*, experimental, state-of-the art, generally accepted scientific knowledge); and
- Quantitative data presented in an easily understandable form, such as tables and graphics.

At EPA, risk characterization takes many different forms depending on the nature of the risk assessment. The level of detail in each risk characterization varies according to the type of assessment for which the characterization is written and the audience for which the characterization is intended. The goal of risk characterization is to clearly communicate the strengths and limitations of the risk assessment so it can be put into context with the other information critical to evaluating options for rules, regulations, and negotiated agreements (*e.g.*, economics, social values, public perception, policies) in the decision-making stage.

The general content of risk characterization is defined by the NAS and, to a limited degree, in each of the EPA risk assessment guidelines (*e.g.*, U.S. EPA 1996a). More specifically, however, the Agency issued its first policy for risk characterization in 1992 (Habicht 1992). This policy was intended to strengthen the reporting of the Agency's risk assessment results. Previously, risk information was sometimes presented to the decision-maker and the public in a form reduced to a simple point-estimate of risk. Such "short-hand" approaches did not fully convey the range of information used in developing the assessment because the numbers alone do not provide an accurate picture of the assessment.

More recently, the Agency updated its policy and issued guidance for the preparation of risk characterizations (Browner 1995, U.S. EPA 1995a, U.S. EPA 1995b). The policy called for all risk assessments performed at EPA to include a risk characterization to ensure that the risk assessment process is transparent and that the risk assessments are clear, reasonable, and consistent with other risk assessments of similar scope prepared by programs across the Agency. In issuing the policy and guidance, the Administrator emphasized the importance of a set of core values to guide risk characterization activities. These core values are transparency, clarity, consistency, and reasonableness (TCCR).

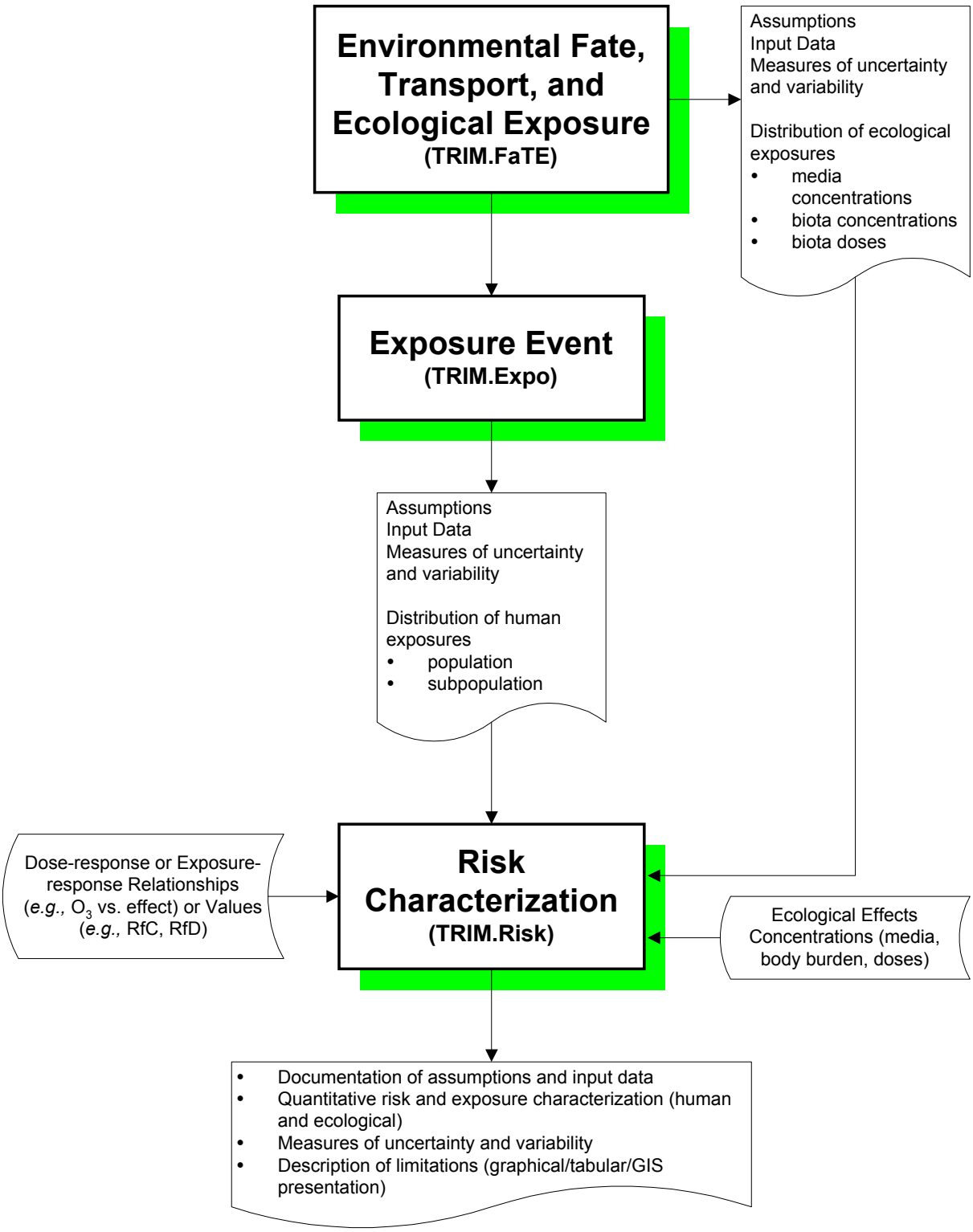
To implement the policy, an Agency-wide document, the *Risk Characterization Handbook*, is being developed (U.S. EPA 1998c). The previously issued policy and guidance, as well as the *Risk Characterization Handbook* under development, will be used to guide the design and implementation of the TRIM.Risk module. Therefore, this chapter includes text drawing from specific discussions and recommendations outlined in these documents along with a description of how TRIM.Risk will conceptually address these recommendations.

## 9.2 PURPOSE OF TRIM.Risk

In order to develop a full risk characterization, information from each of the risk assessment components needs to be characterized separately. These individual characterizations carry forward the key findings, assumptions, strengths, and limitations, and provide a fundamental set of information that must be conveyed in an informative risk characterization. The purpose of the TRIM.Risk module is to summarize and integrate key information from other TRIM modules in addition to other information sources (Figure 9-1) and to facilitate the preparation of a risk characterization. In general, TRIM.Risk will (1) document assumptions and input data, (2) perform risk calculations and data analysis, and (3) present results and supporting information. Where possible, these actions will be automated. It should be noted that while TRIM.Risk is the module with the primary purpose of preparing information to support risk characterization, the guiding principles for risk characterization are also being followed in the development of other TRIM modules (*e.g.*, documenting setup, runs, output), which will facilitate the development of TRIM.Risk.

It is anticipated that TRIM.Risk will be developed in a phased approach similar to other TRIM modules. Ideally, the TRIM.Risk module will provide all of the information required to prepare a full risk characterization. However, the type and variability of information needed for this purpose is vast. Therefore, the type of information generated by TRIM.Risk will evolve over time as the Agency gains experience and has the resources to implement more flexibility. For example, early versions of TRIM.Risk will be limited to preparing quantitative summaries of input data and results, without supporting text. However, as the Agency gains experience, it may be possible to incorporate language to more fully describe the information required for a full risk characterization.

**Figure 9-1**
**Conceptual Diagram of the TRIM.Risk Module**



The purpose of TRIM.Risk is to provide information to risk managers, the public, and stakeholders to support decision-making. To be effective, TRIM.Risk must communicate information that is readily understandable. Specifically, TRIM.Risk is responsible for conveying the information for a specific risk assessment. However, because risk assessments are often used to inform choices between policy alternatives, care will be taken to insure that outputs from TRIM.Risk are formatted to facilitate comparisons (including statistical comparisons) between alternatives.

## 9.3 DESIGN GOALS OF TRIM.Risk

As described in Chapter 1, EPA has established specific goals for the design of TRIM which can be used to measure progress and performance of either the overall modeling system or its individual components. These overall design features of scientific defensibility, flexibility, and accessibility (user-friendliness) apply to the TRIM.Risk module as well. How TRIM.Risk will meet these major design goals is summarized below.

- *Scientific defensibility*. The scientific defensibility of TRIM.Risk will be assured by adherence to the applicable risk characterization guidance (U.S. EPA 1995a, U.S. EPA 1998c) and by full utilization of the abilities of the other TRIM modules to describe uncertainty and variability surrounding their outputs. Consistent with the Agency's guidance for risk characterization to clearly communicate the key strengths and weaknesses of any assessment, the TRIM.Risk module will have the capability to present the variety of important information generated by any of the other TRIM modules. The capability of addressing uncertainty and variability in an integrated manner is critical to presenting risk information beyond deterministic single-point estimates of risk, which is essential in a full characterization of risk. Furthermore, the integrated uncertainty and variability analysis capabilities of the TRIM modules also enhance the ability to identify critical assumptions and data and determine their contributions to overall uncertainty.

- *Flexibility*. The flexibility designed within the TRIM framework will be maintained in TRIM.Risk. Specifically, TRIM.Risk will accommodate and present information for the variety of spatial and temporal scales of analysis possible for other TRIM modules. The value of any risk characterization lies in its ability to convey useful and, most importantly, understandable information to risk managers. An OAQPS evaluation of information needs of risk managers found that because different people process information differently, it is appropriate to provide more than one format for presenting the same information (U.S. EPA 1993). As a result, TRIM.Risk will be designed in such a way that using a specific user interface, outputs may be presented in user-specified formats (*e.g.*, tables, charts, graphics).

- *Accessibility*. As with all TRIM modules, TRIM.Risk will be publicly available and easily obtainable by all interested parties, along with user guides, and will be designed to be user-friendly.

## 9.4 OVERVIEW OF TRIM.RISK

Current and proposed EPA guidance on risk characterization are serving as the basis for designing TRIM.Risk. Therefore, the major elements identified in the guidance with respect to TCCR will be explicitly addressed in TRIM.Risk and are described below. In addition, some discussion is provided on how TRIM.Risk will provide such information and conduct its three primary functions: (1) documenting assumptions and input data, (2) risk calculation and data analysis, and (3) presentation of results.

### 9.4.1 DOCUMENTATION OF ASSUMPTIONS AND INPUT DATA

One purpose of a full risk characterization is to inform the risk manager and others of why EPA assessed the risk the way it did in terms of the available data, the analysis used, uncertainties, alternative analyses, and science policy choices. Risk characterization is not only about science, but also about making clear that current scientific knowledge does not provide all that is needed to perform the analysis, and consequently science policy judgments must be made. Every risk assessment involves a multiplicity of choices and options, and the Agency's *Policy for Risk Characterization* (U.S. EPA 1995b) calls for a highly visible presentation of the explanation for these choices. When appropriate, a recognition and discussion of how others have assessed the same risks should be included.

The computer framework of TRIM (described in Chapter 10) provides an excellent opportunity for documenting assumptions and input data. The algorithm library and parameter database approach used in the TRIM.FaTE and TRIM.Expo modules allows for easy documentation of the algorithms and parameters used in an analysis. Although each module contains default inputs and algorithms, the user can replace these values with alternatives to support site-specific analysis or alternative assumptions. To provide transparency in interpreting results, the TRIM modules will be self-documenting (see Chapter 10), with the ability to catalog the data and algorithms used for every model run, thereby identifying any changes in parameters or algorithms. Therefore, it can be readily determined if differences between model runs are attributable to differences in parameters or algorithms. The algorithm library and parameter database also have comment fields, which provide the opportunity for articulating the rationale for such changes. In addition, the design of user interfaces for each model run within individual modules will document the major assumptions of the analysis.

### 9.4.2 RISK CALCULATION AND ANALYSIS

A variety of risk calculations and analyses is performed by the Agency in risk assessments for the hazardous and criteria air pollutant programs. The TRIM.Risk module is intended to perform this full spectrum of analyses to support characterizations of both human health and environmental risks.

### 9.4.2.1 Human Health Risks

Because cancer and noncancer dose-response assessment have traditionally been different (*i.e.*, assumption of threshold for noncancer versus no threshold for cancer), the current methods for risk assessment also differ and are discussed separately below. In some cases, available data and information do not support the estimation of quantitative estimates of risk. In those cases, the risk characterization may rely on data analyses that summarize risks in a semi-quantitative or qualitative manner, such as comparing exposure concentrations to exposure levels of concern.

#### *Quantification of Cancer Risks*

Cancer risk is defined as the predicted excess probability of contracting cancer over a 70-year period (*i.e.*, assumed human lifespan) following exposure to a pollutant at the estimated concentration for a specified time period. This estimated risk focuses on the additional risk of cancer predicted from the exposure being analyzed, beyond that due to any other factors. Individual cancer risks or population cancer risks associated with an exposure can be calculated by multiplying the individual or population exposure estimate, respectively, by the unit risk estimate (URE). Estimates of risk to an individual are usually expressed as a probability represented in scientific notation as a negative exponent of 10. For example, an additional risk of contracting cancer of one chance in 10,000 (or one additional person in 10,000) is written as $1x10^{-4}$.

In quantitative risk assessment, population risk is an estimate that applies to the entire population within the given area of analysis. The population risk often is expressed as a predicted annual cancer incidence, which is the annual number of excess cancer cases predicted in the exposed population. Each estimated exposure level is multiplied by the number of individuals exposed to that level and by the URE. This provides a prediction of risk for that group after a 70-year exposure to that level. The risks for each exposure group are summed to provide the number of excess cancer cases predicted for the entire exposed population. This 70-year risk estimate can be divided by 70 to estimate the predicted annual incidence in units of cancer cases per year.

People often are exposed to multiple chemicals rather than a single chemical. For analysis of cancer risk from multiple chemical exposures, TRIM.Risk will be consistent with the Agency's *Guidelines for the Health Risk Assessment of Chemical Mixtures* (U.S. EPA 1986a). In developing TRIM.Risk, activities to update these guidelines (*e.g.*, U.S. EPA 1999c) will be followed closely to ensure consistency.

In those few cases where cancer potency values are available for the chemical mixture of concern or for a similar mixture, risk characterization can be conducted on the mixture using the same procedures used for a single compound. However, cancer dose-response assessments usually are available only for individual compounds within a mixture. In such cases, based on the assumption that the risks associated with the individual chemicals in the mixture are additive, the cancer risks predicted for individual chemicals are sometimes added to estimate total risk. The following equation estimates the predicted incremental individual cancer risk for simultaneous exposures to several carcinogens:

$$Risk_T = Risk_1 + Risk_2 + .... + Risk_i$$

where:

$Risk_T$ = the total cancer risk (expressed as a probability of contracting cancer over a lifetime)
$Risk_i$ = the risk estimate for the $i^{th}$ substance.

As described in the proposed revisions to the guidelines for carcinogen risk assessment (U.S. EPA 1996b), when sufficient information is known on the mode of action for a pollutant, dose-response may be better defined by a non-linear relationship. In cases of non-linearity, risk is not extrapolated as the probability of an effect at low doses. In these cases, a margin of exposure analysis is used to evaluate concern for levels of exposure. The margin of exposure is the "point of departure" from the health effects data divided by a human environmental exposure(s) of interest – either actual or hypothetical. Exposures may be of interest because they are associated with actual or projected exposure scenarios or because they are levels that may result from alternative control actions. The risk manager decides whether a given margin of exposure is acceptable within a given regulatory program context. The risk assessment provides an analysis with supporting information and advice to assist the decision-maker in considering aspects of the exposure scenarios at issue in light of the mode of action. A margin of exposure analysis presents all of the pertinent hazard and dose-response factors together. The TRIM.Risk module will be designed to provide analyses and output consistent with the revised guidelines for carcinogen risk assessment.

***Analysis of Noncancer Risks***

Unlike cancer risk characterization, noncancer risks for hazardous air pollutants currently are not expressed as a probability of an individual suffering an adverse effect (*e.g.*, reproductive, neurological, behavioral). Instead, the potential for noncancer effects often is evaluated by comparing an exposure estimate over a specified period of time (*e.g.*, lifetime) with a health reference value, such as a reference concentration (RfC). "Risk" for noncancer effects is quantified by comparing the exposure to the reference level (or benchmark) as a ratio. The resultant Hazard Quotient (HQ) is expressed as:

HQ = Exposure/Benchmark.

Exposures or doses below the benchmark (HQ<1) are not likely to be associated with adverse health effects. With exposures increasingly greater than the reference level (*i.e.*, HQs increasingly greater than 1), the potential for adverse effects increases. The HQ, however, should not be interpreted as a probability. Comparisons of HQs across substances may not be valid, and the level of concern does not increase linearly as exposures approach or cross the reference level. This is because reference levels are derived using different methods and because the slope of the dose-response curve above the benchmark can vary depending on the substance.

As with the evaluation of cancer risks described above, analysis of mixtures in TRIM.Risk will be consistent with Agency guidelines (U.S. EPA 1986a, U.S. EPA 1999c). In

screening-level assessments for such cases, a Hazard Index (HI) approach is sometimes used. This approach is based on the assumption that even when individual pollutant levels are lower than the corresponding reference levels, some pollutants may work together such that their potential for harm is additive and the combined exposure to the group of chemicals poses harm. The assumption of dose additivity is most appropriate to compounds that induce the same effect by similar modes of action (U.S. EPA 1986a). The HI (for a mixture of *i* compounds) is calculated as:

$$HI = HQ_1 + HQ_2 + ...+ HQ_i.$$

As with risk measures for individual pollutants, the HI should not be interpreted as a probability of effect, nor as strict delineation of "safe" and "unsafe" levels (U.S. EPA 1999f, U.S. EPA 1986a). Rather, the HI is a rough measure of potential for risk and needs to be interpreted carefully. Although the HI approach may be appropriate for a screening-level study (U.S. EPA 1999f), it is important to note that application of the HI equation to compounds that may produce different effects or that act by different mechanisms could overestimate or underestimate the potential for effects. Calculating a separate HI for each noncancer endpoint of concern when mechanisms of action are known to be the same is scientifically more appropriate (U.S. EPA 1999f, U.S. EPA 1986a).

It should be noted that, in some instances, the noncancer toxicity of a particular pollutant is well characterized, either because the biokinetics and toxicokinetics are well known or because substantial information on dose- or exposure-response relationships are well known. In these circumstances, probabilistic risk estimates similar to those described for cancer risks above may be possible. For example, risk assessments for criteria air pollutants, and potentially future risk assessments for hazardous air pollutants, utilize a variety of dose- or exposure-response tools in place of the RfC or RfD values. For example, risk assessments for carbon monoxide (CO) include a step in which a population distribution of response (*i.e.*, carboxyhemoglobin production in the blood) is modeled from the population distribution of CO exposures. In ozone risk assessments, population distributions of exposure are modeled against an exposure-response relationship (derived from either controlled human exposures or epidemiological analyses) to predict the distribution of responses in the exposed population or subpopulation. In the case of lead risk assessments, exposure estimates are entered into the IUBK (Intake, Uptake, Biokinetic) model to predict blood levels of lead, which can be compared to levels of concern in the risk characterization step.

#### 9.4.2.2 Environmental Risk

Some components of environmental risk assessment are integral to the assessment of human health risks. For example, the concentrations of pollutants in the environment and their fate and transport can represent a significant part of human exposure assessment. In addition, laboratory animal toxicity data are often used to extrapolate effects of chemical exposures on humans. However, because ecosystems consist of living and non-living entities linked together in numerous interdependent relationships, the scope of an environmental risk assessment can range from very simple to very broad and complex and must be defined at the outset. As an assessment moves from the level of the individual organism to species or populations of species,

communities of several species, and to whole ecosystems, the level of complexity increases. To an even greater degree than for human health, environmental risk assessments rely on qualitative information or expert judgments.

***Individual and Population Levels***

When the scope of an environmental risk assessment is set at the level of an individual organism within a species or an entire population or subpopulation of that species (*e.g.*, threatened or endangered species, sentinel species), the assessment may use types of information and tools analogous to those used for human health risk assessments. In some cases, animal toxicity data developed for human health risk assessments may be directly applicable to the animal species of concern (*e.g.*, when species-specific toxicity values, such as $EC_{50}$, $EC_{10}$, $LC_{50}$, NOAEC, LOAEC, MATC, already exist).

The TRIM.Risk module will have the ability to compare these ecological toxicity values or endpoints with the outputs of TRIM.FaTE (or another source of data) – including (1) concentration of pollutant in relevant media, such as air, soil, water, sediments, (2) tissue concentrations or body burdens in organisms based on ingestion, dermal contact or absorption, or inhalation, and (3) the dose or amount entering organism per unit time. This information can then be used to derive hazard quotients or display the distributions of exposures relative to toxicity values or endpoints.

Because of the paucity of ecological toxicity data for most species, however, extrapolation from one species to the other and from laboratory to field conditions is required, introducing significant uncertainties into the calculation of risk. With respect to animals, a primary effect of concern is mortality. However, because most ecological species live in a much more competitive environment than humans, noncancer effects (*e.g.*, reproductive, neurological, behavioral, growth) can also play a large role in individual and species survival (*e.g.*, reduced ability to avoid predators, defend territory, attract a mate), though they are much more difficult to measure.

Because populations are made up of individual organisms, if enough individuals of a species are adversely affected by exposure to a chemical, the population also will be adversely affected. In order to evaluate population effects from data on individuals, it is necessary to know what kind of life history strategy is employed by that species. In addition to direct effects of exposure, an organism may be indirectly affected by the presence of a toxic chemical in the environment (*e.g.*, through effects on a prey species or on some other aspect of the environment that reduces habitat quality). The EPA's water quality criteria for the protection of aquatic life are an example of an indicator as to the suitability of the aquatic habitat for certain species as well as providing information to assist in the evaluation of the potential for ecosystem impacts.

As with humans, other species are often exposed to multiple chemicals simultaneously or in close temporal proximity so that there may be interactions occurring between them (*e.g.*, synergistic effects, antagonistic effects). Although little is known about these interactions in the field, where information does exist for chemical mixtures, it can be used in the same way as that

for a single compound. Where information does not exist about chemical interactions, it may be necessary to make assumptions in order to assess the risk posed by mixtures.

***Communities and Whole Environments***

Although TRIM.Risk will have the ability to provide distributions of hazard quotients around the modeled site for species of concern, it is expected that substantial additional information will be needed in order to sufficiently characterize risks occurring from HAP exposure at the community and ecosystem levels. Such a refined analysis may require information such as detailed descriptions of the particular ecosystem in which the exposures are occurring; the temporal and spatial scales of the exposures; the significance of the effect of the exposure in the larger landscape; and the ecosystem services and functions affected. Some of this information may be available from TRIM.FaTE or by accessing GIS databases. Thus, the complete ecological risk characterization would combine the outputs of TRIM.Risk with other relevant information in a weight-of-evidence approach.

## 9.4.3 PRESENTATION OF RESULTS

As stated above, there are two elements required for a full characterization of risk. First, the characterization must address qualitative and quantitative features of the assessment, namely clearly identify assumptions (covered under documentation of assumptions and inputs above) as well as quantitative estimates of risk. Second, the characterization must identify any important uncertainties in the assessment as part of a discussion on confidence in the assessment. TRIM.Risk, in presenting results, will address these two points.

### 9.4.3.1 Risk Descriptors for Human Health

The Agency's *Guidance for Risk Characterization* (U.S. EPA 1995a) recommends that EPA risk assessments address or provide descriptors of (1) individual risk, to include the central tendency and high-end portions of the risk distribution, (2) population risk, and (3) important subgroups of the populations such as highly exposed or highly susceptible groups or individuals, if known. Assessors may also use additional descriptors of risk as needed when these add to the clarity of the presentation. With the exception of assessments where particular descriptors clearly do not apply, some form of these three types of descriptors should generally be developed and presented for EPA risk assessments.

- **Individual Risk.** Individual risk descriptors are intended to estimate the risk borne by individuals within a specified population or subpopulation. These descriptors are used to answer questions concerning the affected population, the risk levels of various groups within the population, and the average or maximum risk for individuals within the populations of interest.

- **Population Risk.** Population risk descriptors are intended to estimate the extent of harm for the population as a whole. This typically represents the sum of individual risks within the exposed population. Two important population risk descriptors should be estimated and presented (Habicht 1992): (1) the probabilistic number of health effect cases

estimated in the population of interest over a specified time period; and (2) the percentage of the population, or the number of persons, above a specified level of risk or range of health benchmark levels.

- **Highly Exposed or Highly Susceptible Subpopulations.** Risk descriptors also may be developed for specific segments of the exposed population. These include highly exposed and highly susceptible groups (U.S. EPA 1995a). Use of a risk descriptor for highly exposed subgroups is useful when there is expected to be a subgroup experiencing significantly greater exposures than those of a larger population (*e.g.*, high fish consumers, children playing outdoors all day). Use of a risk descriptor for highly susceptible subgroups is useful when the susceptibility to the health effect being assessed is expected to be significantly greater for a specific population subgroup than it is for the larger population. For example, upon exposure to a chemical, pregnant women, elderly people, children, and people with certain illnesses or nutritional status may each be more sensitive than the population as a whole.

Consistent with Agency guidance, TRIM.Risk will provide central tendency and high-end estimates of risk. Use of several descriptors, rather than a single descriptor, will result in a more complete picture of risk that corresponds to the range of different exposure conditions encountered by various populations exposed to most environmental chemicals. Central tendency estimates of risk are intended to give a characterization of risk for the typical situation in which an individual is likely to be exposed. This may be either the arithmetic mean risk (*i.e.*, average estimate) or the median risk (*i.e.*, median estimate) and should be clearly labeled (Habicht 1992). High-end estimates of risk are intended to estimate the risk that is expected to occur in a small but definable segment of the population. The intent is to "convey an estimate of risk in the upper range of the distribution, but to avoid estimates which are beyond the true distribution. Conceptually, high-end risk means risk above about the 90th percentile of the population distribution, but not higher than the individual in the population who has the highest risk" (Habicht 1992).

#### 9.4.3.2 Presentation of Ecological Risk Assessment Results

In the problem formulation stage of ecological risk assessment, the specific analyses that will be performed for the assessment are identified. Depending on how these analyses are framed, the assessment could focus on either population risk or ecosystem risk. The TRIM.Risk module will be designed with the flexibility for the user to specify the focus of the assessment and the relevant risk analyses. The results will be presented in a form relevant to the specific focus (*e.g.*, a presentation of population risk or ecosystem risk information).

To present outputs for ecological risk, in some cases (*e.g.*, with endangered or indicator species) HQs may be useful by themselves, where the distribution of HQs may be graphically displayed on a map of the study area. In most cases, however, a weight-of-evidence approach will be needed. In these cases, a suite of GIS maps showing different layers of information could be used by experts to evaluate the meaning and context of the HQ. These GIS maps might include media concentrations for both single and multiple HAPs, land use, terrain/topography, soil types, hydrology, distributions of flora/fauna, distributions of endangered species, and

temporal variations (*e.g.*, between years, seasons). In the case of contamination by or exposure to multiple HAPs, GIS overlays might help with the identification of ecological "hotspots" that might not be identified by evaluating the pollutants separately. In addition to GIS maps, graphical displays of distributions of effects within a population would be useful. In cases where TRIM.Risk is used for a simple screening exercise, site-specific information would not be needed and TRIM.Risk can provide more simple outputs.

#### 9.4.3.3 Uncertainty

Uncertainty can be introduced into a risk assessment at every step in the process. Even using the most accurate data with the most sophisticated models, uncertainty is inherent in the process because risk assessment is a complex process. The degree to which all types of uncertainty need to be quantified and the amount of uncertainty that is acceptable vary, depending on the purpose and intended use of the risk assessment. For a screening-level analysis, a high degree of uncertainty often is acceptable, provided that conservative assumptions are used to bias potential error toward protecting human health or the environment. Similarly, the concentrations at a specific location in a region-wide or nationwide assessment will be more uncertain than the concentrations at a specific location in a site-specific assessment because there is more variability in the input parameters for larger scale assessments.

#### 9.4.3.4 Outputs

Because there is more than one audience for each risk assessment, there will probably be more than one risk characterization for a risk assessment. Different types of risk assessment also vary in length and degree of detail, and each risk characterization is as simple or complex as the assessment from which it is derived. While the full risk characterization is written for the type of assessment conducted, as it is presented to various audiences, the characterization product should be tailored to that audience. For fellow risk assessors and other scientists, the full characterization is most appropriate. If the risk characterization is presented to non-technical colleagues and to those whose time is limited (*e.g.*, managers), it should shortened and focused, but the characterization should always include the fundamental, irreducible set of key points that must be communicated to characterize adequately the essence of any risk assessment.

OAQPS recognizes that individuals process information differently and it is, therefore, appropriate to provide more than one format for presenting the same information. Therefore, each TRIM module will be designed so that the output can be presented in various ways in an automated manner (*e.g.*, Chart Wizard in Excel), allowing the user to select a preferred format.

The TRIM.Risk module will provide quantitative estimates of risk for both human and ecological risks. At a minimum, the following risk measures will be presented as outputs of TRIM.Risk.

**EXAMPLES OF RISK MEASURES TO BE INCLUDED IN TRIM.Risk**

| | |
|---|---|
| **Human Risks** | |
| Cancer | Distributions of excess cancer, MOE within exposed population<br>(Note: deterministic values may be used for screens)<br>Estimate of predicted cancer incidence |
| Noncancer | Distribution of HQ or HI within exposed population<br>(Note: deterministic values may be used for screens)<br>Distribution of exposure (dose) relative to exposure (dose) levels of concern<br>Distribution of probability of effect within exposed population (estimated incidence) |
| **Ecological Risks** | Distribution of concentration/criteria (similar to HQ or HI)<br>Distribution of probability of effect within population |

## 9.5 CURRENT STATUS AND FUTURE PLANS FOR TRIM.Risk

At present, only the conceptual design of TRIM.Risk has been developed. Development of a TRIM.Risk prototype will begin after SAB comments are received on the conceptual design. Module development will include identification of data needs and formatting of data outputs. Programming for a TRIM.Risk prototype is expected to be completed in 2000.

# 10. DEVELOPMENT OF TRIM COMPUTER FRAMEWORK

This chapter describes the computer framework that will be used for each of the TRIM modules and that is currently being implemented for TRIM.FaTE. Therefore, much of this discussion is specific to TRIM.FaTE, but it can be generalized to all of the TRIM modules. Additional information about these aspects of TRIM.FaTE Version 1.0 can be found in Appendix F of Volume I of the TRIM.FaTE TSD and in Fine et al. (1998a, 1998b).

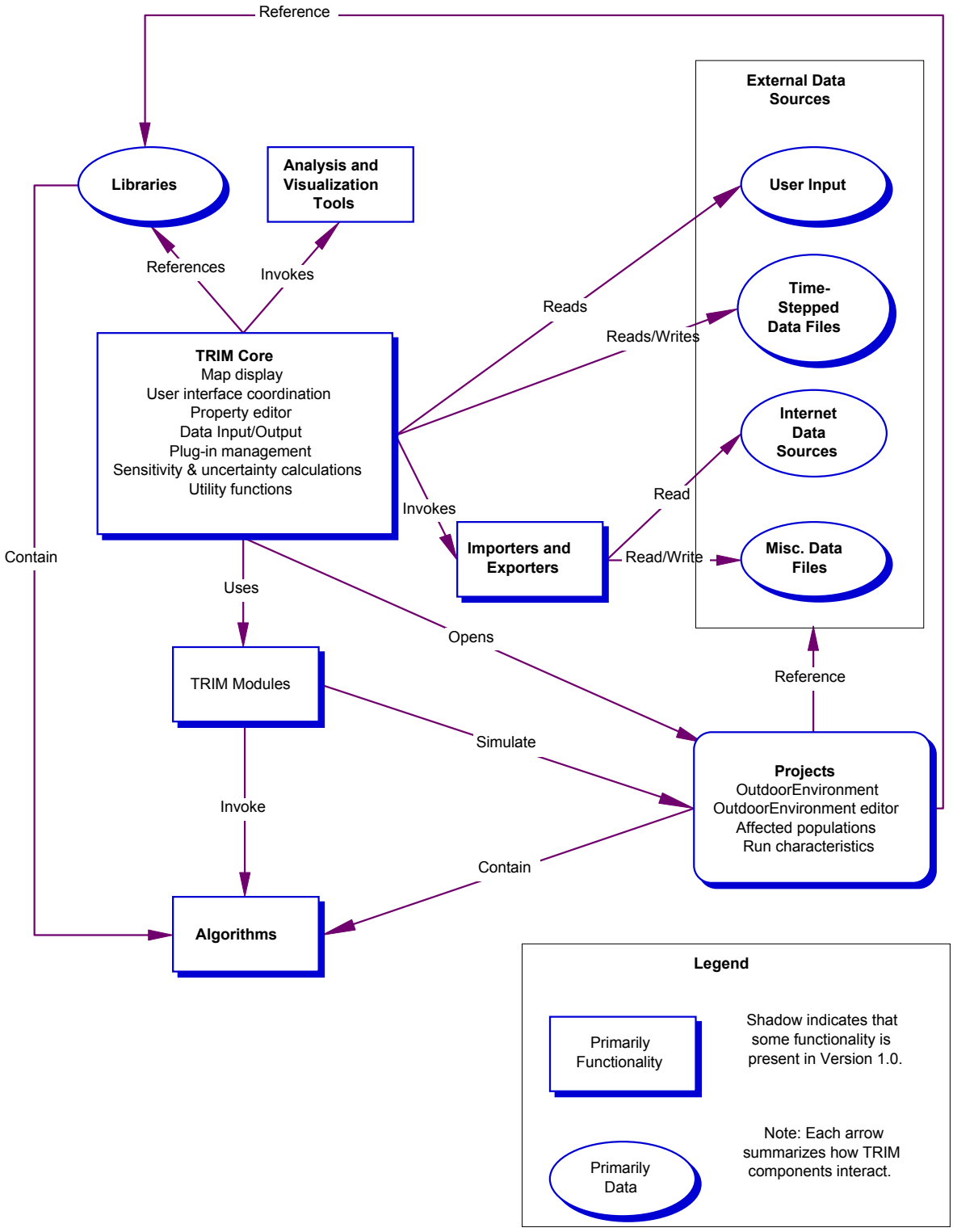
The development of TRIM.FaTE Version 1.0 began in 1998 and was completed in September 1999. Version 1.0 differs from the prototype in several ways. Specifically, Version 1.0 (1) is compatible with operating systems beyond Microsoft Windows, such as UNIX, (2) provides improved management of multiple modeling scenarios, and (3) is easier to use and more reliable. Similar to Prototype V of TRIM.FaTE, TRIM.FaTE Version 1.0 provides users with the following options:

- Define the parameters of each specific assessment, including time period, geographic region, pollutants, environmental media, and populations of interest;
- Choose appropriate pollutant fate and transport algorithms for use in assessments;
- Select modeling parameters, including emissions sources, characteristics of the environment (*e.g.*, air temperature, soil permeability), and simulation time step (*e.g.*, hourly, daily);
- Identify and access input data sets, and identify and create output data sets;
- Execute the assessment; and
- Export results.

## 10.1 ARCHITECTURE

As shown in Figure 10-1, the TRIM computer system architecture is complex but flexible, allowing it to be applied in developing each of the different TRIM modules. The architecture components used to describe TRIM are classified as those that primarily provide (1) functionality (rectangles), and (2) data (ovals). However, each of the components except for external data sources provide both functionality and data. The architectural components that have been implemented to some degree in Version 1.0 are depicted with shadows. This figure is designed to represent the relationships within the TRIM computer framework, rather than the data flow within the system. Therefore, the word along an arrow forms a sentence where the verb on the arrow connects the two architecture components at the end of an arrow. For example, in the upper left hand corner of the figure, the TRIM Core "invokes" Analysis and Visualization Tools. Each of the TRIM components shown in Figure 10-1 are described below.

**Figure 10-1**
**TRIM Computer System Architecture**



### 10.1.1 TRIM CORE

The TRIM Core component primarily provides services required by multiple architectural components or integrates those components. The following items are included in the Core.

- A mapping tool shows volume elements and associated information, such as predicted chemical concentrations, and is based on an off-the-shelf software component that provides some GIS-like capabilities. The mapping tool allows users to view geospatial data from external sources, such as soil type layers generated by a GIS and stored in a SHAPE file, with an overlay of TRIM information.

- A simple graphical user interface allows the user to invoke TRIM modules, such as TRIM.FaTE, and that maintains lists of open windows.

- A property editor enables users to edit and view property values, where a property value describes an attribute (*e.g.*, molecular weight) of an entity that is simulated by the module, such as a chemical or compartment or volume element. Examples of attributes for which property values are used include air temperature, scavenging coefficients, and chemical reaction rates.

- A management system allows user to plug in data importers and exporters.

- An analysis feature calculates sensitivity, uncertainty, and variability of outputs using TRIM modules (Note: this may not be supported in Version 1.0).

- Utility functions, such as routines that assist with data storage and retrieval, are used by TRIM modules.

### 10.1.2 PROJECTS

Projects in TRIM are used to store all information pertinent to an individual assessment. A project contains "scenarios," where each scenario contains a description of the outdoor environment being simulated, populations being studied, and model parameters, such as the simulation time step. Each project also displays the information it contains and allows the user to change that information. In some cases, the information display and manipulation functions of a project rely on a TRIM Core functionality, such as the property editor.

### 10.1.3 TRIM MODULES

Each TRIM module, such as TRIM.FaTE, is a component that allows for simulation or analysis. Where required, modules also provide specialized graphical user interfaces that support their functionality. Version 1.0 includes only the TRIM.FaTE module. Future TRIM versions will include additional TRIM modules.

### 10.1.4 LIBRARIES

A substantial amount of relatively static information is required to conduct assessments of multimedia chemical fate and transport and subsequent exposures and effects on selected populations. For instance, static information includes the measured properties of chemicals that change infrequently or the boundaries of a study region that might stay constant for years. Because of the static nature of this information and because a large amount of static information may be needed for a single assessment, users can store such information in TRIM libraries. Users can then easily reuse selected information from a library in future projects. Changes may be made to the library over time to ensure that the most current science is used in assessments. However, when a user creates a project that accesses information from a library, a copy of the information is made to protect the project from future changes to the library.

The TRIM.FaTE module uses a number of chemical fate and transport algorithms that compute chemical transfer coefficients between and chemical transformation coefficients within compartments. As new chemicals, ecosystems, and relationships are studied, new algorithms will be required. In anticipation of this need, TRIM.FaTE has been designed to allow users to add algorithms. The algorithms are stored in libraries and can be applied to various projects, as designated by the user. Specifically, a user can manually assign algorithms stored in libraries to links or can request that TRIM.FaTE assign applicable algorithms based on the compartments that are connected by a link. For instance, some algorithms might only be applicable for transfer from surface water to fish. Even when TRIM.FaTE assigns algorithms, the user can review the assignments and make changes before the simulation starts. Before or after a simulation, the user can export the simulation scenario and its results (if available) to a set of HTML files. These HTML files show which algorithms were used for each link and the formulation of each algorithm.

### 10.1.5 EXTERNAL DATA SOURCES, IMPORTERS, AND EXPORTERS

Given the diversity of potential applications of TRIM, data required to address those applications, and formats used for storing that data, it is difficult to construct a computer framework that provides all potentially required capabilities. The TRIM architecture addresses this issue in several ways.

The architecture allows the user to add data importers and exporters in a relatively easy manner, as needed. Data importers read non-TRIM data sets and create and/or set appropriate TRIM objects and properties. For instance, Version 1.0 contains a data importer that can read a text file describing volume elements and can create the corresponding elements in a TRIM project. Another data importer can read a textual description of algorithms, compartments, chemicals, and sources and can create the corresponding objects in a TRIM library. Data exporters can write TRIM configurations and results in a format that is suitable for use by another computer program or for interactive review. Version 1.0 can export the configuration of a simulation scenario and its results to HTML files and simulation results to a text file that can be imported by Microsoft® Excel. Future data importers and exporters could provide many other capabilities. Examples include reading data produced by a GIS (*e.g.*, SHAPE files) and interpolating values to TRIM volume elements, writing results in a format that could be further

processed by a GIS, importing information directly from a web site or database, and transferring results to a statistical package that is executing concurrently with TRIM. To provide additional flexibility, future versions of TRIM may allow knowledgeable users to apply data importers and exporters that users develop without modifying TRIM.

The TRIM.FaTE module, in specific, allows users to provide environmental data in binary files that can be read as needed by a TRIM.FaTE simulation. This streamlines the use of large data sets, such as hourly temperatures or concentrations over a 30-year period. Binary files can also be used for storing TRIM.FaTE results. The TRIM Core supports reading data from and writing data to file formats that are based on the Environmental Decision Support System/Models-3 Input/Output Applications Programming Interface (I/O API) (Coats 1998). The I/O API format can be easily read and written from several programming languages, is platform-independent, is suitable for large data sets, is self-describing (*i.e.*, contains information about variables and time periods contained in the file), and is computationally efficient.

### 10.1.6 ANALYSIS AND VISUALIZATION TOOLS

Version 1.0 does not include any analysis or visualization tools. Instead, simulation results can be easily exported to Microsoft® Excel or other analysis packages. In the future, TRIM will include some analysis and visualization capabilities and may allow users to develop and plug in additional capabilities.

## 10.2 IMPLEMENTATION APPROACHES AND TECHNOLOGIES

The TRIM is being developed using an object-oriented approach. There has been much discussion in the software engineering literature, such as Booch (1993), on the benefits of this approach, including increased software extensibility, reusability, and maintainability. The essence of object-oriented software development is that concepts, such as a volume element, are represented as a unit that contains internal data (*e.g.*, the boundaries of a volume element) and operations on the data (*e.g.*, computation of volume), and that one class of objects (*e.g.*, volume element with vertical sides) can be a specialization of another class of objects (*e.g.*, volume element). Being able to specialize classes of objects allows general functionality to be shared by several specialized classes. The TRIM's representation of the outdoor environment (with volume elements that contain compartments) and the development of associated graphical user interfaces are well suited for an object-oriented treatment.

The TRIM is being developed in an iterative manner. The major components and responsibilities of a class of objects are understood before implementation, but some details may need to be resolved as implementation proceeds. Prior to implementation, graphical user interface mock-ups and significant new capabilities are shown to potential users. During implementation, the design is modified as needed. This user-oriented development approach helps highlight potential problems before undesirable approaches become embedded in the system. Furthermore, the object-oriented, open-ended structure of TRIM is intended to make future changes and additions a relatively simple process.

For Version 1.0 of TRIM, simpler and/or more reliable approaches were used in preference to faster and/or less resource-intensive approaches. In cases where simple approaches did not have adequate performance or significantly limited the potential for future changes, more complex approaches were used. Operations that caused noticeable speed or resource problems were optimized as time and resources permitted.

The TRIM computer framework and TRIM.FaTE module have been developed primarily, but not entirely, in the Java programming language. Some parts of TRIM.FaTE, such as the differential equation solver, and other TRIM modules, such as TRIM.Expo, ultimately will be implemented in the FORTRAN programming language. Advantages of using Java include the following.

- Java code is portable across different hardware and operating systems. This is especially important for graphical user interfaces, which will comprise a large fraction of the TRIM code and which can be difficult to develop for multiple platforms.

- Java offers a combination of speed of development, dependable system behavior, and support for object-oriented designs.

- Java is supported by multiple vendors, often leading to competitive pressures to improve development tools. In addition, it reduces the likelihood that one vendor's product strategy or financial problems will negatively affect TRIM development.

- Java provides built-in support for multithreading (*i.e.*, allowing multiple operations to proceed simultaneously) and networking (*i.e.*, communicating with software on remote computers, such as extracting simulation properties from a web-based data repository).

The disadvantages of using Java as the primary programming language for TRIM include the following.

- Programs written in Java typically execute more slowly than programs written in C++ or BASIC. However, as the technologies for compiling and executing Java programs advance, the execution time for Java programs should decrease.

- Fewer plug-in components (*e.g.*, mapping tools) and libraries (*e.g.*, matrix manipulation) are available for Java than are available for languages such as C++ or BASIC on Windows. However, the number of plug-in components available for Java is continuing to grow.

- Java development tools are not as mature (*e.g.*, fewer tools, lower performance, greater probability of system errors) as tools for other languages, but that situation is improving.

## 10.3 USING TRIM.FaTE VERSION 1.0

Version 1.0 of TRIM.FaTE as completed in September 1999. This section provides a general discussion of how a user would set up and run a simulation using Version 1.0.

After starting TRIM.FaTE Version 1.0, the user can create a new project or library or open an existing project or library. A library populated with objects must be created by the user before any meaningful work can be performed with a project. Note that when TRIM.FaTE is distributed in the future, some pre-loaded libraries will be included. From the library window (shown in Figure 10-2), the user can choose to create new or examine existing algorithms, chemicals, compartments, point sources, or property types. TRIM.FaTE Version 1.0 also allows the user to import objects from text files rather than creating objects from the Graphical User Interface (GUI).

Properties are an important concept in TRIM.FaTE Version 1.0 because they store information about the objects in the system. Examples of properties for a chemical include melting point, vapor pressure, and molecular weight. Examples of properties for an algorithm include the receiving compartment type, the sending compartment type, and whether it transforms a chemical. Each property references a property type that defines the type of data (*e.g.*, real number, date and time, true or false), a default value, a description, units, and for numeric data types recommended minimum and maximum values. In TRIM.FaTE Version 1.0, a GUI component, the Property Editor (shown on the right sides of Figures 10-2 and 10-3), is used throughout the system to add properties to objects and to view and edit the values of properties. For some properties in Figure 10-1, the value field contains "<See Below>." These are special properties for which the value is a formula. An example of the use of formulas as properties is specifying how transfer factors are calculated for algorithm objects.

After creating a library that contains the algorithms, chemicals, compartments, and point sources to be used in the simulations, a project can be created with scenarios that will run the simulations. New projects are created with one scenario by default, and additional scenarios can be added as needed. Generally, the scenarios in a project are related in some manner. Libraries are attached to projects and serve as sources of objects for the scenarios. Typically, after creating a scenario, the user sets its properties. These include the begin and end times for and the time step for the simulation. After setting the properties, volume elements can be imported from a text file into the scenario. In a later version of TRIM.FaTE, a GUI will be available for defining and viewing volume elements.

The outdoor environment window (shown in Figure 10-3) is organized as a set of tabbed panes that allow the user to define the sources, chemicals, compartments, links, and algorithms that comprise the outdoor environment. The general procedure for populating the outdoor environment is to copy objects from libraries into the scenario's outdoor environment, and then to customize the objects as needed. Abiotic compartments are automatically added to the outdoor environment when the volume elements are imported, whereas biotic compartments can be manually added and deleted from the Compartments tab. A function called "Smart Add" is available to intelligently add biotic compartments to the abiotic compartments based on their properties. The volume elements, compartments, and links in the outdoor environment are

displayed in an outline form that can be expanded and collapsed to display varying levels of detail. Links can be created manually using the Links tab or automatically using the "Smart Link" function. With "Smart Link," links are created between adjacent or co-located compartments if algorithms that connect their compartment types exist in the project's libraries. Algorithms on links can be viewed and added or removed manually from the Algorithms tab.

After the properties for the scenario are set and the sources, chemicals, compartments, links, and algorithms are assigned to the outdoor environment, it is possible to run a simulation. The Verify button on the scenario window can be used before running the simulation to ensure that all necessary information is available (*i.e.*, all properties needed by the simulation have values). The Run button on the window is used to start the simulation. After the simulation is executed, the results can be exported to HTML and to text files that can be imported by Microsoft® Excel or another spreadsheet program.

**Figure 10-2**
**Library Window of TRIM.FaTE Version 1.0**

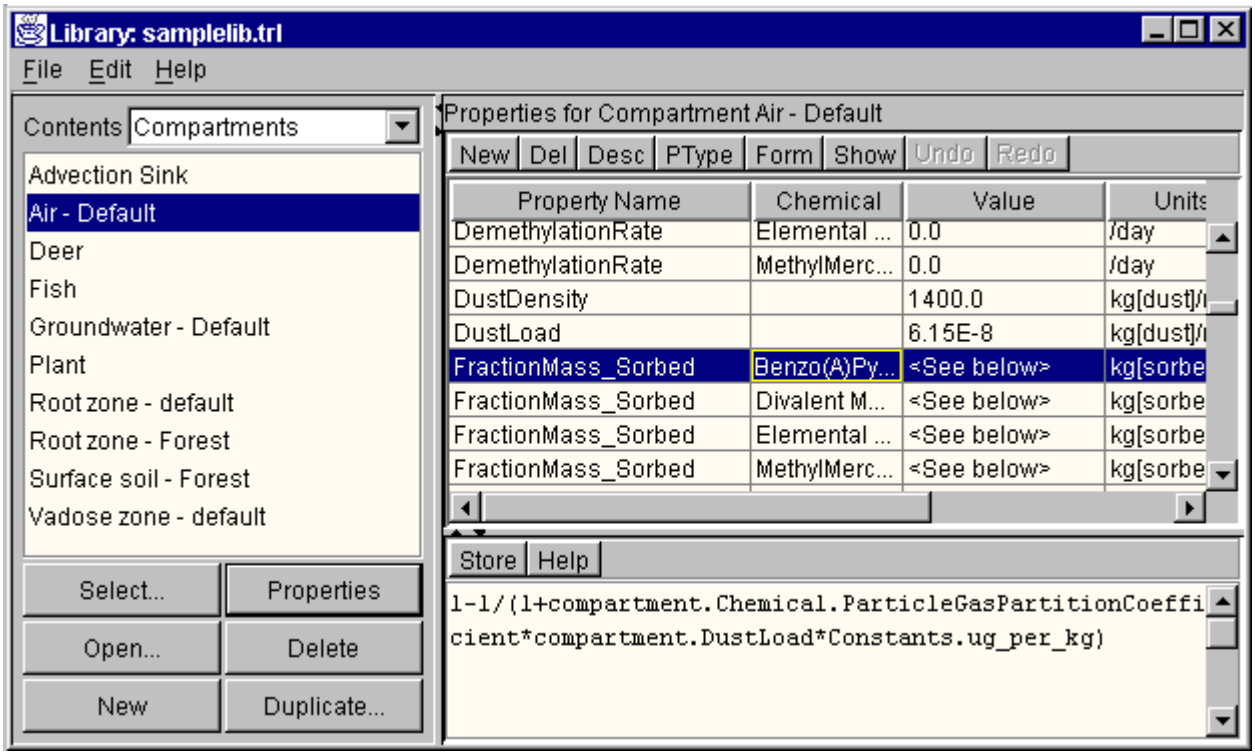
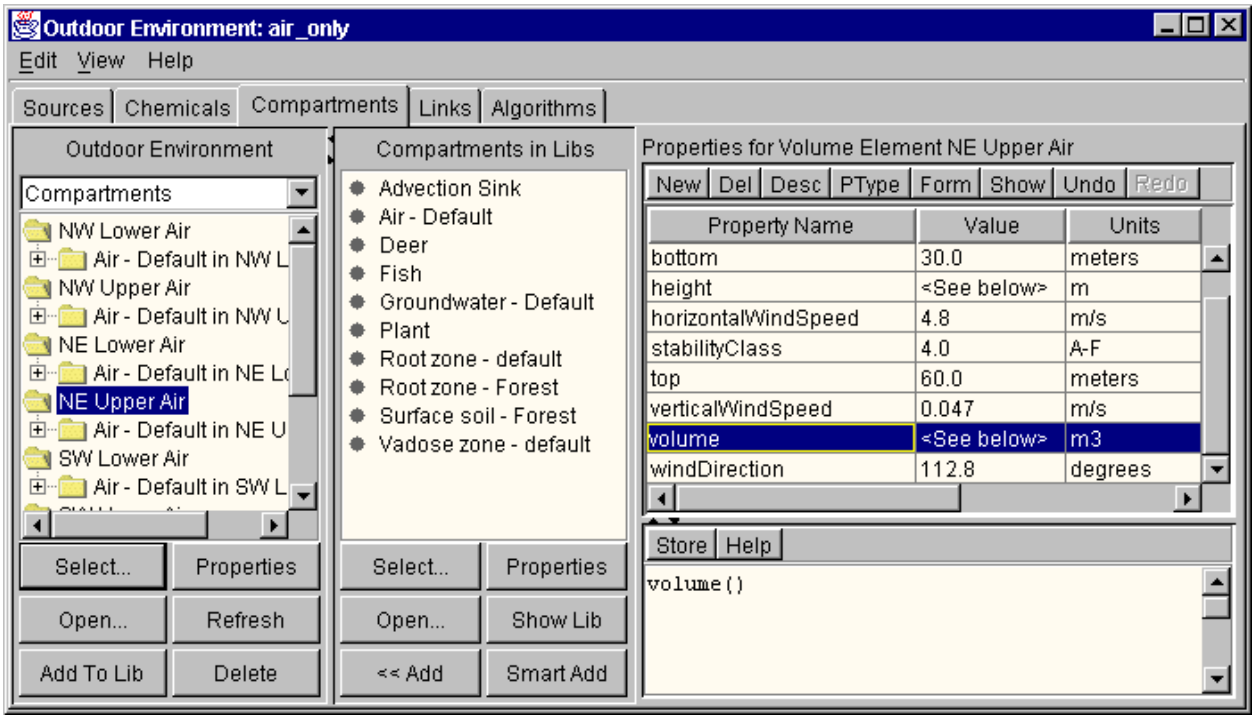


**Figure 10-3**
**Outdoor Environment Window of TRIM.FaTE Version 1.0**




## 10.4 IMPLEMENTATION STATUS

Version 1.0 provides all of the functionality listed at the beginning of this chapter. The software is currently being evaluated to identify problems and to gain confidence in the system. Major additions that will be implemented in the future include data analysis tools, sensitivity and uncertainty studies, and the display of geographic data.

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# APPENDIX A
# Glossary

**Abiotic Compartment Type** — A compartment type consisting primarily of a non-living environmental medium (*e.g.*, air, soil) for which TRIM.FaTE calculates chemical masses and concentrations; it may also contain biota, such as the microorganisms responsible for chemical transformation (see also compartment type).

**Activity Patterns** — A series of discrete events of varying time intervals describing information about an individual's lifestyle and routine. The information contained in an activity pattern typically includes the locations that the individual visited (usually described in terms of microenvironments), the amount of time spent in those locations, and a description of what the individual was doing in each location (*e.g.*, sleeping, eating, exercising). All of the information for an activity pattern is gathered during an "activity pattern survey," usually through the use of questionnaires or diaries. Each activity pattern survey is designed to collect information on activities needed for a particular study or purpose. Activity patterns are also referred to as "time/activity patterns."

**Biotic Compartment Type** — A compartment type consisting of a population or community of living organisms (*e.g.*, bald eagle, benthic invertebrate), or in the case of terrestrial plants, portions of living organisms (*e.g.*, stems, leaves), for which TRIM.FaTE calculates chemical masses and concentrations (see also compartment type).

**Chemical** — A unit whose mass is being modeled by TRIM.FaTE. A chemical can be any element or compound, or even group of compounds, assuming the necessary parameters (*e.g.,* molecular weight, diffusion coefficient in air) are defined.

**Cohort** — A group of people within a population who are assumed to have similar exposures and whose demographic variables are taken from the same probability distribution during a specified exposure period.

The use of cohorts is useful when modeling the exposures of a large population. Since adequate data on the exposures of each individual in a population does not exist, information about people who are expected to have similar exposures are aggregated together in order to make better use of the limited data that is available.

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| | Cohorts can be defined for each application or situation. In the latest pNEM/CO model, for example, cohort exposure was taken to be a function of demographic group, location of residence, location of work place, and type of cooking fuel (natural gas or other). Specifying the home and work district of each cohort provided a means of linking cohort exposure to ambient CO concentrations. Specifying the demographic group provided a means of linking cohort exposure to activity patterns which vary with age, work status, and other demographic variables. Specifying the type of cooking fuel provided a means of linking cohort exposure to proximity to a particular emission source. In some analyses, cohorts are further distinguished according to factors relating to time spent in particular microenvironments. In the pNEM analyses, the population-of-interest is divided into a set of cohorts such that each person is assigned to one and only one cohort. |
| **Compartment** | A homogeneous unit of space characterized by its physical composition and within which it is assumed, for modeling purposes, that all chemical mass is in equilibrium. |
| **Compartment Type** | A specific kind of compartment, such as an air compartment type or a mule deer compartment type. Compartment types are distinguished from each other by the way they exchange chemical mass with other compartment types. |
| **Conceptual Model Evaluations** | Evaluations focused on the theory and assumptions underlying the model. These activities seek to determine if the model is conceptually sound. |
| **Criteria Air Pollutants** | Air pollutants for which national ambient air quality standards (NAAQS) have been established under the Clean Air Act (CAA); at present, the six criteria air pollutants are particulate matter, ozone, carbon monoxide, nitrogen oxides, sulfur dioxide, and lead. |
| **Exposure** | The contact between a target organism and a pollutant at the outer boundary of the organism. Exposure may be quantified as the amount of pollutant available at the boundary of the receptor organism per specified time period. As an example, inhalation exposure over a period of time may be represented by a time-dependent profile of the exposure concentrations. |
| **Exposure District** | A geographic location within a defined physical or political region where there is potential contact between an organism and a pollutant, and for which environmental media |

APPENDIX A
GLOSSARY

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| | concentrations have been estimated either through modeling or measurement. |
| **Exposure Event** | A human activity that results in contact with a contaminated medium within a specified microenvironment at a given geographic location. |
| **Functionality** | The capability to perform computational operations. |
| **Hazardous Air Pollutant** | Any air pollutant listed under Clean Air Act (CAA) section 112(b); currently, there are 188 air pollutants designated as Hazardous Air Pollutants (HAPs). |
| **Link** | A connection that allows the transfer of chemical mass between any two compartments. Each link is implemented by an algorithm or algorithms that mathematically represent the mass transfer. |
| **Mechanistic and Data Quality Evaluations** | Evaluations focused on the specific algorithms and assumptions used in the model. These activities seek to determine if the individual process models and input data used in the model are scientifically sound, and if they properly "fit together." |
| **Microenvironment** | A defined space in which human contact with an environmental pollutant takes place and which can be treated as a well-characterized, relatively homogeneous location with respect to pollutant concentrations for a specified time period. |
| **Model Evaluation** | The broad range of review, analysis, and testing activities designed to examine and build consensus about a model's performance. |
| **Parcel** | A planar (*i.e.*, two-dimensional) geographical area used to subdivide a modeling region. Parcels, which can be virtually any size or shape, are the basis for defining volume elements. There can be air, land, and surface water parcels. |
| **Performance Evaluations** | Evaluations focused on the output of the full model. These activities seek to determine if the output is relevant, reliable, and useful. |
| **Scenario** | A specified set of conditions (*e.g.*, spatial, temporal, environmental, source, chemical) used to define a model setup for a particular simulation or set of simulations. |

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| **Sensitivity** | The rate of change of the model output with respect to changes in an input parameter. |
| **Simulation** | A single application of a model to estimate environmental conditions, based on a given scenario and any initial input values needed. |
| **Source** | An external component that introduces chemical mass directly into a compartment. |
| **Structural evaluations** | Evaluations focused on how changes in modeling complexity affect model performance. These activities seek to determine how the model will respond to being set up differently for different applications. |
| **Uncertainty** | The lack of knowledge regarding the actual values of model input variables (parameter uncertainty) and of physical systems (model uncertainty). |
| **Variability** | The diversity or heterogeneity in a population or parameter; sometimes referred to as natural variability. |
| **Volume Element** | A bounded three-dimensional space that defines the location of one or more compartments. This term is introduced to provide a consistent method for organizing objects that have a natural spatial relationship. |

# APPENDIX B
# Review of Methods for Conducting Uncertainty Analyses

As part of the TRIM model development process, the Agency has conducted and will continue to conduct uncertainty and variability analyses. To ensure that the most appropriate methods were selected for use in this effort, EPA conducted a literature search to identify the full range of the available methods and developed a set of selection criteria against which to compare those methods. This appendix describes the selection criteria and the review of available methods for use in connection with uncertainty and variability analyses for TRIM. The method that was selected is a two-stage approach consisting of a sensitivity/screening analysis followed by a detailed analysis of uncertainty and variability, as described in Chapter 3 and Section 4.7 of this report and in Chapter 6 of the TRIM.FaTE TSD Volume I.

## B.1 CRITERIA FOR METHOD SELECTION

The primary objectives for the overall approach for TRIM uncertainty and variability analyses were articulated as detailed criteria that characterize the desirable and undesirable features of the candidate uncertainty and variability analysis methods. These criteria were used to distinguish the available methods according to how well they might serve the objectives. Most of the criteria described below are necessary or highly desirable to support the analysis of uncertainty and variability for TRIM. The required criteria for a method to be used are listed first, followed by additional criteria that are desirable but not absolutely necessary for a method to be used in TRIM uncertainty and variability analyses.

### B.1.1 REQUIRED CRITERIA

- **Estimate uncertainty and variability separately, and maintain this separation throughout risk characterization and across module interfaces.** Uncertainty and variability have different meanings, and uncertainty may be reducible, while variability is not. The method should follow the distributions of both uncertainty and variability through the model, yielding uncertainty and variability distributions of the model outputs. The modular design of TRIM poses challenges for the propagation and analysis of uncertainty and variability, and it is important that the selected method be able to fit smoothly and accurately within the modular design and be able to transfer information between connected TRIM modules.

- **Evaluate sensitivity of both specific model inputs and model components.** In addition to the changes in the results which occur when the values of input variables are changed, it is useful to examine the changes in the results which occur when different algorithms are used in the mechanistic model.

- **Evaluate uncertainty and variability importance.** One of the key functions of the analysis methodology is to evaluate the importance, in terms of both uncertainty and variability, of specific model inputs and model components in relation to other inputs and components. This type of analysis provides insight into priorities for reducing uncertainty and allocating resources to the improved representation of uncertain and variable inputs. The ability to rank input parameters in order of their influence on the uncertainty of the model results is an important component of this function.

- **Identify and represent correlations and other interdependencies.** Physical processes or relationships can dictate that certain variable values change in concert with other variable values. The correlations can be weak or strong and can be negative or positive. Ignoring these relationships can introduce error into the risk assessment effort. Tracking these relationships can add substantial complexity and increase the computational resources necessary for the risk assessment effort. These correlations can exist between model input parameters or can be introduced within the model. The selected method should represent the input parameter correlations and follow these through the model with the structural correlations introduced by the model. It also should be able to identify correlations between sets of model inputs and outputs and between sets of intermediate variables.

- **Treat tails of distributions.** Some methods focus more on the central region of probability distributions and are less accurate in their treatment of extreme values. For risk assessment applications, accuracy in the tails of the probability distributions is very important. Therefore, the selected method should adequately treat infrequent but important events.

- **Evaluate relevant temporal and spatial scales.** The selected method should facilitate comparison of the results when different temporal or spatial scales are used, as the appropriate scale to use for modeling can directly impact model uncertainties.

- **Limit computational requirements.** The method should be computationally efficient and should not require excessive effort to set up or run.

- **Handle complex mathematical relationships.** Some available methods are designed for and more suited to models with simple mathematical constructs and cannot feasiblely handle more complex models. Other methods are designed to handle very mathematically complex models. The selected method for TRIM must be able to handle complex models.

- **Be easily automated.** Propagation and analysis of uncertainty and variability can require considerable effort, often in the form of large numbers of repetitions of model runs for numerical techniques and large numbers of algebraic manipulations for analytical techniques. The ability to automate the procedures is highly desirable to minimize effort and can provide the added advantage of reducing human errors.

### B.1.2 DESIRABLE CRITERIA

- **Use input distributions directly without further approximations or need to fit input distributions to standard analytical forms.** When the values for the input variables arise from certain specific types of physical processes or have certain natural properties, they may be accurately represented by standard analytical forms (*e.g.*, normal or lognormal probability density functions). When conditions are less than ideal, fitting the values to such distributions can introduce unnecessary error into the risk assessment effort, and the use of nonparametric representations may be preferable. Some of the methods evaluated assume analytical forms, while other methods handle a wide variety of representations of probability distributions. Some available methods require discretization of continuous distributions to be applied. The selected method should be able to handle the basic types of distributions that will be encountered.

- **Increase the level of precision in a simple manner.** Most of the uncertainty methodologies have some means of increasing the precision of uncertainty analysis results. For some methods, however, the procedures for doing so are substantially more difficult or require substantially more effort. The method selected for TRIM needs to provide a balance between precision and necessary effort.

- **Support investigation of model behavior and changes to the model.** Insight into the structure of the model can reveal the effects of model changes and why changes affect uncertainty as they do. Obtaining this insight typically involves analysis of the intermediate calculations performed within the model and keeping track of the uncertainties of the intermediate values calculated.

- **Reduce opportunities for human error in the uncertainty and variability analysis.** Complex models, large numbers of variables, significant amounts of hand processing for data entry, debugging, and programming of transfers across modules among other processes all create significant opportunities for error. A desirable method for uncertainty analysis will not increase the opportunities for error and, ideally, will expose errors of this type.

- **Maintain ability to track causal links and support auditing.** This feature involves maintaining an audit trail of processing within the model, keeping track of where significant changes occur through the model data flow. Primarily useful during the development of an application, this ability supports the interpretation of the meaning of results as well as the need to check for errors. This desired characteristic can be partially fulfilled by retaining intermediate results (*e.g.*, input and output distributions) and tracking linkages within the model.

- **Provide capabilities for additional analysis.** A single method may not be able to perform all of the envisioned types of uncertainty analyses, and other methods might be used to perform specific analyses in conjunction with the primary method selected. It is desirable for a method to be able to interface with other analysis tools.

- **Support model evaluation efforts.** A major effort during the development of TRIM is model evaluation (see Chapter 6 of this report), and it would be advantageous for the method to be capable of supporting this effort.

- **Build a reduced form model.** While not a method for analysis of uncertainty *per se*, some methods used in connection with uncertainty analyses are able to produce a "reduced form model" (an approximation to the simulation model which runs much faster while giving results reasonably consistent with the results of the full simulation model). This can be advantageous when the uncertainty method requires thousands of simulations by using the reduced form model for some of the simulations.

# B.2 DESCRIPTION OF AVAILABLE METHODS

Table B-1 presents descriptions of a number of available methods for analysis of model uncertainty and variability that were identified by EPA in its literature review. For each method, the strengths, weaknesses, and applicability for TRIM uncertainty analysis are summarized, with particular focus on TRIM.FaTE. The recommended uses of the methods reviewed, which are appropriate for a TRIM uncertainty and variability analysis, are summarized in Table B-2 and are described below.

## B.2.1 THE CORE UNCERTAINTY ANALYSIS METHOD

The core uncertainty analysis method selected for use in TRIM must be able to handle propagation of uncertainty and variability of the model input parameters, taking into account distributions of parameter uncertainty and variability and parameter dependencies. The method will be used to provide uncertainties of model outputs in terms of distributions of model outputs, joint distributions of model inputs and outputs, and summary scalar measures.

For performing a thorough uncertainty and variability analysis, the Monte Carlo method has a number of advantages over other methods described in Table B-1, and therefore it has been selected as the core uncertainty analysis method for TRIM. The primary advantages of this method are the reduction of the number of simulations required, the ability to use different ways of specifying parameter distributions, the ability to handle very complex models, and the propagation of variability, uncertainty, and parameter dependencies through the model that are reflected in the distributions of model outputs. The Monte Carlo method is a widely used method, with numerous papers and other publications describing the method and how to apply it (Frey and Rhodes 1996, Morgan and Henrion 1990, Thompson et al. 1992, U.S. EPA 1997, Vose 1996, SRA 1993).

**Table B-1**
**Available Methods for Analysis of Model Uncertainty and Variability**

| Method | Technique | Assumptions | Strengths | Weaknesses | Applicability to TRIM |
|---|---|---|---|---|---|
| **Monte Carlo** | Monte Carlo uses multiple iterations of random samples from model input distributions. Four sampling techniques include:<br>• Simple Monte Carlo;<br>• Latin Hypercube Sampling (LHS);<br>• Midpoint LHS; and<br>• Importance sampling. | • There are no specific assumptions; it works with any reasonable data set and does not require distributional assumptions other than reasonably complete distributions and correlations. | • Varied parameter distributions can be specified.<br>• It can handle correlations, dependencies, and complex model algorithms.<br>• Complexity is linear with the number of parameters.<br>• It can find confidence bounds for estimates of output distributions.<br>• Additional iterations increase precision.<br>• It provides insight into behavior of the model.<br>• It is widely used and accepted by the scientific community. | • Large numbers of parameters and correlations between parameters can require many iterations and large computing time requirements. (Note: a reduced form of the model can be used for some applications that significantly reduces the required computing time.) | Highly applicable: listed strengths are all desirable for TRIM.FaTE uncertainty analysis, and any of the four Monte Carlo techniques described would be applicable to TRIM requirements. |
| **Method of Moments (Taylor Series Expansion)** | The method of moments calculates partial derivatives of the mathematical expressions in the model and uses these to calculate effects of perturbing the data. The Taylor series expansion is a case of this method involving only first order derivatives. Analytical expressions for partial derivatives for each equation are coded into the model as a companion set of equations. Distributions of interest can be propagated through the model using derivatives to transform input distribution parameters to output distribution parameters. | • Distributions can be adequately parameterized by their means, variances, and other moments; distribution type/shape known *a priori*.<br>• All parameters are independent of each other.<br>• Mathematical expressions in the model are continuously differentiable. | • A well-known method, it has been extensively applied to a variety of applications.<br>• It can be effective for models where analytic expressions for all derivatives can be derived and coded. | • Techniques are usually very complex.<br>• Errors can be easily introduced when coding expressions for calculating derivatives.<br>• Computation of derivatives can be intractable for all but fairly simple models.<br>• Methods are not appropriate for some normality assumptions and distributional forms. | Not easily applicable: TRIM.FaTE algorithms are too complex to apply this method feasiblely. |

| Method | Technique | Assumptions | Strengths | Weaknesses | Applicability to TRIM |
|---|---|---|---|---|---|
| **Differential Sensitivity Analysis (DSA)** | DSA calculates partial derivatives of the mathematical expressions in the model (like method of moments, but uses additional techniques to reduce intractability of computing derivatives in complex models). Two classes of DSA methods exist: (1) specialized numerical procedures to efficiently calculate derivatives, and (2) symbolic differentiation methods to obtain derivatives through the use of computer programs that also generate code. | • Functions in model are continuously differentiable.<br>• Output distributions and the distributions propagated throughout the model are normal. | • It can be a powerful tool for local model sensitivity analysis when coupled with automated procedures for generating code required to calculate derivatives<br>• It can obtain derivatives even for complex models | • Procedures for calculating derivatives can be difficult and time-consuming to implement<br>• Smoothness assumptions may be violated by step-functions or discrete distributions used in risk assessment<br>• May not be able to integrate correlations unless DSA method is nested within a method that can | Not easily applicable for all cases; additional code would need to be developed to handle any discrete distributions due to the smoothness assumptions of DSA. |
| **Classification and Regression Trees (CART)** | CART uses a nonparametric, binary tree method to simultaneously treat ordered and categorical data in the same problem. It produces tree structures rather than predictive algorithms. | • No specific assumptions; it works with any reasonable data set and does not require distributional assumptions other than reasonably complete distributions and correlations | • It is applicable to large, high-dimensional data sets, non-homogeneous data, and sets with missing data.<br>• It can account for masking of variables in ranking parameters according to their influence on the classification of outcomes.<br>• It is robust with respect toward outliers.<br>• It uses conditional information and dependencies in the data<br>• Graphical tree structure produced can be relatively easy to understand and interpret. | • Complexity of results for complex models can hinder interpretation of analysis. | Possibly applicable through three uses:<br>• Reduced-form model that allows for faster simulations;<br>• A tool to examine model sensitivity to individual parameters; or<br>• A method that provides initial importance-ranking of parameters, taking into account dependencies. |

| Method | Technique | Assumptions | Strengths | Weaknesses | Applicability to TRIM |
|---|---|---|---|---|---|
| **Bootstrap Method** | Bootstrap uses Monte Carlo algorithms to sample the data for multiple replications in order to obtain a confidence interval or other measure of accuracy for an estimated statistic. It is used primarily to assess the accuracy of estimated parameters and model predictions. | • Sufficient data are available to generate distributions (specific amount of data required depends on the particular application). | • It can be used to assess accuracy for complex procedures relatively easily.<br>• It can be applied parametrically or nonparametrically<br>• It can use importance sampling methods to improve efficiency of estimating tail probabilities.<br>• With careful setup, it can be used with data having dependencies. | • It can give incorrect results if the nonparametric empirical distribution function deviates from the true distribution function in the tails<br>• It can give downwardly biased estimates when used for assessment of model prediction accuracy. (Note: modified bootstrap methods can help to alleviate this problem.) | Possibly applicable: it can be used for estimating statistics of the input parameters (*e.g.*, mean, variance, distributions, and confidence intervals). |
| **Response Surface Estimation** | Response Surface Estimation uses sets of inputs and outputs from numerous model runs in a general regression model to produce a sample response surface that functions as an estimate of the actual model response surface. The fitted response surface can be used to predict outcomes of the model given values of the input parameters. Usually, factorial-type designs are used to specify the model runs used to fit the surface. Model inputs can be sampled carefully to give higher importance to more influential parameters and to ensure full representation of distribution tails. | • Simulations performed to develop the surface will provide adequate coverage of the parameter-outcome space at resolutions that will capture variability and dependencies.<br>• Continuity and boundedness of response surface function exists.<br>• Response surface should not be extended beyond the region represented by the simulations. | • It is widely used, well understood, and simple to interpret.<br>• It is useful as an approximation of a reduced form of a complex model.<br>• It provides an overview of how a model responds to variations in the input values. | • It requires a very large number of model runs to estimate the fitted response surface, particularly if there are many correlated parameters.<br>• It can be tedious to estimate the accuracy of the sample response surface with respect to the full model response surface; this usually requires a second set of simulations . | It can serve as a reduced form replacement for TRIM.FaTE for fast simulations. Also, it could be used for sensitivity analyses in the initial ranking of model inputs according to contributions to model variability. |

| Method | Technique | Assumptions | Strengths | Weaknesses | Applicability to TRIM |
|---|---|---|---|---|---|
| **Combinatorial Scenarios / Discrete Probability Trees** | It produces *combinatorial scenarios* by selecting a small set of values for each input parameter and then running the model for all physically possible combinations of these parameters to form a grid on the response surface of the model. A *discrete probability tree* then analyzes results of these scenarios by using information about each parameter's probability. | • Chosen scenarios are representative of a range of scenarios. | • For models with few parameters, it provides insight into the structure of the influence of parameter uncertainty and variability on the model outcomes.<br>• Tree diagrams present results relatively clearly for models with few parameters. | • Number of combinatorial scenarios increases exponentially with the number of parameters, leading to extremely long analysis times for models with many variables | Not applicable: the large number of uncertain parameters and the complexity inherent to TRIM.FaTE renders the use of these methods computationally infeasible. |
| **Generalized Linear Models (GLM)** | This class of classical linear models includes the use of techniques like analysis of variance (ANOVA), linear regression, logit/probit, log-linear, and multinomial response models. These models can calculate an uncertainty partitioning based on deviance or the generalized Pearson chi-squared statistic. | • It uses second-order moment assumptions, primarily on how moments vary with respect to each other. | • Restrictive assumptions on the form of distributions are not needed.<br>• It handles both discrete and continuous covariates.<br>• It is relatively easy to apply. | • As a parametric method, it does not have the flexibility of nonparametric methods like classification and regression tree methods. | May be applicable as a first-order type analysis of importance of parameters, taking into account interactions between pairs of parameters. |
| **Neural Networks (artificial)** | Neural Networks consist of a collection of techniques for estimating functions. Networks are composed of a large number of simple processing elements and connections between the elements. Elements operate only on local information and store information via a training process where the network "learns" about the data using observed data. The trained network can then make predictions of model outputs. | • For neural networks without smoothing, no assumptions made regarding parameter distributions or complexity of the model. Networks with smoothing limit the complexity of the fitted model. | • It provides models that are flexible and non-linear.<br>• With sufficient training data, it can approximate any reasonable function of any degree of complexity.<br>• Complexity of the network can be controlled.<br>• As the number of model input parameters increases, computational complexity of the network does not increase exponentially. | • It has a tendency to overfit by using too many parameters.<br>• There are high time requirements for the analyst to properly apply the appropriate neural network techniques.<br>• For many applications, it offers no advantage over more simple standard statistical methods.<br>• Poor model performance results if a small amount of data is available for training the network. | Applicability uncertain: probably not enough data to make use of neural networks directly for TRIM.FaTE uncertainty procedures. Method may be applicable for developing a reduced model that would execute faster than TRIM.FaTE; however, other approaches may be more favorable for the analysis due to the weaknesses. |

**Table B-2**
**Recommended Uses of Applicable Methods**

| Method | Uncertainty Analysis Methods | Sensitivity Analysis Methods | Supplementary Analysis Methods | Reduced Form Models |
|---|---|---|---|---|
| Direct Sensitivity Calculations | | ✔ | | |
| Monte Carlo | ✔ | ✔ | | |
| Classification and Regression Trees | | | ✔ | ✔ |
| Response Surfaces | | | ✔ | |
| Combinatorial Methods | | | ✔ | |
| Generalized Linear Models | | | ✔ | |

Compared to the Monte Carlo approach, the other methods reviewed in Table B-1 would not function as well for the core uncertainty analysis method for TRIM.FaTE, for different reasons. Taylor series expansion and methods of moments only treat local sensitivity analyses and are not feasible for this application due to the complexity of the TRIM.FaTE algorithms. The number of uncertain parameters and the complexity of TRIM.FaTE also make the use of combinatorial methods (*e.g.*, discrete probability trees) computationally infeasible for a full analysis. Neural network approaches require more simulations than Monte Carlo and operate on an approximation to the model. Treatment of parameter and model dependencies in a neural network approach is not straightforward and would entail development of additional techniques, as would the use of differential sensitivity analysis. The remaining methods reviewed (*i.e.*, response surface estimation, bootstrap, generalized linear models, and classification and regression trees (CART)) do not adequately address the primary requirements for uncertainty analysis (*e.g.*, propagation of uncertainty).

### B.2.2 SENSITIVITY ANALYSIS METHODS

Sensitivity analysis and screening analysis are fast techniques for measuring changes in model results relative to changes in input parameters. These analyses provide a first-order determination of the influential parameters that will need to be included in the detailed uncertainty analysis. Sensitivity analyses often are conducted not only for the full model, but also for each modular component within the model. They also can be employed to uncover anomalies and verify that the model is performing as expected.

In addition to directly calculating parameter sensitivities (*e.g.*, elasticity and normalized sensitivity scores), response surface estimation and generalized linear models (GLM) can be used to characterize model sensitivity. These approaches require that a set of model simulations be performed that vary the parameter values according to some experimental design. Response surfaces involving many parameters are difficult to display and interpret and require more

simulations than direct calculation and therefore are not appropriate for TRIM sensitivity analysis. Measures of parameter importance are the primary result of sensitivity analysis and can be presented visually using graphs.

### B.2.3 SUPPLEMENTARY ANALYSIS METHODS

Much of the uncertainty and variability analysis will involve direct computation of measures of uncertainty and variability and summaries of relationships between different input parameter variability/uncertainty distributions as well as dependencies of the input distributions with model output distributions. Some of the methods described in Table B-1 can be used to perform supplementary analyses of results of the Monte Carlo simulations. The use of these methods can provide a better understanding of the uncertainty and variability process and can provide additional measures. These methods include response surface estimation, combinatorial scenarios, discrete probability trees, GLM, and CART.

### B.2.4 REDUCED FORM MODELS

Some of the available methods can be used to construct reduced form models (*i.e.*, simplified "models of the model") that, in the context of an uncertainty analysis, could be used for uncertainty propagation simulations. By substantially reducing the computational burden of model runs, the use of a reduced form model allows for a larger number of parameters to be treated and for more detailed results to be generated. This analysis would only need to be performed if the computational requirements for the detailed analysis using the full model are excessive. Reduced form models can be built using a variety of non-linear regression methods. CART could be used for this because it typically produces good models of non-linear systems, it is relatively easy to implement, it provides insight into the model itself, and the way that CART functions is not difficult to conceptualize and explain.

## References for Appendix B

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# APPENDIX C
# Input Values Being Developed for TRIM.FaTE Mercury Case Study

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| **SOURCE DATA** (for each source) | | | |
| Location of source | UTM coordinates (x,y) | [specific coordinates] | supplied by state agency |
| Height of emission source | m | specified by height of source compartment | supplied by state agency |
| Emission rate (for each chemical) | g/s | 1.75E-03 | supplied by state agency |
| **BACKGROUND DATA** (for each modeled chemical) | | | |
| Background concentration in each compartment | Soil: ng/$m^3$<br>Water: ng/l<br>Air: ng/$m^3$ | Soil: 100 [98% Hg(2), 2% MHg]<br>Water: 1000 [90% Hg(2), 10% MHg]<br>Air: 1 [100% Hg(0)] | based on ranges reported in U.S. EPA 1997 |
| **METEOROLOGICAL DATA** | | | |
| Horizontal wind speed | m/s | varies over time | NCDC 1997 |
| Horizontal wind direction | degrees | varies over time | NCDC 1997 |
| Vertical wind speed | m/s | varies over time | NCDC 1997 |
| Air temperature | °K | varies over time | NCDC 1997 |
| Precipitation | m/day | varies over time | NCDC 1997 |
| Mixing height | m | varies over time | NCDC 1997 |
| Relative humidity | unitless | varies over time | NCDC 1997 |
| **SPATIAL DATA** | | | |
| Height of each air VE[b] | m | Equal to mixing height | NCDC 1997 |
| Surface soil depth (for each surface soil VE) | m | 0.01 | professional judgment |
| Root zone depth (for each root zone VE) | m | 0.55 | McKone et al. 1998 |
| Vadose zone depth (for each vadose zone VE) | m | 0.76 | McKone et al. 1998 |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| Ground water layer depth (for each aquifer layer VE) | m | 3 | professional judgment |
| Surface water depth (for each surface water VE) | m | ponds: 3.0<br>rivers: [being developed] | supplied by state agency |
| Sediment layer depth (for each sediment layer VE) | m | ponds: 0.05<br>rivers: [being developed] | based on default from U.S. EPA 1997 |
| **ABIOTIC ENVIRONMENTAL SETTING DATA** | | | |
| **Air** (assumed same for all air compartments) | | | |
| Atmospheric dust load | kg[dust] / $m^3$[air] | 6.15E-08 | Bidleman 1988 |
| Dust density | kg[dust] / $m^3$[dust] | 1.40E+03 | Bidleman 1988 |
| Dry deposition velocity of air particulates | m / day | 5.00E+02 | McKone et al. 1998 |
| Washout ratio | [mass chem/volume rain] /[ mass chem/volume air] | 2.00E+05 | U.S. EPA 1997 |
| Surface area per volume of particles | $m^2$[area] / $m^3$[particles] | 5.71E-04 | Bidleman 1988 |
| Junge_C | m-Pa | 1.72E-01 | Pankow 1987 |
| Density of air | $g/cm^3$ | 1.20E-03 | U.S. EPA 1997 |
| Fraction organic matter on particulates | unitless | 2.00-01 | Harner and Bidleman 1998 |
| Diffusion coefficient of water in air | $m^2/d$ | 2.16E+00 | Riederer 1995 |
| Boundary layer thickness in air above soil | m | 5.00E-03 | McKone et al. 1998 |
| **Surface Soil** (assumed same for all surface soil compartments) | | | |
| Water content | volume[water] / volume[compartment] | 1.60E-01 | McKone et al. 1998 |
| Air content | volume[air] / volume[compartment] | 4.38E-01 | McKone et al. 1998 |
| Soil material density | kg[soil] / $m^3$[soil] | 2.60E+03 | McKone et al. 1998 |
| Organic carbon fraction | unitless | 1.66E-02 | McKone et al. 1998 |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| Air soil boundary thickness | m | 5.00E-03 | Thibodeaux 1996 |
| Default depth of runoff water | m | 5.00E-03 | approximated from a typical runoff rate and number of rain events |
| Fraction of area available for vertical diffusion | $m^2$[area available] / $m^2$[total] | 1.00E+00 | area assumed rural |
| Fraction of area available for erosion | $m^2$[area available] / $m^2$[total] | 1.00E+00 | area assumed rural |
| Fraction of area available for runoff | $m^2$[area available] / $m^2$[total] | 1.00E+00 | area assumed rural |
| **Root Zone** (assumed same for all root zone compartments) | | | |
| Water content | volume[water] / volume[compartment] | 1.61E-01 | McKone et al. 1998 |
| Air content | volume[air] / volume[compartment] | 3.60E-01 | McKone et al. 1998 |
| Soil material density | kg[soil] / $m^3$[soil] | 2.60E+03 | Siever 1986 |
| Organic carbon fraction | unitless | 1.66E-02 | McKone et al. 1998 |
| **Vadose Zone** (assumed same for all vadose zone compartments) | | | |
| Water content | volume[water] / volume[compartment] | 1.60E-01 | McKone et al. 1998 |
| Air content | volume[air] / volume[compartment] | 2.16E-01 | McKone et al. 1998 |
| Soil material density | kg[soil] / $m^3$[soil] | 2.60E+03 | McKone et al. 1998 |
| Organic carbon fraction | unitless | 1.28E-03 | McKone et al. 1998 |
| **Ground Water** (assumed same for all ground water compartments) | | | |
| Porosity | volume[total pore space] / volume[compartment] | 2.00E-01 | McKone et al. 1998 |
| Solid material density in aquifer | kg[soil] / $m^3$[soil] | 2.60E+03 | McKone et al. 1998 |
| Organic carbon fraction | unitless | 1.00E-02 | Schwarzenbach et al. 1993 |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| **Surface Water** (depends on water body type - values provided have been developed for an initial simple water body scenario) | | | |
| Flush rate | flushes/year | 4.31 | supplied by state agency |
| Suspended sediment concentration | kg[sediment] / $m^3$[water column] | 0.8E-03 | Schwalen and Kiefer 1996 |
| Evaporation of water | $m^3$[water] / $m^2$[area]-day | 9.45E-05 | van der Leeden et al. 1990 |
| Current velocity | m/s | 0 | professional judgment |
| Organic carbon fraction in suspended sediments | unitless | 0.02 | McKone et al. 1998 |
| Suspended sediment density | kg[sediment] / $m^3$[sediment] | 2600 | McKone et al. 1998 |
| Boundary layer thickness above sediment | m | 2.00E-02 | McKone et al. 1998 |
| Drag coefficient for water body | unitless | 0.0011 | Ambrose et al. 1995 |
| Viscous sublayer thickness | m | 4 | Ambrose et al. 1995 |
| pH | unitless | 6.5 | supplied by state agency |
| Chloride concentration | mg/L | 56 | supplied by state agency |
| **Sediment** (depends on associated water body type) | | | |
| Organic carbon fraction | unitless | 2.00E-02 | McKone et al. 1998 |
| Solid material density in sediment | kg[sediment] / $m^3$[sediment] | 2.60E+03 | McKone et al. 1998 |
| Porosity of the sediment zone | volume[total pore space] / volume[sediment compartment] | 2.00E-01 | McKone et al. 1998 |
| Benthic solids concentration | kg[sediment] / $m^3$[sediment compartment] | 2.08E+03 | professional judgment |

| Input Parameter | Input Units | Value[a] | | | Reference |
|---|---|---|---|---|---|
| **ABIOTIC CHEMICAL-SPECIFIC DATA** (for each chemical) | | | | | |
| **General to All Media** | | | | | |
| | | **Hg(0)** | **Hg(2)** | **MHg** | |
| Molecular weight | g/mol | 2.01E+02 | 2.01E+02 | 2.16E+02 | U.S. EPA 1997 |
| Octanol-water partition coefficient ($K_{ow}$) | L[water] / L[octanol] | 4.15E+00 | 3.33E+00 | 1.70E+00 | Mason et al. 1996 |
| Melting point | °K | 2.34E+02 | 5.50E+02 | 4.43E+02 | CARB 1994 |
| Water solubility | mol / $m^3$ | 3.00E-04 | 3.30E+02 | NA | CARB 1994 |
| Henry's Law constant | Pa-$m^3$ / mol | 7.10E-03 | 7.10E-10 | 4.70E-07 | U.S. EPA 1997 |
| Diffusion coefficient in pure air | $m^2$ / day | 4.78E-01 | 4.78E-01 | 4.56E-01 | U.S. EPA 1997 |
| Diffusion coefficient in pure water | $m^2$ / day | 5.54E-05 | 5.54E-05 | 5.28E-05 | U.S. EPA 1997 |
| **Surface Soil** | | | | | |
| Methylation rate constant for Hg(2) to MHg | 1/day | 1.00E-03 | | | range reported in Porvari and Verta (1995) is 2E-4 to 1E-3 /day; value is average maximum potential methylation rate constant under anaerobic conditions |
| Demethylation rate constant for MHg to Hg(2) | 1/day | 0.06 | | | range reported in Porvari and Verta (1995) is 3E-2 to 6E-2 /day; value is average maximum potential demethylation rate constant under anaerobic conditions |
| Reduction rate constant for Hg(2) to Hg(0) | 1/day | 1.25E-05 | | | value used for untilled surface soil (2cm), 10% moisture content, in U.S. EPA 1997; general range is (0.0013/day)*moisture content to (0.0001/day)*moisture content for forested region (Lindberg 1996; Carpi and Lindberg 1997) |
| Oxidation rate constant for Hg(0) to Hg(2) | 1/day | 1.00E-08 | | | small default nonzero value (0 assumed in U.S. EPA 1997) |
| **Root Zone** | | | | | |
| Methylation rate constant for Hg(2) to MHg | 1/day | 1.00E-03 | | | range reported in Porvari and Verta (1995) is 2E-4 to 1E-3 /day; value is average maximum potential methylation rate constant under anaerobic conditions |
| Demethylation rate constant for MHg to Hg(2) | 1/day | 0.06 | | | range reported in Porvari and Verta (1995) is 3E-2 to 6E-2 /day; value is average maximum potential demethylation rate constant under anaerobic conditions |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| Reduction rate constant for Hg(2) to Hg(0) | 1/day | 3.25E-06 | value used for tilled surface soil (20cm), 10% moisture content in U.S. EPA 1997 (Lindberg 1996; Carpi and Lindberg, 1997) |
| Oxidation rate constant for Hg(0) to Hg(2) | 1/day | 1.00E-08 | small default nonzero value (0 assumed in U.S. EPA 1997) |
| **Vadose Zone** | | | |
| Methylation rate constant for Hg(2) to MHg | 1/day | 1.00E-03 | range reported in Porvari and Verta (1995) is 2E-4 to 1E-3 /day; value is average maximum potential methylation rate constant under anaerobic conditions |
| Demethylation rate constant for MHg to Hg(2) | 1/day | 0.06 | range reported in Porvari and Verta (1995) is 3E-2 to 6E-2 /day; value is average maximum potential demethylation rate constant under anaerobic conditions |
| Reduction rate constant for Hg(2) to Hg(0) | 1/day | 3.25E-06 | value used for tilled surface soil (20cm), 10% moisture content in U.S. EPA 1997 (Lindberg 1996; Carpi and Lindberg 1997) |
| Oxidation rate constant for Hg(0) to Hg(2) | 1/day | 1.00E-08 | small default nonzero value (0 assumed in U.S. EPA 1997) |
| **Ground Water** | | | |
| Methylation rate constant for Hg(2) to MHg | 1/day | 1.00E-03 | range reported in Porvari and Verta (1995) is 2E-4 to 1E-3 /day; value is average maximum potential methylation rate constant under anaerobic conditions |
| Demethylation rate constant for MHg to Hg(2) | 1/day | 0.06 | range reported in Porvari and Verta (1995) is 3E-2 to 6E-2 /day; value is average maximum potential demethylation rate constant under anaerobic conditions |
| Reduction rate constant for Hg(2) to Hg(0) | 1/day | 3.25E-06 | value used for tilled surface soil (20cm), 10% moisture content in U.S. EPA 1997 (Lindberg 1996; Carpi and Lindberg, 1997) |
| Oxidation rate constant for Hg(0) to Hg(2) | 1/day | 1.00E-08 | small default nonzero value (0 assumed in U.S. EPA 1997) |
| **Surface Water** | | | |
| Methylation rate constant for Hg(2) to MHg | 1/day | 1.00E-03 | value used in U.S. EPA 1997; range is from 1E-4 to 3E-4/day (Gilmour and Henry 1991) |
| Demethylation rate constant for MHg to Hg(2) | 1/day | 0.0130 | average of range of 1E-3 to 2.5E-2/day from Gilmour and Henry (1991) |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| Reduction rate constant for Hg(2) to Hg(0) | 1/day | 7.50E-03 | value used in U.S. EPA 1997; reported values range from less than 5E-3/day for depths greated than 17m, up to 3.5/day (Xiao et al. 1995; Vandal et al. 1995; Mason et al. 1995a; Amyot et al. 1997) |
| Oxidation rate constant for Hg(0) to Hg(2) | 1/day | 1.00E-08 | small default nonzero value (0 assumed in U.S. EPA 1997) |
| **Sediment** | | | |
| Methylation rate constant for Hg(2) to MHg | 1/day | 1.00E-04 | value used in U.S. EPA 1997; range is from 1E-5 to 1E-1/day (Gilmour and Henry 1991) |
| Demethylation rate constant for MHg to Hg(2) | 1/day | 0.0501 | average of range of 2E-4 to 1E-1/day from Gilmour and Henry (1991) |
| Reduction rate constant for Hg(2) to Hg(0) | 1/day | 1.00E-06 | inferred value based on presence of Hg(0) in sediment porewater (U.S. EPA 1997; Vandal et al. 1995) |
| Oxidation rate constant for Hg(0) to Hg(2) | 1/day | 1.00E-08 | small default nonzero value (0 assumed in U.S. EPA 1997) |
| **ABIOTIC FLOW DATA** | | | |
| Total erosion rate from soil | kg[soil] / $m^2$[area]-day | 2.89E-04 | van der Leeden et al. 1990 |
| Erosion rates between soil and soil | kg[soil] / $m^2$[area]-day | parcel-specific | professional judgment |
| Erosion rates between soil and surface water | kg[soil] / $m^2$[area]-day | parcel-specific | professional judgment |
| Total runoff rate from soil | $m^3$[water] / $m^2$[area]-day | 1.01E-03 | van der Leeden et al. 1990 |
| Runoff rates between soil and soil | $m^3$[water] / $m^2$[area]-day | parcel-specific | professional judgment |
| Runoff rates between soil and surface water | $m^3$[water] / $m^2$[area]-day | parcel-specific | professional judgment |
| Percolation rates between soil and soil | $m^3$[water] / $m^2$[area]-day | 0.2 x rainfall rate | professional judgement |
| Surface water flow between surface water compartments | $m^3$[water] / $m^2$[area]-day | ponds: 0<br>rivers: NA | professional judgment |
| Recharge from ground water to surface water | $m^3$[water] / $m^2$[area]-day | being developed | professional judgment |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| Deposition of suspended sediment in the water column to the sediment bed | kg[sediment] / $m^2$[area]-day | 1.3E+01 | McKone et al. 1998 |
| Resuspension of sediment from the sediment bed to the water column | kg[sediment] / $m^2$[area]-day | 1.00E-04 | McKone et al. 1998 |
| Burial rate of sediment in the sediment bed | kg[sediment] / $m^2$[area]-day | calculated assuming net solid deposition to sediment is zero | professional judgment |
| **BIOTIC ENVIRONMENTAL SETTING DATA** (for each relevant compartment) | | | |
| **ANIMALS - AQUATIC** | | | |
| **Water Column Carnivore - Bass** | | | |
| Body weight (BW) | kg | 2.00E+00 | professional judgment |
| Fraction lipid weight | unitless | 1.00E-01 | value from Thomann 1989 |
| Biomass per area | km/ $m^2$ | 5.97E-04 | mean of data from 11 lakes in Kelso and Johnson (1991) |
| Population per area | # / $m^2$ | calculated | biomass per area divided by body weight of individual |
| Ventilation rate | ml / min / kg | 5.00E+02 | low end of range, 500-6000, in Thomann 1989 |
| Fraction of food diet comprised of fish omnivores | unitless | 1.00E+00 | value set based on definition of trophic levels |
| Fraction of food diet comprised of fish herbivores | unitless | 0.00E+00 | value set based on definition of trophic levels |
| Fraction of food diet comprised of fish carnivores | unitless | 0.00E+00 | value set based on definition of trophic levels |
| Fraction of food diet comprised of mayfly nymph | unitless | 0.00E+00 | value set based on definition of trophic levels |
| **Water Column Herbivore - Bluegill** | | | |
| Body weight (BW) | kg | 2.50E-02 | professional judgment |
| Fraction lipid weight | unitless | 1.00E-01 | value from Thomann 1989 |
| Biomass per area | kg / $m^2$ | 1.65E-03 | based on data from 11 lakes in Kelso and Johnson (1991) |
| Population per area | # / $m^2$ | calculated | biomass per area divided by body weight of individual |
| Ventilation rate | ml / min / kg | 5.00E+02 | low end of range, 500-6000, in Thomann 1989 |
| Fraction of food diet comprised of phytoplankton (algae) | unitless | 1.00E+00 | value set based on definition of trophic levels |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| Fraction of food diet comprised of macrophyte | unitless | 0.00E+00 | value set based on definition of trophic levels |
| Fraction of diet_mayfly | unitless | 0.00E+00 | value set based on definition of trophic levels |
| **Water Column Omnivore - Channel Catfish** | | | |
| Body weight (BW) | kg | 5.00E-01 | professional judgment |
| Fraction lipid weight | unitless | 0.1 | value from Thomann 1989 |
| Biomass per area | kg/ $m^2$ | 1.67E-04 | mean of data from 11 lakes in Kelso and Johnson (1991) |
| Population per area | # / $m^2$ | calculated | biomass per area divided by body weight of individual |
| Ventilation rate | ml / min / kg | 500 | low end of range, 500-6000, in Thomann 1989 |
| Fraction of food diet comprised of macrophyte | unitless | 0.00E+00 | value set based on definition of trophic levels |
| Fraction of food diet comprised of mayfly nymph | unitless | 0.00E+00 | value set based on definition of trophic levels |
| Fraction of food diet comprised of omnivore | unitless | 0.00E+00 | value set based on definition of trophic levels |
| Fraction of food diet comprised of fish herbivores | unitless | 1.00E+00 | value set based on definition of trophic levels |
| **Benthic Omnivore** | | | |
| Body weight (BW) | kg | 0.500 | professional judgment |
| Fraction lipid weight | unitless | 0.1 | value from Thomann 1989 |
| Biomass per area | kg/$m^2$ | 1.39E-03 | mean of data from 11 lakes in Kelso and Johnson (1991) |
| Population per area | # / $m^2$ | calculated | biomass per area divided by body weight of individual |
| Ventilation rate | ml / min / kg | 500 | low end of range, 500-6000, in Thomann 1989 |
| Fraction of diet comprised of benthic invertebrates | unitless | 1.00E+00 | value set based on definition of trophic levels |
| **Benthic Carnivore** | | | |
| Body weight (BW) | kg | 2.0 | professional judgment |
| Fraction lipid weight | unitless | 0.1 | value from Thomann 1989 |
| Biomass per area | kg/$m^2$ | 7.14E-04 | mean of data from 11 lakes in Kelso and Johnson (1991) |
| Population per area | # / $m^2$ | calculated | biomass per area divided by body weight of individual |
| Ventilation rate | ml / min / kg | 500 | low end of range, 500-6000, in Thomann 1989 |
| Fraction of diet comprised of benthic omnivores | unitless | 1.00E+00 | value set based on definition of trophic levels |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| **PLANTS - AQUATIC** | | | |
| **Macrophyte** | | | |
| Biomass per area | $kg/m^2$ | 0.1 | Bonar et al. 1993 |
| Density of macrophytes | $kg/m^3$ | 1000 | professional judgment |
| **Phytoplankton - Algae** | | | |
| Diameter of algae | μm | 2.5 | Mason et al. 1995b |
| Average cell density (per vol cell, not water) | $g/\mu m^3$ | 1.00E-12 | Mason et al. 1995b, Mason et al. 1996 |
| Algae growth rate | 1/day | 0.7 | Hudson et al. 1994 as cited in Mason et al. 1995b |
| Algae density in water column | g[algae]/L[water] | 2.50E-03 | derived from Millard et al. 1996 |
| Algae carbon content (fraction) | unitless | 4.65E-01 | APHA 1995 |
| Algae water content (fraction) | unitless | 9.00E-01 | APHA 1995 |
| **ANIMALS - TERRESTRIAL** | | | |
| **Soil Detritivore - Earthworm** | | | |
| Density per soil area, deciduous forest | kg[worm] / $m^2$ [area] | 4.50E-02 | avg of oak and beech values in Satchell 1983 |
| Density per soil area, coniferous forest | kg[worm] / $m^2$ [area] | 2.20E-02 | pine forest in Satchell 1983 |
| Density per soil area, grass/herb | kg[worm] / $m^2$ [area] | 5.00E-03 | avg of 0.0032 and 0.0075, range on grassland in Tennessee, Lee 1985 |
| Density | kg[worm] / L[volume] | 1.00E+00 | professional judgment |
| Water content of worm | mass fraction | 8.40E-01 | U.S. EPA 1993 |
| **Soil Detritivore - Soil Arthropod** | | | |
| Body weight (BW) | kg | 1.31E-04 | grasshopper, Porter et al. 1996 |
| Biomass per area | kg / $m^2$ | 3.01E-04 | grasshopper, Porter et al. 1996 |
| **Terrestrial Ground-Invertebrate Feeder - Black-capped Chickadee** | | | |
| Body weight (BW) | kg | 1.08E-02 | Dunning 1993 |
| Population per area | # / $m^2$ | 3.50E-05 | avg of 0.2 and 0.3 /ha in British Columbia, Smith 1993 |
| Soil ingestion rate | kg[soil] / kg BW-day | 0.00E+00 | assumed, rarely observed on ground, Smith 1993 |
| Water_a | unitless | 5.90E-02 | Calder and Braun 1983 |
| Water_b | unitless | 6.70E-01 | Calder and Braun 1983 |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| Inhalation_a | unitless | 4.09E-01 | Lasiewski and Calder 1971 |
| Inhalation_b | unitless | 8.00E-01 | Lasiewski and Calder 1971 |
| Food ingestion rate | kg[food] / kg BW-day | 7.40E-01 | calculated from Bell 1990, Dunning 1993 |
| Fraction of food diet comprised on plants | unitless | 3.00E-01 | Sample et al. 1993, Smith 1993, Martin et al. 1951 |
| Fraction of food diet comprised of benthic invertebrates | unitless | 7.00E-01 | Sample et al. 1993, Smith 1993, Martin et al. 1951 |
| Fraction excretion to soil | unitless | 1.00E+00 | professional judgment |
| Fraction excretion to water | unitless | 0.00E+00 | professional judgment |
| **Semiaquatic Piscivore - Kingfisher** | | | |
| Body weight (BW) | kg | 1.48E-01 | Dunning 1993 |
| Population per area | # / $m^2$ | 4.00E-07 | Fry and Fry 1992 |
| Soil ingestion rate | kg[soil] / kg BW-day | 0.00E+00 | professional judgment |
| Water_a | unitless | 5.90E-02 | Calder and Braun 1983 |
| Water_b | unitless | 6.70E-01 | Calder and Braun 1983 |
| Inhalation_a | unitless | 4.09E-01 | Lasiewski and Calder 1971 |
| Inhalation_b | unitless | 8.00E-01 | Lasiewski and Calder 1971 |
| Food ingestion rate | kg[food] / kg BW-day | 7.40E-02 | Alexander 1977 |
| Fraction of food diet comprised of water column herbivore | unitless | 0.16 | assumed based on approximate trophic levels of several consumed fish species |
| Fraction of food diet comprised of water column omnivore | unitless | 0.16 | assumed based on approximate trophic levels of several consumed fish species |
| Fraction of food diet comprised of benthic omnivore | unitless | 0.325 | assumed based on approximate trophic levels of several consumed fish species |
| Fraction excretion to soil | unitless | 5.00E-01 | professional judgment |
| Fraction excretion to water | unitless | 5.00E-01 | professional judgment |
| **Semiaquatic Predator/Scavenger - Bald eagle** | | | |
| Body weight (BW) | kg | 4.74E+00 | Dunning 1993 |
| Population per area | # / $m^2$ | 1.30E-08 | supplied by state agency |
| Soil ingestion rate | kg[soil] / kg BW-day | 0.00E+00 | professional judgment |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| Water_a | unitless | 5.90E-02 | Calder and Braun 1983 |
| Water_b | unitless | 6.70E-01 | Calder and Braun 1983 |
| Inhalation_a | unitless | 4.09E-01 | Lasiewski and Calder 1971 |
| Inhalation_b | unitless | 8.00E-01 | Lasiewski and Calder 1971 |
| Food ingestion rate | kg[food] / kg BW-day | 7.40E-02 | U.S. EPA 1995 |
| Fraction of food diet comprised of mouse | unitless | 2.30E-01 | professional judgment |
| Fraction of food diet comprised of chickadee | unitless | 1.00E-01 | professional judgment |
| Fraction of food diet comprised of water column herbivore | unitless | 0.11 | assumed based on approximate trophic levels of several consumed fish species |
| Fraction of food diet comprised of water column omnivore | unitless | 0.11 | assumed based on approximate trophic levels of several consumed fish species |
| Fraction of food diet comprised of water column carnivore | unitless | 0.11 | assumed based on approximate trophic levels of several consumed fish species |
| Fraction of food diet comprised of benthic omnivore | unitless | 0.17 | assumed based on approximate trophic levels of several consumed fish species |
| Fraction of food diet comprised of benthic carnivore | unitless | 0.17 | assumed based on approximate trophic levels of several consumed fish species |
| Fraction excretion to soil | unitless | 5.00E-01 | professional judgment |
| Fraction excretion to water | unitless | 5.00E-01 | professional judgment |
| **Semiaqautic Piscivore - Common Loon** | | | |
| Body weight (BW) | kg | 4.13E+00 | Dunning 1993 |
| Population per area | # / $m^2$ | 4.90E-08 | W. Jakubas, Maine Dept Inland Fisheries & Wildlife |
| Soil ingestion rate | kg[soil] / kg BW-day | 0.00E+00 | professional judgment |
| Water_a | unitless | 5.90E-02 | Calder and Braun 1983 |
| Water_b | unitless | 6.70E-01 | Calder and Braun 1983 |
| Inhalation_a | unitless | 4.09E-01 | Lasiewski and Calder 1971 |
| Inhalation_b | unitless | 8.00E-01 | Lasiewski and Calder 1971 |
| Food ingestion rate | kg[food] / kg BW-day | 2.30E-01 | Barr 1996 |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| Fraction of diet comprised of water column herbivore | unitless | 1.00E+00 | assumed based on approximate size range of fish consumed |
| Fraction excretion to soil | unitless | 5.00E-01 | professional judgment |
| Fraction excretion to water | unitless | 5.00E-01 | professional judgment |
| **Semiaquatic Omnivore - Mallard** | | | |
| Body weight (BW) | kg | 1.13E+00 | Nelson and Martin 1953 |
| Population per area | # / $m^2$ | 9.30E-06 | average of 0.012 and 0.174/ha, North Dakota, U.S. EPA 1993 |
| Soil ingestion rate | kg[soil] / kg BW-day | 3.30E-03 | Beyer et al. 1994 |
| Water_a | unitless | 5.90E-02 | Calder and Braun 1983 |
| Water_b | unitless | 6.70E-01 | Calder and Braun 1983 |
| Inhalation_a | unitless | 4.09E-01 | Lasiewski and Calder 1971 |
| Inhalation_b | unitless | 8.00E-01 | Lasiewski and Calder 1971 |
| Food ingestion rate | kg[food] / kg BW-day | 1.00E-01 | Heinz et al. 1987 |
| Fraction of food diet comprised of plant | unitless | 6.65E-01 | Martin et al. 1951 |
| Fraction of food diet comprised of benthic invertebrate | unitless | 3.35E-01 | professional judgment |
| Fraction excretion to soil | unitless | 5.00E-01 | professional judgment |
| Fraction excretion to water | unitless | 5.00E-01 | professional judgment |
| **Terrestrial Predator/Scavenger - Red-tailed Hawk** | | | |
| Body weight (BW) | kg | 1.13E+00 | North America, Dunning 1993 |
| Population per area | # / $m^2$ | 7.00E-07 | average of range 0.0034 and 0.01 for Colorado, U.S. EPA 1993 |
| Soil ingestion rate | kg[soil] / kg BW-day | 0.00E+00 | professional judgment |
| Water_a | unitless | 5.90E-02 | Calder and Braun 1983 |
| Water_b | unitless | 6.70E-01 | Calder and Braun 1983 |
| Inhalation_a | unitless | 4.09E-01 | Lasiewski and Calder 1971 |
| Inhalation_b | unitless | 8.00E-01 | Lasiewski and Calder 1971 |
| Food ingestion rate | kg[food] / kg BW-day | 1.20E-01 | Preston and Beane 1993 |
| Fraction of food diet comprised of soil arthropod | unitless | 4.00E-02 | approximate from Sherrod 1978 |
| Fraction of food diet comprised of chickadee | unitless | 2.57E-01 | approximate from Sherrod 1978 |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| Fraction of food diet comprised of mouse | unitless | 3.03E-01 | approximate from Sherrod 1978 |
| Fraction of food diet comprised of short tailed shrew | unitless | 2.00E-01 | approximate from Sherrod 1978 |
| Fraction of food diet comprised of vole | unitless | 2.00E-01 | approximate from Sherrod 1978 |
| Fraction excretion to soil | unitless | 1.00E+00 | professional judgment |
| Fraction excretion to water | unitless | 0.00E+00 | professional judgment |
| **Terrestrial Insectivore - Tree Swallow** | | | |
| Body weight (BW) | kg | 2.01E-02 | Dunning 1993 |
| Population per area | # / $m^2$ | 7.00E-04 | De Graaf et al. 1981 |
| Soil ingestion rate | kg[soil] / kg BW-day | 0.00E+00 | professional judgment |
| Water_a | unitless | 5.90E-02 | Calder and Braun 1983 |
| Water_b | unitless | 6.70E-01 | Calder and Braun 1983 |
| Inhalation_a | unitless | 4.09E-01 | Lasiewski and Calder 1971 |
| Inhalation_b | unitless | 8.00E-01 | Lasiewski and Calder 1971 |
| Food ingestion rate | kg[food] / kg BW-day | 1.98E-01 | Preston and Beane 1993 |
| Fraction of food diet comprised of benthic invertebrate | unitless | 1.00E+00 | professional judgment |
| Fraction excretion to soil | unitless | 1.00E+00 | professional judgment |
| Fraction excretion to water | unitless | 0.00E+00 | professional judgment |
| **Terrestrial Herbivore - Meadow Vole** | | | |
| Body weight (BW) | kg | 4.41E-02 | Reich 1981 |
| Population per area | # / $m^2$ | 6.00E-03 | average of 0.011/$m^2$, Klaas et al. 1998, and 0.0015/$m^2$, Getz 1961 |
| Soil ingestion rate | kg[soil] / kg BW-day | 2.30E-03 | Beyer et al. 1994 |
| Water_a | unitless | 9.90E-02 | Calder and Braun 1983 |
| Water_b | unitless | 9.00E-01 | Calder and Braun 1983 |
| Inhalation_a | unitless | 5.46E-01 | Stahl 1967 |
| Inhalation_b | unitless | 8.00E-01 | Stahl 1967 |
| Food ingestion rate | kg[food] / kg BW-day | 9.70E-02 | mean for Microtus spp., Dark et al. 1983 |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| Fraction of food diet comprised of plant | unitless | 1.00E+00 | professional judgment |
| Fraction excretion to soil | unitless | 1.00E+00 | professional judgment |
| Fraction excretion to water | unitless | 0.00E+00 | professional judgment |
| **Terrestrial Predator/Scavenger - Long-tailed Weasel** | | | |
| Body weight (BW) | kg | 1.47E-01 | Mumford and Whitaker 1982 |
| Population per area | # / $m^2$ | 6.50E-06 | average of 6-7/ha, Svendsen 1982 |
| Soil ingestion rate | kg[soil] / kg BW-day | 0.00E+00 | professional judgment |
| Water_a | unitless | 9.90E-02 | Calder and Braun 1983 |
| Water_b | unitless | 9.00E-01 | Calder and Braun 1983 |
| Inhalation_a | unitless | 5.46E-01 | Stahl 1967 |
| Inhalation_b | unitless | 8.00E-01 | Stahl 1967 |
| Food ingestion rate | kg[food] / kg BW-day | 7.35E-02 | calc from Brown and Lasiewski 1972, Golley 1961, U.S. EPA 1993 |
| Fraction of food diet comprised of mouse | unitless | 5.00E-01 | professional judgment |
| Fraction of food diet comprised of vole | unitless | 2.50E-01 | professional judgment |
| Fraction of food diet comprised of shrew | unitless | 2.50E-01 | professional judgment |
| Fraction excretion to soil | unitless | 1.00E+00 | professional judgment |
| Fraction excretion to water | unitless | 0.00E+00 | professional judgment |
| **Semiaquatic Omnivore - Mink** | | | |
| Body weight (BW) | kg | 8.32E-01 | Mumford and Whitaker 1982 |
| Population per area | # / $m^2$ | 5.75E-05 | avg of 0.01 and 0.1/ha for general US, U.S. EPA 1993 |
| Soil ingestion rate | kg[soil] / kg BW-day | 0.00E+00 | professional judgment |
| Water_a | unitless | 9.90E-02 | Calder and Braun 1983 |
| Water_b | unitless | 9.00E-01 | Calder and Braun 1983 |
| Inhalation_a | unitless | 5.46E-01 | Stahl 1967 |
| Inhalation_b | unitless | 8.00E-01 | Stahl 1967 |
| Food ingestion rate | kg[food] / kg BW-day | 1.40E-01 | mink in captivity, Bleavins and Aulerich 1981 |
| Fraction of food diet comprised of mouse | unitless | 2.30E-01 | Hamilton 1940, Sealander 1943, Korschgen 1958, Burgess and Bider 1980 |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| Fraction of food diet comprised of vole | unitless | 2.30E-01 | Hamilton 1940, Sealander 1943, Korschgen 1958, Burgess and Bider 1980 |
| Fraction of diet comprised of water column herbivore | unitless | 7.00E-02 | assumed based on approximate trophic levels of several consumed fish species |
| Fraction of diet comprised of water column omnivore | unitless | 7.00E-02 | assumed based on approximate trophic levels of several consumed fish species |
| Fraction of diet comprised of benthic omnivore | unitless | 1.50E-01 | assumed based on approximate trophic levels of several consumed fish species |
| Fraction of food diet comprised of benthic invertebrate | unitless | 1.70E-01 | Hamilton 1940, Sealander 1943, Korschgen 1958, Burgess and Bider 1980 |
| Fraction of food diet comprised of chickadee | unitless | 8.00E-02 | Hamilton 1940, Sealander 1943, Korschgen 1958, Burgess and Bider 1980 |
| Fraction excretion to soil | unitless | 5.00E-01 | professional judgment |
| Fraction excretion to water | unitless | 5.00E-01 | professional judgment |
| **Terrestrial Omnivore - White-footed Mouse** | | | |
| Body weight | kg | 2.12E-02 | North America, Silva and Downing 1995 |
| Population per area | # / $m^2$ | 3.15E-03 | average of range 6-57/ha, Wolff 1985 |
| Soil ingestion rate | kg[soil] / kg BW-day | 2.00E-02 | Beyer et al. 1994 |
| Water_a | unitless | 9.90E-02 | Calder and Braun 1983 |
| Water_b | unitless | 9.00E-01 | Calder and Braun 1983 |
| Inhalation_a | unitless | 5.46E-01 | Stahl 1967 |
| Inhalation_b | unitless | 8.00E-01 | Stahl 1967 |
| Food ingestion rate | kg[food] / kg BW-day | 1.51E-01 | Green and Millar 1987 |
| Fraction of food diet comprised of worm | unitless | 5.00E-01 | professional judgment |
| Fraction of food diet comprised of plant | unitless | 5.00E-01 | professional judgment |
| Fraction excretion to soil | unitless | 5.00E-01 | professional judgment |
| Fraction excretion to water | unitless | 5.00E-01 | professional judgment |
| **Terrestrial Herbivore - White-tailed Deer** | | | |
| Body weight (BW) | kg | 7.48E+01 | Silva and Downing 1995 |
| Population per area | # / $m^2$ | 4.60E-05 | 12-80/ha, forest avg from Smith 1987, Torgerson and Porath 1984,Wishart 1984,Cook 1984 |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| Soil ingestion rate | kg[soil] / kg BW-day | 1.00E-03 | Beyer et al. 1994 |
| Water_a | L[water] / kg BW-day | 9.90E-02 | Calder and Braun 1983 |
| Water_b | L[water] / kg BW-day | 9.00E-01 | Calder and Braun 1983 |
| Inhalation_a | unitless | 5.46E-01 | Stahl 1967 |
| Inhalation_b | unitless | 8.00E-01 | Stahl 1967 |
| Food ingestion rate | kg[food] / kg BW-day | 5.00E-02 | Mautz et al. 1976 |
| Fraction of food diet comprised of plant | unitless | 1.00E+00 | professional judgment |
| Fraction excretion to soil | unitless | 1.00E+00 | professional judgment |
| Fraction excretion to water | unitless | 0.00E+00 | professional judgment |
| **Semiaquatic Omnivore - Raccoon** | | | |
| Body weight (BW) | kg | 6.35E+00 | Lotze and Anderson 1979 |
| Population per area | # / $m^2$ | 2.15E-05 | average of range 0.023 to 0.2/ha, Lotze and Anderson 1979 |
| Soil ingestion rate | kg[soil] / kg BW-day | 9.40E-02 | Beyer et al. 1994 |
| Water_a | L[water] / kg BW-day | 9.90E-02 | Calder and Braun 1983 |
| Water_b | L[water] / kg BW-day | 9.00E-01 | Calder and Braun 1983 |
| Inhalation_a | unitless | 5.46E-01 | Stahl 1967 |
| Inhalation_b | unitless | 8.00E-01 | Stahl 1967 |
| Food ingestion rate | kg[food] / kg BW-day | 5.20E-01 | calc from Teubner and Barrett 1983, Tyson 1950, U.S. EPA 1993 |
| Fraction of food diet comprised of benthic invertebrate | unitless | 6.90E-01 | representing molluscs, crustacea, Tyson 1950 |
| Fraction of diet comprised of water column herbivore | unitless | 3.00E-02 | assumed based on approximate trophic levels of several consumed fish species |
| Fraction of diet comprised of water column omnivore | unitless | 3.00E-02 | assumed based on approximate trophic levels of several consumed fish species |
| Fraction of diet comprised of benthic omnivore | unitless | 4.00E-02 | assumed based on approximate trophic levels of several consumed fish species |
| Fraction of food diet comprised of worm | unitless | 2.10E-01 | coastal mudflats of SW Washington, Tyson 1950 |
| Fraction excretion to soil | unitless | 5.00E-01 | professional judgment |
| Fraction excretion to water | unitless | 5.00E-01 | professional judgment |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| **Terrestrial Ground-Invertebrate Feeder - Short-tailed Shrew** | | | |
| Body weight (BW) | kg | 2.20E-02 | 0.015-0.029 kg reported for Manitoba, Silva and Downing 1995 |
| Population per area | # / $m^2$ | 6.10E-04 | average value for Maine, A. Fuller, U. Maine |
| Soil ingestion rate | kg[soil] / kg BW-day | 6.11E-02 | Talmage and Walton 1993 |
| Water_a | L[water] / kg BW-day | 9.90E-02 | Calder and Braun 1983 |
| Water_b | L[water] / kg BW-day | 9.00E-01 | Calder and Braun 1983 |
| Inhalation_a | unitless | 5.46E-01 | Stahl 1967 |
| Inhalation_b | unitless | 8.00E-01 | Stahl 1967 |
| Food ingestion rate | kg[food] / kg BW-day | 4.70E-01 | Barrett and Stueck 1976 |
| Fraction of food diet comprised of worm | unitless | 5.85E-01 | Whitaker and Ferraro 1963, slugs represented by earthworms, Ithaca, NY |
| Fraction of food diet comprised of soil arthropod | unitless | 4.15E-01 | Whitaker and Ferraro 1963 |
| Fraction excretion to soil | unitless | 1.00E+00 | professional judgment |
| Fraction excretion to water | unitless | 0.00E+00 | professional judgment |
| **PLANTS - TERRESTRIAL** | | | |
| **Deciduous Forest Leaf** | | | |
| Water content | unitless | 8.00E-01 | Paterson et al. 1991 |
| Lipid content | kg/kg wet weight | 2.24E-03 | European beech, Riederer 1995 |
| Correction exponent, octanol to lipid | unitless | 7.60E-01 | from roots, Trapp 1995 |
| Volume of wet leaf weight per unit area | $m^3$ / $m^2$ | calculated | calculated |
| Density of wet leaf | kg / $m^3$ | 8.20E+02 | Paterson et al. 1991 |
| Mass of leaf per unit area | kg[fresh leaf] / $m^2$[area] | 6.00E-01 | calc from LAI[c], leaf thickness (Simonich and Hites 1994), density of wet foliage |
| Dry mass of leaf per unit area | kg[dry leaf] / $m^2$[area] | calculated | calculated |
| Leaf wetting factor | m | 3.00E-04 | 1E-04 to 6E-04 for different crops and elements, Muller and Prohl 1993 |
| 1-sided leaf area index[c] | $m^2$[leaf] / $m^2$[area] | 3.40E+00 | Harvard Forest, dom. red oak and red maple, http://cdiac.esd.ornl.gov/ |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| Vegetation attenuation factor (to calc interception fraction) | unitless | 2.90E+00 | grass/hay, Baes et al. 1984 |
| Particle washoff rate constant | 1 / day | 5.76E+01 | conifer leaves, McCune and Lauver 1986 |
| Length of leaf | m | 1.00E-01 | professional judgment |
| **Coniferous Forest Leaf** | | | |
| Water content | unitless | 8.00E-01 | Paterson et al. 1991 |
| Lipid content | kg/kg wet weight | 2.24E-03 | European beech, Riederer 1995 |
| Correction exponent, octanol to lipid | unitless | 7.60E-01 | from roots, Trapp 1995 |
| Volume of wet leaf weight per unit area | $m^3 / m^2$ | calculated | calculated |
| Density of wet leaf | $kg / m^3$ | 8.20E+02 | Paterson et al. 1991 |
| Mass of leaf per unit area | kg[fresh leaf] / $m^2$[area] | 2.00E+00 | calc from LAI[c], leaf thickness (Simonich and Hites 1994), density of wet foliage |
| Dry mass of leaf per unit area | kg[dry leaf] / $m^2$[area] | calculated | calculated |
| Leaf wetting factor | m | 3.00E-04 | 1E-04 to 6E-04 for different crops and elements, Muller and Prohl 1993 |
| 1-sided leaf area index[c] | $m^2$[leaf] / $m^2$[area] | 5.00E+00 | rep. value for conifers, Ned Nikolov, Oak Ridge National Lab |
| Vegetation attenuation factor (to calc interception fraction) | unitless | 2.90E+00 | grass/hay, Baes et al. 1984 |
| Particle washoff rate constant | 1 / day | 5.76E+01 | conifer leaves, McCune and Lauver 1986 |
| Length of leaf | m | 1.00E-02 | professional judgment |
| **Herb/Grassland Leaf** | | | |
| Water content | unitless | 8.00E-01 | Paterson et al. 1991 |
| Lipid content | kg/kg wet weight | 2.24E-03 | European beech, Riederer 1995 |
| Correction exponent, octanol to lipid | unitless | 7.60E-01 | from roots, Trapp 1995 |
| Volume of wet leaf weight per unit area | $m^3 / m^2$ | calculated | calculated |
| Density of wet leaf | $kg / m^3$ | 8.20E+02 | Paterson et al. 1991 |
| Mass of leaf per unit area | kg[fresh leaf] / $m^2$[area] | 1.00E+00 | calc from LAI[c] and Maddelena 1998 |
| Dry mass of leaf per unit area | kg[dry leaf] / $m^2$[area] | calculated | professional judgment |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| Leaf wetting factor | m | 3.00E-04 | 1E-04 to 6E-04 for different crops and elements, Muller and Prohl 1993 |
| 1-sided leaf area index[c] | $m^2$[leaf] / $m^2$[area] | 5.00E+00 | range for old field about 4 to 6, R. J. Luxmoore, Oak Ridge National Lab. |
| Vegetation attenuation factor (to calc interception fraction) | unitless | 2.90E+00 | grass/hay, Baes et al. 1984 |
| Particle washoff rate constant | 1 / day | 5.76E+01 | conifer leaves, McCune and Lauver 1986 |
| Length of leaf | m | 5.00E-02 | professional judgment |
| **Root – Nonwoody Only** | | | |
| Wet density of root | kg / $m^3$ | 8.30E+02 | soybean, Paterson et al. 1991 |
| Water content of root | unitless | 0.8 | professional judgment |
| Lipid content of root | kg/kg wet weight | 1.10E-02 | calculated |
| Correction exponent for the differences between octanol and lipids | unitless | 0.76 | Trapp 1995 |
| Total volume of dry roots in domain per unit area | $m^3$ / $m^2$ | calculated | calculated |
| Areal density grass/herb | kg / $m^2$ | 1.40E+00 | temperate grassland , Jackson et al. 1996 |
| **Stem – Nonwoody Only** | | | |
| Density | g/$cm^3$ | 9.00E-01 | professional judgment |
| Water content of stem | unitless | 8.00E-01 | Paterson et al. 1991 |
| Lipid content | kg/kg wet weight | 2.24E-03 | leaves of European beech, Riederer 1995 |
| Volume of wet stem per unit area | $m^3/m^2$ | 10% of volume of foliage | professional judgment |
| Density of phloem fluid | kg/$m^3$ | 1.00E+03 | professional judgment |
| Density of xylem fluid | kg/$cm^3$ | 9.00E+02 | professional judgment |
| Volume of wet weight in domain per unit area | $m^3/m^2$ | 0.4 times volume of foliage per unit area | professional judgment |
| Flow rate of transpired water per leaf area | $m^3$[water]/$m^2$ [leaf] | 4.80E-03 | Crank et al. 1981 |
| Fraction of transpiration flow rate that is phloem rate | unitless | 0.05 | Paterson et al. 1991 |
| Correction exponent between foliage lipids and octanol | unitless | 7.60E-01 | Trapp 1995 |

| Input Parameter | Input Units | Value[a] | | | Reference |
|---|---|---|---|---|---|
| **TEMPORAL ENVIRONMENTAL SETTING DATA** | | | | | |
| **Site-specific** | | | | | |
| Day of first frost | unitless | Sept 30 | | | Hampden, ME, value for northeastern US |
| Day of last frost | unitless | May 12 | | | Hampden, ME, value for northeastern US |
| **Deciduous Forest and Grassland** | | | | | |
| Litterfall begin date | unitless | Day 273 (Sept 30) | | | assumed equivalent to date of first frost (W. W. Hargrove, U. of Tenn., pers. comm., 2/99) |
| Litterfall end date | unitless | Day 302 (Oct 29) | | | professional judgment |
| Uptake by leaf, end date | unitless | Day 273 (Sept 30) | | | assumed equivalent to date of first frost (W. W. Hargrove, U. of Tenn., pers. comm., 2/99) |
| Uptake by root (herb/grass), end date | unitless | Day 273 (Sept 30) | | | assumed equivalent to date of first frost (W. W. Hargrove, U. of Tenn., pers. comm., 2/99) |
| $LAI^c = 0$, date | unitless | Day 273 (Sept 30) | | | assumed equivalent to date of first frost (W. W. Hargrove, U. of Tenn., pers. comm., 2/99) |
| Uptake by leaf, begin date | unitless | Day 132 (May 12) | | | assumed equivalent to date of last frost (W. W. Hargrove, U. of Tenn., pers. comm., 2/99) |
| $LAI^c$ = default value, date | unitless | Day 132 (May 12) | | | assumed equivalent to date of last frost (W. W. Hargrove, U. of Tenn., pers. comm., 2/99) |
| Litterfall rate constant | 1/ day | 1.50E-01 | | | assumes 99% of leaves have fallen during 30 days of litterfall |
| **Coniferous Forest** | | | | | |
| Uptake by leaf, end date | unitless | Day 303 (Oct 30) | | | assumed to be one month after date of first frost |
| Uptake by leaf, end date | unitless | Day 102 (Apr 12) | | | assumed to be one month before date of last frost |
| Litterfall rate constant | 1/ day | being developed | | | 2-10 yr turnover, WM Post, Oak Ridge Natl |
| **BIOTIC CHEMICAL-SPECIFIC DATA** | | | | | |
| **ANIMALS - AQUATIC** | | | | | |
| **Water-column Carnivore - Bass** | | | | | |
| | | **Hg(0)** | **Hg(2)** | **MHg** | |
| Carnivore-omnivore partition coefficient | kg/kg | NA | 8.81E-02 | 3.50E+00 | 1 trophic level transfer, Hg(2) - Watras and Bloom 1992, MHg - Lindqvst et al. 1991 |
| Alpha for carnivore | unitless | NA | 9.50E-01 | 9.50E-01 | professional judgment |
| $t_{alpha}$ | day | NA | 4.38E+04 | 4.38E+04 | derived from Lindqvist et al. 1991 |
| Assimilation efficiency | percent | NA | 9 | 90 | Hg(2): Trudel and Rasmussen 1997; MHg: Odin et al. 1995 |

| Input Parameter | Input Units | Value[a] | | | Reference |
|---|---|---|---|---|---|
| **Water-column Herbivore - Bluegill** | | | | | |
| | | **Hg(0)** | **Hg(2)** | **MHg** | |
| Herbivore-algae partition coefficient | kg/kg | NA | 1.41E-01 | 1.20E+01 | zooplankton intermediate trophic level, Hg(2) - Watras and Bloom 1992; MHg - Lindqvst et al. 1991 |
| Alpha for herbivore | unitless | NA | 9.50E-01 | 9.50E-01 | professional judgment |
| $t_{alpha}$ | day | NA | 5.48E+02 | 5.48E+02 | derived from Lindqvist et al. 1991 |
| Assimilation efficiency | percent | NA | 9 | 90 | Hg(2): Trudel and Rasmussen 1997; MHg: Odin et al. 1995 |
| **Water-column Omnivore - Channel Catfish** | | | | | |
| | | **Hg(0)** | **Hg(2)** | **MHg** | |
| Omnivore-herbivore partition coefficient | kg/kg | NA | 8.81E-02 | 3.50E+00 | zooplankton to planktiverous fish, Hg(2) - Watras and Bloom 1992; MHg - Lindqvst et al. 1991 |
| Alpha for omnivore | unitless | NA | 9.50E-01 | 9.50E-01 | professional judgment |
| $t_{alpha}$ | days | NA | 1.46E+03 | 1.46E+03 | derived from Lindqvist et al. 1991 |
| Assimilation efficiency | percent | NA | 9 | 90 | Hg(2): Trudel and Rasmussen 1997; MHg: Odin et al. 1995 |
| **Benthic Invertebrate (represented by Mayfly)** | | | | | |
| | | **Hg(0)** | **Hg(2)** | **MHg** | |
| Benthic invertebrate-sediment partition coefficient | kg/kg | NA | 8.24E-02 | 5.04E+00 | Hg(0) - assumed based on Hg(2) value; Hg(2) and MHg - Saouter et al. 1991 |
| Alpha for omnivore | unitless | NA | 9.50E-01 | 9.50E-01 | professional judgment |
| $t_{alpha}$ | days | NA | 1.40E+01 | 1.40E+01 | experiment duration from Saouter 1991 |
| **Benthic Carnivore (represented by Largemouth Bass)** | | | | | |
| Carnivore-omnivore partition coefficient | kg/kg | NA | 8.81E-02 | 3.50E+00 | zooplankton to planktiverous fish, Hg(2) - Watras and Bloom 1992; MHg - Lindqvst et al. 1991 |
| Alpha for omnivore | unitless | NA | 9.50E-01 | 9.50E-01 | professional judgment |
| $t_{alpha}$ | day | NA | 4.38E+04 | 4.38E+04 | derived from Lindqvist et al. 1991 |
| Assimilation efficiency | percent | NA | 9 | 90 | Hg(2): Trudel and Rasmussen 1997; MHg: Odin et al. 1995 |
| **Benthic Omnivore (represented by Channel Catfish)** | | | | | |
| | | **Hg(0)** | **Hg(2)** | **MHg** | |
| Omnivore-invertebrate partition coefficient | kg]/kg | NA | 8.81E-02 | 3.50E+00 | zooplankton to planktiverous fish, Hg(2) - Watras and Bloom 1992; MHg - Lindqvst et al. 1991 |
| Alpha for omnivore | unitless | NA | 9.50E-01 | 9.50E-01 | professional judgment |
| $t_{alpha}$ | day | NA | 1.46E+03 | 1.46E+03 | derived from Lindqvist et al. 1991 |
| Assimilation efficiency | percent | NA | 8 | 80 | Hg(2): Trudel and Rasmussen 1997; MHg: Odin et al. 1995 |

| Input Parameter | Input Units | Value[a] | | | Reference |
|---|---|---|---|---|---|
| **PLANTS - AQUATIC** | | | | | |
| **Macrophyte** | | | | | |
| | | **Hg(0)** | **Hg(2)** | **MHg** | |
| Macrophyte-water partition coefficient | L/g | NA | 8.83E-01 | 4.40E+00 | Elodea densa, Ribeyre and Boudou 1994 |
| Alpha for macrophyte | unitless | NA | 9.50E-01 | 9.50E-01 | professional judgment |
| $t_{alpha}$ | days | NA | 1.80E+01 | 1.80E+01 | experiment duration from Ribeyre and Boudou 1994 |
| **Phytoplankton - Algae** | | | | | |
| | | **Hg(0)** | **Hg(2)** | **MHg** | |
| $D_{ow}$ | unitless | NA | depends on pH and Cl conc | depends on pH and Cl conc | look-up table of pH and Cl concentrations derived from graph in Mason et al. 1996 |
| Uptake rate | $\mu m^{-2}$-$d^{-1}$-L | NA | 4.00E-11 | 7.07E-11 | assumes radius = 2.5mm, Mason et al. 1995b, Mason et al. 1996 |
| **ANIMALS - TERRESTRIAL** | | | | | |
| **Soil Detritivore - Earthworm** | | | | | |
| | | **Hg(0)** | **Hg(2)** | **MHg** | |
| Earthworm-soil partitition coefficient, dry | mg/kg per mg/kg | NA | 3.60E-01 | 3.60E-01 | Bull et al. 1977 |
| $t_{alpha}$ for worm ↔ soil | day | 2.10E+01 | 2.10E+01 | 2.10E+01 | assumed same as earthworms, Janssen et al. 1997 |
| Alpha for worm ↔ soil | unitless | 9.50E-01 | 9.50E-01 | 9.50E-01 | specified |
| **Soil Detritivore - Soil Arthropod** | | | | | |
| | | **Hg(0)** | **Hg(2)** | **MHg** | |
| Arthropod-soil partition coefficient | kg/kg wet weight | NA | 4.60E-01 | 2.90E+00 | Hg(2) - median from Talmage and Walton 1993; MHg - median from Nuorteva and Nuorteva 1982 |
| $t_{alpha}$ for arthropod ↔ soil | day | 2.10E+01 | 2.10E+01 | 2.10E+01 | assumed same as earthworms, Janssen et al. 1997 |
| Alpha for arthropod ↔ soil | unitless | 9.50E-01 | 9.50E-01 | 9.50E-01 | professional judgment |
| **Terrestrial Ground-Invertebrate Feeder - Black-capped Chickadee** | | | | | |
| First-order transformation rate constant for Hg(0)→Hg(2) | 1/day | 1.00E+00 | | | professional judgment |
| First-order transformation rate constant for MHg→Hg(2) | 1/day | 9.00E-02 | | | calculated from rats in Takeda and Ukita 1970 |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| First-order transformation rate constant for Hg(0)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| Assimilation efficiency for inhalation for Hg(0) | unitless | 0.75 | human, ATSDR 1997, Teisinger and Fiserova-Bergova 1965 |
| Assimilation efficiency for inhalation for Hg(2) | unitless | 0.4 | value for dog, U.S. EPA 1997 |
| Assimilation efficiency for inhalation for MHg | unitless | 0.75 | assume same as value of Hg(0) |
| **Semiaquatic Piscivore - Kingfisher** | | | |
| First-order transformation rate constant for Hg(0)→Hg(2) | 1/day | 1.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(2) | 1/day | 9.00E-02 | calculated from rats in Takeda and Ukita 1970 |
| First-order transformation rate constant for Hg(0)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→Hg(0) | 1/day | 0.00E+00 | professional judgment |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| First-order transformation rate constant for MHg→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| Assimilation efficiency for inhalation for Hg(0) | unitless | 0.75 | human, ATSDR 1997, Teisinger and Fiserova-Bergova 1965 |
| Assimilation efficiency for inhalation for Hg(2) | unitless | 0.4 | value for dog, U.S. EPA 1997 |
| Assimilation efficiency for inhalation for MHg | unitless | 0.75 | assume same as value of Hg(0) |
| **Semiaquatic Predator/Scavenger - Bald Eagle** | | | |
| First-order transformation rate constant for Hg(0)→Hg(2) | 1/day | 1.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(2) | 1/day | 9.00E-02 | calculated from rats in Takeda and Ukita 1970 |
| First-order transformation rate constant for Hg(0)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| Assimilation efficiency for inhalation for Hg(0) | unitless | 0.75 | human, ATSDR 1997, Teisinger and Fiserova-Bergova 1965 |
| Assimilation efficiency for inhalation for Hg(2) | unitless | 0.4 | value for dog, U.S. EPA 1997 |
| Assimilation efficiency for inhalation for MHg | unitless | 0.75 | assume same as value of Hg(0) |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| **Semiaquatic Piscivore - Common Loon** | | | |
| First-order transformation rate constant for Hg(0)→Hg(2) | 1/day | 1.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(2) | 1/day | 9.00E-02 | calculated from rats in Takeda and Ukita 1970 |
| First-order transformation rate constant for Hg(0)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| Assimilation efficiency for inhalation for Hg(0) | unitless | 0.75 | human, ATSDR 1997, Teisinger and Fiserova-Bergova 1965 |
| Assimilation efficiency for inhalation for Hg(2) | unitless | 0.4 | value for dog, U.S. EPA 1997 |
| Assimilation efficiency for inhalation for MHg | unitless | 0.75 | assume same as value of Hg(0) |
| **Semiaquatic Omnivore - Mallard** | | | |
| First-order transformation rate constant for Hg(0)→Hg(2) | 1/day | 1.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(2) | 1/day | 9.00E-02 | calculated from rats in Takeda and Ukita 1970 |
| First-order transformation rate constant for Hg(0)→MHg | 1/day | 0.00E+00 | professional judgment |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| First-order transformation rate constant for Hg(2)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| Assimilation efficiency for inhalation for Hg(0) | unitless | 0.75 | human, ATSDR 1997, Teisinger and Fiserova-Bergova 1965 |
| Assimilation efficiency for inhalation for Hg(2) | unitless | 0.4 | value for dog, U.S. EPA 1997 |
| Assimilation efficiency for inhalation for MHg | unitless | 0.75 | assume same as value of Hg(0) |
| **Terrestrial Predator/Scavenger - Red-tailed Hawk** | | | |
| First-order transformation rate constant for Hg(0)→Hg(2) | 1/day | 1.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(2) | 1/day | 9.00E-02 | calculated from rats in Takeda and Ukita 1970 |
| First-order transformation rate constant for Hg(0)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| Assimilation efficiency for inhalation for Hg(0) | unitless | 0.75 | human, ATSDR 1997, Teisinger and Fiserova-Bergova 1965 |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| Assimilation efficiency for inhalation for Hg(2) | unitless | 0.4 | value for dog, U.S. EPA 1997 |
| Assimilation efficiency for inhalation for MHg | unitless | 0.75 | assume same as value of Hg(0) |
| **Terrestrial Insectivore - Tree Swallow** | | | |
| First-order transformation rate constant for Hg(0)→Hg(2) | 1/day | 1.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(2) | 1/day | 9.00E-02 | calculated from rats in Takeda and Ukita 1970 |
| First-order transformation rate constant for Hg(0)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| Assimilation efficiency for inhalation for Hg(0) | unitless | 0.75 | human, ATSDR 1997, Teisinger and Fiserova-Bergova 1965 |
| Assimilation efficiency for inhalation for Hg(2) | unitless | 0.4 | value for dog, U.S. EPA 1997 |
| Assimilation efficiency for inhalation for MHg | unitless | 0.75 | assume same as value of Hg(0) |
| **Terrestrial Herbivore - Meadow Vole** | | | |
| First-order transformation rate constant for Hg(0)→Hg(2) | 1/day | 1.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(2) | 1/day | 9.00E-02 | calculated from rats in Takeda and Ukita 1970 |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| First-order transformation rate constant for Hg(0)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| Assimilation efficiency for inhalation for Hg(0) | unitless | 0.75 | human, ATSDR 1997, Teisinger and Fiserova-Bergova 1965 |
| Assimilation efficiency for inhalation for Hg(2) | unitless | 0.4 | value for dog, U.S. EPA 1997 |
| Assimilation efficiency for inhalation for MHg | unitless | 0.75 | assume same as value of Hg(0) |
| **Terrestrial Herbivore - Long-tailed Vole** | | | |
| First-order transformation rate constant for Hg(0)→Hg(2) | 1/day | 1.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(2) | 1/day | 9.00E-02 | calculated from rats in Takeda and Ukita 1970 |
| First-order transformation rate constant for Hg(0)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→Hg(0) | 1/day | 0.00E+00 | professional judgment |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| First-order transformation rate constant for MHg→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| Assimilation efficiency for inhalation for Hg(0) | unitless | 0.75 | human, ATSDR 1997, Teisinger and Fiserova-Bergova 1965 |
| Assimilation efficiency for inhalation for Hg(2) | unitless | 0.4 | value for dog, U.S. EPA 1997 |
| Assimilation efficiency for inhalation for MHg | unitless | 0.75 | assume same as value of Hg(0) |
| **Terrestrial Predator/Scavenger - Long-tailed Weasel** | | | |
| First-order transformation rate constant for Hg(0)→Hg(2) | 1/day | 1.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(2) | 1/day | 9.00E-02 | calculated from rats in Takeda and Ukita 1970 |
| First-order transformation rate constant for Hg(0)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| Assimilation efficiency for inhalation for Hg(0) | unitless | 0.75 | human, ATSDR 1997, Teisinger and Fiserova-Bergova 1965 |
| Assimilation efficiency for inhalation for Hg(2) | unitless | 0.4 | value for dog, U.S. EPA 1997 |
| Assimilation efficiency for inhalation for MHg | unitless | 0.75 | assume same as value of Hg(0) |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| **Semiaquatic Omnivore - Mink** | | | |
| First-order transformation rate constant for Hg(0)→Hg(2) | 1/day | 1.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(2) | 1/day | 9.00E-02 | calculated from rats in Takeda and Ukita 1970 |
| First-order transformation rate constant for Hg(0)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| Assimilation efficiency for inhalation of Hg(0) | unitless | 0.75 | human, ATSDR 1997, Teisinger and Fiserova-Bergova 1965 |
| Assimilation efficiency for inhalation of Hg(2) | unitless | 0.4 | value for dog, U.S. EPA 1997 |
| Assimilation efficiency for inhalation of MHg | unitless | 0.75 | assume same as value of Hg(0) |
| **Terrestrial Omnivore - White-footed Mouse** | | | |
| First-order transformation rate constant for Hg(0)→Hg(2) | 1/day | 1.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(2) | 1/day | 9.00E-02 | calculated from rats in Takeda and Ukita 1970 |
| First-order transformation rate constant for Hg(0)→MHg | 1/day | 0.00E+00 | professional judgment |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| First-order transformation rate constant for Hg(2)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| Assimilation efficiency for inhalation for Hg(0) | unitless | 0.75 | human, ATSDR 1997, Teisinger and Fiserova-Bergova 1965 |
| Assimilation efficiency for inhalation for Hg(2) | unitless | 0.4 | value for dog, U.S. EPA 1997 |
| Assimilation efficiency for inhalation for MHg | unitless | 0.75 | assume same as value of Hg(0) |
| **Terrestrial Herbivore - Mule Deer/Black-tailed Deer** | | | |
| First-order transformation rate constant for Hg(0)→Hg(2) | 1/day | 1.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(2) | 1/day | 9.00E-02 | calculated from rats in Takeda and Ukita 1970 |
| First-order transformation rate constant for Hg(0)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| Assimilation efficiency for inhalation for Hg(0) | unitless | 0.75 | human, ATSDR 1997, Teisinger and Fiserova-Bergova 1965 |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| Assimilation efficiency for inhalation for Hg(2) | unitless | 0.4 | value for dog, U.S. EPA 1997 |
| Assimilation efficiency for inhalation for MHg | unitless | 0.75 | assume same as value of Hg(0) |
| **Terrestrial Herbivore - White-tailed Deer** | | | |
| First-order transformation rate constant for Hg(0)→Hg(2) | 1/day | 1.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(2) | 1/day | 9.00E-02 | calculated from rats in Takeda and Ukita 1970 |
| First-order transformation rate constant for Hg(0)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| Assimilation efficiency for inhalation for Hg(0) | unitless | 0.75 | human, ATSDR 1997, Teisinger and Fiserova-Bergova 1965 |
| Assimilation efficiency for inhalation for Hg(2) | unitless | 0.4 | value for dog, U.S. EPA 1997 |
| Assimilation efficiency for inhalation for MHg | unitless | 0.75 | assume same as value of Hg(0) |
| **Semiaquatic Omnivore - Raccoon** | | | |
| First-order transformation rate constant for Hg(0)→Hg(2) | 1/day | 1.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(2) | 1/day | 9.00E-02 | calculated from rats in Takeda and Ukita 1970 |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| First-order transformation rate constant for Hg(0)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(0) | 1/day | 0.00E+00 | professional judgment |
| Assimilation efficiency for inhalation for Hg(0) | unitless | 0.75 | human, ATSDR 1997, Teisinger and Fiserova-Bergova 1965 |
| Assimilation efficiency for inhalation for Hg(2) | unitless | 0.4 | value for dog, U.S. EPA 1997 |
| Assimilation efficiency for inhalation for MHg | unitless | 0.75 | assume same as value of Hg(0) |
| **Terrestrial Ground-Invertebrate Feeder - Short-tailed Shrew** | | | |
| First-order transformation rate constant for Hg(0)→Hg(2) | 1/day | 1.00E+00 | professional judgment |
| First-order transformation rate constant for MHg→Hg(2) | 1/day | 9.00E-02 | calculated from rats in Takeda and Ukita 1970 |
| First-order transformation rate constant for Hg(0)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→MHg | 1/day | 0.00E+00 | professional judgment |
| First-order transformation rate constant for Hg(2)→Hg(0) | 1/day | 0.00E+00 | professional judgment |

| Input Parameter | Input Units | Value[a] | | | Reference |
|---|---|---|---|---|---|
| First-order transformation rate constant for MHg→Hg(0) | 1/day | 0.00E+00 | | | professional judgment |
| Assimilation efficiency for inhalation for Hg(0) | unitless | 0.75 | | | human, ATSDR 1997, Teisinger and Fiserova-Bergova 1965 |
| Assimilation efficiency for inhalation for Hg(2) | unitless | 0.4 | | | value for dog, U.S. EPA 1997 |
| Assimilation efficiency for inhalation for MHg | unitless | 0.75 | | | assume same as value of Hg(0) |
| **PLANTS - TERRESTRIAL** | | | | | |
| **Leaf** | | | | | |
| First-order transformation rate constant for Hg(0)→Hg(2) | 1/day | 1.00E+06 | | | value used for rate constants that are judged to be close to instantaneous |
| First-order transformation rate constant for Hg(2)→MHg | 1/day | 0.00E+00 | | | assumed from Gay 1975, Bache et al. 1973, Lindberg pers comm |
| First-order transformation rate constant for MHg →Hg(2) | 1/day | 3.00E-02 | | | calc from Bache et al. 1973 |
| Washout ratio Hg(2) vapor | unitless | 1.60E+06 | | | U.S. EPA 1997 based on Petersen et al. 1995 |
| Washout ratio Hg(0) vapor | unitless | 1.20E+03 | | | U.S. EPA 1997 based on Petersen et al. 1995 |
| Washout ratio Hg particulate | unitless | 5.00E+05 | | | U.S. EPA 1997 based on Petersen et al. 1995 |
| **Root** | | | | | |
| | | **Hg(0)** | **Hg(2)** | **MHg** | |
| Alpha for root ↔ root-zone soil | unitless | 9.50E-01 | 9.50E-01 | 9.50E-01 | professional judgment |
| $t_{alpha}$ | day | NA | 2.10E+01 | 2.10E+01 | professional judgment |
| Dry root/root-zone-soil partition coefficient | mg/kg per mg/kg | NA | 9.00E-01 | 6.00E+00 | Hg(2) - geom mean Leonard et al. 1998, John 1972, Hogg et al. 1978; MHg - assumed, based on Hogg et al. 1978 |
| **Stem** | | | | | |
| Transpiration stream concentration factor | $kg/m^3$ per $kg/m^3$ | 0 | 0.2 | 0.5 | calculation from Norway spruce, Scots pine, Bishop et al. 1998 |

| Input Parameter | Input Units | Value[a] | Reference |
|---|---|---|---|
| **Leaf Surface** | | | |
| Transfer factor from leaf to leaf surface (Hg) | 1/day | 2.00E-03 | calculated (1% of transfer factor from leaf surface to leaf) |
| Transfer factor from leaf surface to leaf (Hg particulate) | 1/day | 2.00E-01 | professional judgment |

[a] NA = not applicable, parameter does not apply to this species of mercury
[b] VE = volume element
[c] LAI = leaf area index

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# APPENDIX D
# Summary of Available Monitoring Data for TRIM.FaTE Mercury Case Study

The test site used to compare TRIM.FaTE module outputs to environmental monitoring data was selected, in part, due to the amount and kinds of monitoring data available for comparison. This appendix provides a summary of the mercury monitoring data that are currently available for the selected test site. The data sets are organized into primarily on-site and primarily off-site monitoring efforts, with abiotic data sets presented first followed by biotic data sets. Note that several of the data sets that are listed as on-site include one or two off-site reference location measurements.

***Note: Data sources are not provided because they could reveal the location and identity of the case study site.***

## D.1 ON-SITE MONITORING DATA

### D.1.1 ON-SITE SOIL MONITORING DATA

**Environmental Medium:** Surface soil

**Number of Data Points:** 11 data points from 11 locations

**Measurement Endpoint(s) (Units):** Total mercury dry weight concentration (mg/kg)

**Sampling Date(s):** June 6-7, 1995, October 27, 1997

**Sample Location(s):** 10 data points from 10 on-site and 1 data point from a reference location

**Purpose of Monitoring:** 1995 and 1997 site investigations

**Range:** 0.18 - 10.3 mg/kg, dry weight

**Mean and Standard Deviation:** 5.05 ± 3.47 mg/kg, dry weight (median = 4.8 mg/kg, dry weight)

**Other Information:** These data correspond in time and location to the earthworm monitoring data (see below) and overlap with 6 of the 61 surface soil samples listed below. Some of these samples maybe contaminated by on-site point source releases.

**Environmental Medium:** Surface and subsurface soil

**Number of Data Points:** 113 data points of which 61 are from 0 - 0.5 feet including 2 not analyzed (NA) and 6 duplicates, and 52 are from 1 - 1.5 feet including 2 ND at detection level of 0.1 mg/kg, 4 NA, and 4 duplicates

**Measurement Endpoint(s) (Units):** Total mercury dry weight concentration (mg/kg)

**Sampling Date(s):** August 16, 1994, August 17, 1994, August 18, 1994, May 3, 1995, May 4, 1995, June 6, 1995, June 7, 1995

**Sample Location(s):** On-site from 56 locations

**Purpose of Monitoring:** 1995 and 1997 site investigations

**Range:** (1) At 0 - 0.5 feet: 0.14 - 310 mg/kg
(2) At 1 - 1.5 feet: $\leq$ 0.1 - 80 mg/kg

**Mean and Standard Deviation:** (1) At 0 - 0.5 feet: 30.1 ± 47.6 mg/kg (median = 13 mg/kg)
(2) At 1 - 1.5 feet: 12.4 ± 16.3 mg/kg (median = 6.2 mg/kg)

**Other Information:** These data also include measurement of soil pH in some cases. Some of these samples maybe contaminated by on-site point source releases.

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**Environmental Medium:** Surface soil

**Number of Data Points:** 56 data points including 6 duplicates from 50 different sampling sites

**Measurement Endpoint(s) (Units):** Total mercury dry weight concentration (mg/kg)

**Sampling Date(s):** September/October 1997

**Sample Location(s):** On-site from 50 locations

**Purpose of Monitoring:** 1997 site investigation

**Range:** < 0.20 - 310 mg/kg dry weight

**Mean and Standard Deviation:** 5.37 ± 11.4 mg/kg, dry weight (median = 1.2 mg/kg, dry weight)

**Other Information:** Some of these samples maybe contaminated by on-site point source releases.

**Environmental Medium:** Surface and subsurface soil.

**Number of Data Points:** 33 data points from 4 locations, including 19 from 0 - 0.5 feet, 8 from 0 - 0.2 feet, and 6 from 1 - 1.5 feet

**Measurement Endpoint(s) (Units):** Total mercury dry weight concentration (mg/kg)

**Sampling Date(s):** November 3, 1997, November 6, 1997, November 14, 1997

**Sample Location(s):** On-site from 14 sites clustered around 1 location, 11 sites clustered around another location, and 4 sites each clustered around 2 other locations

**Purpose of Monitoring:** Delineation soil sampling for 1997 site investigation

**Range:** (1) 0 - 0.5 feet: 0.1 - 42.5 mg/kg, dry weight
(2) 0 - 0.2 feet: 4.5 - 126.9 mg/kg, dry weight
(3) 1-1.5 feet: 0 - 6.4 mg/kg, dry weight

**Mean and Standard Deviation:** (1) 0 - 0.5 feet: 8.3 ± 12.6 mg/kg, dry weight
(2) 0 - 0.2 feet: 23.8 ± 41.8 mg/kg, dry weight
(3) 1-1.5 feet: 3.5 ± 2.5 mg/kg, dry weight

**Other Information:** Some of these samples maybe contaminated by on-site point source releases.

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**Environmental Medium:** Subsurface soil

**Number of Data Points:** 107 data points, including 25 data points from 2 cores in different locations in 1995 including 3 duplicate samples and 9 ND, and 82 data points from 8 cores in different locations in 1997 including 8 duplicate samples and 2 ND. Data are provided in 2 foot intervals from 0 feet to up to 57 feet in some cores.

**Measurement Endpoint(s) (Units):** Total mercury dry weight concentration (mg/kg)

**Sampling Date(s):** 1995 and 1997

**Sample Location(s):** On-site from 10 different locations

**Purpose of Monitoring:** 1995 and 1997 site investigations

**Range:** 0.00 - 239.30 mg/kg (for entire data set, regardless of depth and year)

**Mean and Standard Deviation:** Due to the nature of this data set, a mean and standard deviation were not calculated.

**Other Information:** Some of these samples maybe contaminated by on-site point source releases.

### D.1.2 ON-SITE BIOTA MONITORING DATA

**Environmental Medium:** Deer mouse (Peromyscus maniculatus)

**Number of Data Points:** 9 data points from 9 locations

**Measurement Endpoint(s) (Units):** (1) Total Mercury concentration (mg/kg, wet weight, whole body)
(2) Percent moisture (%)

**Sampling Date(s):** June 1995

**Sample Location(s):** (1) 7 from on-site locations
(2) 2 from an off-site reference location

**Purpose of Monitoring:** 1995 Site Investigation

**Range:** (1) On-site: 0.06 - 0.198 mg/kg, wet weight; 70.4 - 77.1 % moisture
(2) Off-site: 0.016 - 0.087 mg/kg, wet weight; 73.5 - 77.3 % moisture

**Mean and Standard Deviation:** (1) On-site: 0.100 ± 0.063 mg/kg, wet weight; 74.2 ± 2.3 % moisture
(2) Off-site: 0.0515 ± 0.050 mg/kg, wet weight; 75.4 ± 2.7 % moisture

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**Environmental Medium:** Earthworm (Species not specified)

**Number of Data Points:** 11 data points from 11 locations

**Measurement Endpoint(s) (Units):** (1) Total mercury concentration (mg/kg, wet weight)
(2) Percent moisture (%)

**Sampling Date(s):** June 6-7, 1995, October 27, 1997

**Sample Location(s):** 10 data points on-site and 1 data point from a reference location

**Purpose of Monitoring:** 1995 and 1997 site investigations

**Range:** (1) On-site: 0.087 - 2.82 mg/kg, wet weight; 84.3 - 88.6%
(2) Off-site: 0.044 mg/kg, wet weight; 87.9 % (single values)

**Mean and Standard Deviation:** (1) On-site: 0.044 mg/kg, wet weight; 87.9 % (single value, no standard deviation)
(2) Off-site: 0.982 ± 0.79 mg/kg, wet weight; 86.3 ± 1.2 %

**Other Information:** These data correspond in time and location to one set of soil monitoring data (see above)

## D.2 OFF-SITE MONITORING DATA

### D.2.1 OFF-SITE AIR MONITORING DATA

**Environmental Medium:** Ambient air

**Number of Data Points:** Approximately 9,000 data points from 3 continuous monitoring stations. Data quality flags are included indicating automatic calibration, power failure, valid measurement, standard addition, maintenance and manual calibrations, equipment failure or malfunction, no peak (i.e., below detection limit), overload (beyond analyzer range), and suspect data (based on quality assurance measures).

**Measurement Endpoint (Units):** One-hour average total gaseous mercury ($ng/m^3$)

**Sampling Date(s):** September 4, 1998 to January 9, 1999 (hourly samples throughout period)

**Sample Location(s):** (1) Approximately 1,500 feet southeast of facility
(2) approximately 4,300 feet north-northwest of the facility
(3) approximately 6,400 feet north-northwest of the facility

**Purpose of Monitoring:** To provide data to the state environmental agency as a result of a consent agreement enforcement order

**Range:** (1) 0.834 - 157 $ng/m^3$
(2) 0.993 - 25.8 $ng/m^3$
(3) 0.565 - 14.8 $ng/m^3$

**Mean and Standard Deviation:** (1) 9.96 ± 15.52 $ng/m^3$ (includes values with all types of data flags)
(2) 2.46 ± 2.15 $ng/m^3$ (includes values with all types of data flags)
(3) 1.85 ± 1.66 $ng/m^3$ (includes values with all types of data flags)

**Other Information:** Corresponding meteorological data are also available from an on-site monitoring station, including approximately 1,680 data points each for (1) average hourly wind speed (mph), (2) average hourly wind direction (°N), (3) average hourly ambient temperature

(°C), and (4) average hourly solar radiation ($W/m^2$) from 1 continuous monitoring station from November 1, 1998 to January 9, 1999. Another data set of meteorological parameters that can be used as inputs to TRIM.FaTE is available from a continuous monitoring station in Portland, ME. This data set includes approximately 8,760 hourly averaged measurements from each year from 1990 to 1995 for wind speed (m/s), wind direction (degrees), rural and urban mixing height (m), precipitation rate (mm/hour), precipitation type (unitless), ambient temperature (°K), stability class (unitless), friction velocity (m/s), monin-obukhov length (m), and surface roughness length (m).

### D.2.2 OFF-SITE SURFACE WATER MONITORING DATA

**Environmental Medium:** Surface water

**Number of Data Points:** 5 data points in 5 locations

**Measurement Endpoint(s) (Units):** Total mercury concentration (ug/L) (unfiltered samples)

**Sampling Date(s):** June 1995

**Sample Location(s):** (1) 2 samples located in adjacent river upstream of facility
(2) 3 samples located in adjacent river downstream of facility

**Purpose of Monitoring:** 1995 site investigation

**Range:** (1) Upstream: 0.00359 - 0.00529 ug/L
(2) Downstream: 0.000646 - 0.0703 ug/L

**Mean and Standard Deviation:** (1) Upstream: 0.004 ± 0.001 ug/L (median = 0.004 ug/L)
(2) Downstream: 0.034 ± 0.033 ug/L (median = 0.027 ug/L)

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**Environmental Medium:** Surface water

**Number of Data Points:** 50 data points plus 6 not analyzed from 14 locations at ebb tide, flood tide, high tide, and low tide

**Measurement Endpoint(s) (Units):** Total mercury concentration (ng/L)

**Sampling Date(s):** August 18-19, 1997

**Sample Location(s):** In adjacent river

**Purpose of Monitoring:** 1995 site investigation

**Range:** 4.09 (flood tide) - 173 (ebb tide) ng/L

**Mean and Standard Deviation:** 15 ± 37.71 ng/L

### D.2.3 OFF-SITE SEDIMENT MONITORING DATA

**Environmental Medium:** Sediment

**Number of Data Points:** 1 data point based on a single measurement each from 4 different off-site ponds and lakes, including measurements from the pond that is part of the mercury case study

**Measurement Endpoint(s) (Units):** Total mercury concentration in the upper 2 cm of the sediment in the deepest part of the waterbody (mg/kg, dry weight)

**Sampling Date(s):** (1) September 19, 1996
(2) September 26, 1996
(3) September 20, 1996
(4) September 20, 1996

**Sampling Location(s):** four nearby offsite lakes and ponds. Deepest part of each waterbody.

**Purpose of Monitoring:** To determine if lakes and ponds are measurably affected by small, local air emission sources of mercury

**Range:** N/A (single value provided)

**Mean and Standard Deviation:** (1) 0.319 mg/kg (no SD available)
(2) 0.157 mg/kg (no SD available)
(3) 0.201 mg/kg (no SD available)
(4) 0.132 mg/kg (no SD available)

### D.2.4 OFF-SITE BIOTA MONITORING DATA

**Environmental Medium:** Juvenile loon

**Number of Data Points:** 1 data point from 1 location

**Measurement Endpoint(s) (Units):** Blood total mercury concentration (ppm, wet weight) from single loon

**Sampling Date(s):** July 1998

**Sample Location(s):** Pond located southeast of the facility that is part of the mercury case study

**Purpose of Monitoring:** Mercury risk assessment

**Range:** N/A

**Mean and Standard Deviation:** 1.3 ppm, wet weight (single value, no standard deviation)

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**Environmental Medium:** Loon egg

**Number of Data Points:** 3 data points from 1 location

**Measurement Endpoint(s) (Units):** Total average mercury concentration (ppm, wet weight) from multiple measurements

**Sampling Date(s):** June 1998

**Sample Location(s):** Pond located east of the facility

**Purpose of Monitoring:** Mercury risk assessment

**Range:** 1.6 - 1.8 ppm, wet weight

**Mean and Standard Deviation:** 1.73 ± 0.12 ppm, wet weight

**Other Information:** The sediment mercury concentration in this pond is 0.319 mg/kg.

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**Environmental Medium:** Loon egg

**Number of Data Points:** 1 state average based on a sample size of 43

**Measurement Endpoint(s) (Units):** Total mercury concentration (ppm, wet weight)

**Sampling Date(s):** June 1998

**Sample Location(s):** Ponds and lakes in facility's state

**Purpose of Monitoring:** Mercury risk assessment

**Range:** N/A

**Mean and Standard Deviation:** 0.93 ± 0.55 ppm

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**Environmental Medium:** Adult male loon

**Number of Data Points:** (1) 6 data points from 6 locations
(2) 1 state average based on a sample size of 67

**Measurement Endpoint(s) (Units):** Blood total mercury concentration (ppm, wet weight)

**Sampling Date(s):** July - August, 1997-1998

**Sample Location(s):** Ponds and lakes in facility's state

**Purpose of Monitoring:** Mercury risk assessment

**Range:** (1) 0.61 - 3.71 ppm, wet weight for 6 locations
(2) Not provided

**Mean and Standard Deviation:** (1) 2.62 ± 1.23 ppm, wet weight for 6 locations
(2) 2.5 ± 1.1 ppm, wet weight for state average

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**Environmental Medium:** Adult female loon

**Number of Data Points:** (1) 1 data point from 1 location
(2) 1 state average based on a sample size of 64

**Measurement Endpoint(s) (Units):** Mercury total blood concentration (ppm, wet weight)

**Sampling Date(s):** July 1998

**Sample Location(s):** Ponds and lakes in facility's state

**Purpose of Monitoring:** Mercury risk assessment

**Mean and Standard Deviation:** (1) 1.16 ppm, wet weight (single value, no standard deviation) for 1 location
(2) 2.1 ± 1.5 ppm, wet weight for state average

**Range:** (1) N/A for 1 location
(2) Not provided

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**Environmental Medium:** Juvenile loon

**Number of Data Points:** (1) 5 data points from 5 locations
(2) 1 state average based on a sample size of 52

**Measurement Endpoint(s) (Units):** Total mercury blood concentration (ppm, wet weight)

**Sampling Date(s):** July - August, 1997 - 1998

**Sample Location(s):** Ponds and lakes in facility's state

**Purpose of Monitoring:** Mercury risk assessment

**Range:** (1) 0.01 - 0.64 ppm, wet weight for 5 locations
(2) N/A

**Mean and Standard Deviation:** (1) 0.22 ± 0.24 ppm, wet weight for 5 locations
(2) 0.22 ± 0.29 ppm, wet weight for state average

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**Environmental Medium:** White perch

**Number of Data Points:** 35 mercury concentration and fish length data points from 4 waterbodies, including (1) 10 data points from 1 pond, (2) 8 data points from 1 pond, (3) 11 data points from 1 pond, and (4) 6 data points from 1 lake

**Measurement Endpoint(s) (Units):** (1) Total mercury concentration in skinless fillet (mg/kg, wet weight)
(2) Fish length (mm)

**Sampling Date(s):** (1) September 19, 1996
(2) September 20, 1996
(3) September 26, 1996
(4) September 20, 1996

**Sample Location(s):** (1) Southeast of facility
(2) East of facility
(3) East of facility
(4) East of facility

**Purpose of Monitoring:** To determine if lakes and ponds are measurably affected by small, local air emission sources of mercury

**Range:** (1) 0.50 - 1.31 mg/kg, wet weight and 240 - 350 mm in length
(2) 0.28 - 0.72 mg/kg, wet weight and 135 - 270 mm in length
(3) 0.60 - 2.20 mg/kg, wet weight and 186 - 305 mm in length
(4) 0.32 - 0.53 mg/kg, wet weight and 185 - 202 mm in length

**Mean and Standard Deviation:** (1) 0.98 ± 0.25 mg/kg, wet weight and 308 ± 32 mm in length
(2) 0.45 ± 0.14 mg/kg, wet weight and 224 ± 48 mm in length
(3) 1.07 ± 0.43 mg/kg, wet weight and 231 ± 34 mm in length
(4) 0.41 ± 0.08 mg/kg, wet weight and 195 ± 8 mm in length

**Environmental Medium:** Short-tailed Shrew (*Blarina brevicauda*)

**Number of Data Points:** 1 data point from 1 location

**Measurement Endpoint(s) (Units):** (1) Total mercury concentration (mg/kg, wet weight, whole body)
(2) Percent moisture (%)

**Sampling Date(s):** June 1995

**Sample Location(s):** Off-site reference location

**Purpose of Monitoring:** 1995 Site Investigation

**Range: N/A**

**Mean and Standard Deviation:** (1) 0.064 mg/kg, wet weight (single value, no standard deviation)
(2) 73.4 % (single value, no standard deviation)

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**Environmental Medium:** Eel (*Anguilla rostrata*)

**Number of Data Points:** 15 data points, including (1) 6 from upstream of the site and (2) 9 from downstream of the site

**Measurement Endpoint(s) (Units):** (1) Total mercury concentration (mg/kg, dry weight, fillets)
(2) Percent moisture (%)
(3) Total mercury concentration (mg/kg, wet weight, fillets)
(4) Eel weight (grams)
(5) Eel length (cm)

**Sampling Date(s):** June 6, 1995

**Sample Locations:** One location each in the river upstream and downstream of the facility

**Purpose of Monitoring:** 1995 site investigation

**Range:** (1) Upstream: 1.08 - 4.49 mg/kg, dry weight; 74.9 - 80.5 % moisture; 0.271 - 0.876 mg/kg, wet weight; 50 - 200 g; 30 - 46 cm
(2) Downstream: 1.2 - 3.64 mg/kg, dry weight; 70.5 - 81.6 % moisture; 0.259 - 0.678 mg/kg, wet weight; 50 - 375 g; 28 - 56 cm

**Mean and Standard Deviation:** (1) Upstream: 2.5 ± 1.1 mg/kg, dry weight; 78 ± 2 % moisture; 0.53 ± 0.2 mg/kg, wet weight; 110 ± 56.01 g; 37 ± 5.72 cm

(2) Downstream: 2.14 ± 0.81 mg/kg, dry weight; 78 ± 3 % moisture; 0.46 ± 0.14 mg/kg, wet weight; 75 ± 101.64 g; 33 ± 8.92 cm

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**Environmental Medium:** River minnow (killyfish) (*Fundulus heteroclitus*)

**Number of Data Points:** 1 data point from 1 location

**Measurement Endpoint(s) (Units):** Total mercury concentration (mg/kg, dry weight, composite whole body)

**Sampling Date(s):** August 1, 1995

**Sample Location(s):** In river downstream of the facility

**Purpose of Monitoring:** 1995 site investigation

**Range:** N/A

**Mean and Standard Deviation:** 0.447 mg/kg, dry weight (single value, no standard deviation)