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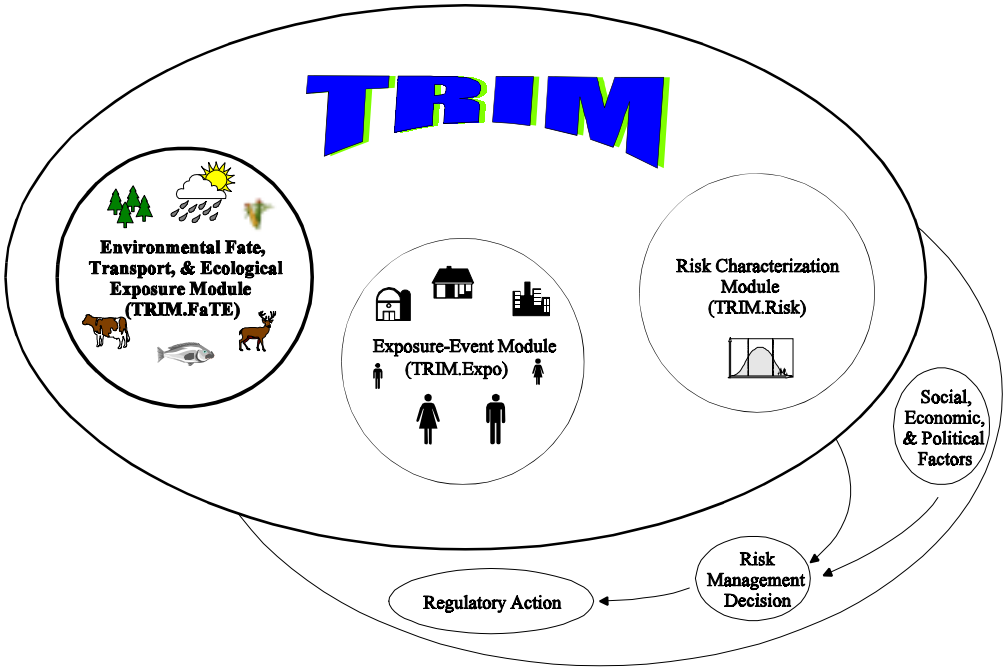
Air

TRIM
Total Risk Integrated Methodology

TRIM.FaTE
TECHNICAL SUPPORT DOCUMENT
Volume I: Description of Module

EXTERNAL REVIEW DRAFT



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Volume I: Description of Module

U.S. ENVIRONMENTAL PROTECTION AGENCY
Office of Air and Radiation
Office of Air Quality Planning and Standards
Research Triangle Park, North Carolina 27711

External Review Draft
November 1999

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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.FaTE 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 draft document, the *TRIM.FaTE Technical Support Document*, is part of a series of documentation for the overall Total Risk Integrated Methodology (TRIM) modeling system. 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. This report, which supersedes an earlier version (U.S. EPA 1998a), documents the Environmental Fate, Transport, and Ecological Exposure module of TRIM (TRIM.FaTE) and is divided into two volumes. The first volume provides a description of terminology, model framework, and functionality of TRIM.FaTE, and the second volume presents a detailed description of the algorithms used in the module.

To date, EPA has issued draft TSDs for TRIM.FaTE (this report) and the Exposure-Event module (*TRIM.Expo TSD*, U.S. EPA 1999a). 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.

The EPA has also issued the 1999 *Total Risk Integrated Methodology (TRIM) Status Report* (U.S. EPA 1999b). The purpose of that 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 1998b). The EPA plans to issue status reports on an annual basis while TRIM is under development.

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

B(a)P	Benzo(a)pyrene
CAA	Clean Air Act
CalTOX	California Department of Toxic Substance Control's Risk Computerized Model
CART	Classification and regression tree
CDF	Cumulative distribution function
CRARM	Presidential/Congressional Commission on Risk Assessment and Risk Management
DOE	United States Department of Energy
EPA	United States Environmental Protection Agency
GIS	Geographic Information System
HAP	Hazardous air pollutant
IEM	Indirect Exposure Methodology
I/O API	Environmental Decision Support System/Models 3 Input/Output Applications Programming Interface
ISMCM	Integrated Spatial Multimedia Compartment Model
LHS	Latin Hypercube Sampling
LSODE	Livermore Solver for Ordinary Differential Equations
MC	Monte Carlo
MCM	Multimedia Compartment Model
MEPAS	Multimedia Environmental Pollutant Assessment System
MPE	Multiple Pathways of Exposure
NAAQS	National ambient air quality standard
NAS	National Academy of Sciences
NATA	National Air Toxics Assessment
OAQPS	EPA Office of Air Quality Planning and Standards
OSWER	EPA Office of Solid Waste and Emergency Response
PAH	Polycyclic aromatic hydrocarbon
PDF	Probability distribution function
RIA	Regulatory impact analysis
SAB	Science Advisory Board
SMCM	Spatial Multimedia Compartment Model
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
WASP	Water Quality Analysis Simulation Program

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TABLE OF CONTENTS

Appendices

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 the TRIM 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 1998b), was reviewed by EPA's Science Advisory Board (SAB) in May 1998 (U.S. EPA 1998c). 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.

This TSD is divided into two volumes. The first volume provides a description of the terminology, model framework, and functionality of TRIM.FaTE. Specifically, Chapter 2 provides an overview of the development and features of TRIM.FaTE, Chapters 3 and 4 discuss the TRIM.FaTE terminology and conceptual design, Chapter 5 provides a general description of how the conceptual design is implemented in TRIM.FaTE, and Chapter 6 explains the treatment of uncertainty and variability in TRIM.FaTE. Volume II of this document presents detailed descriptions of the algorithms used in the TRIM.FaTE module.

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.

[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.

- **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 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 1999c)).

- **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.

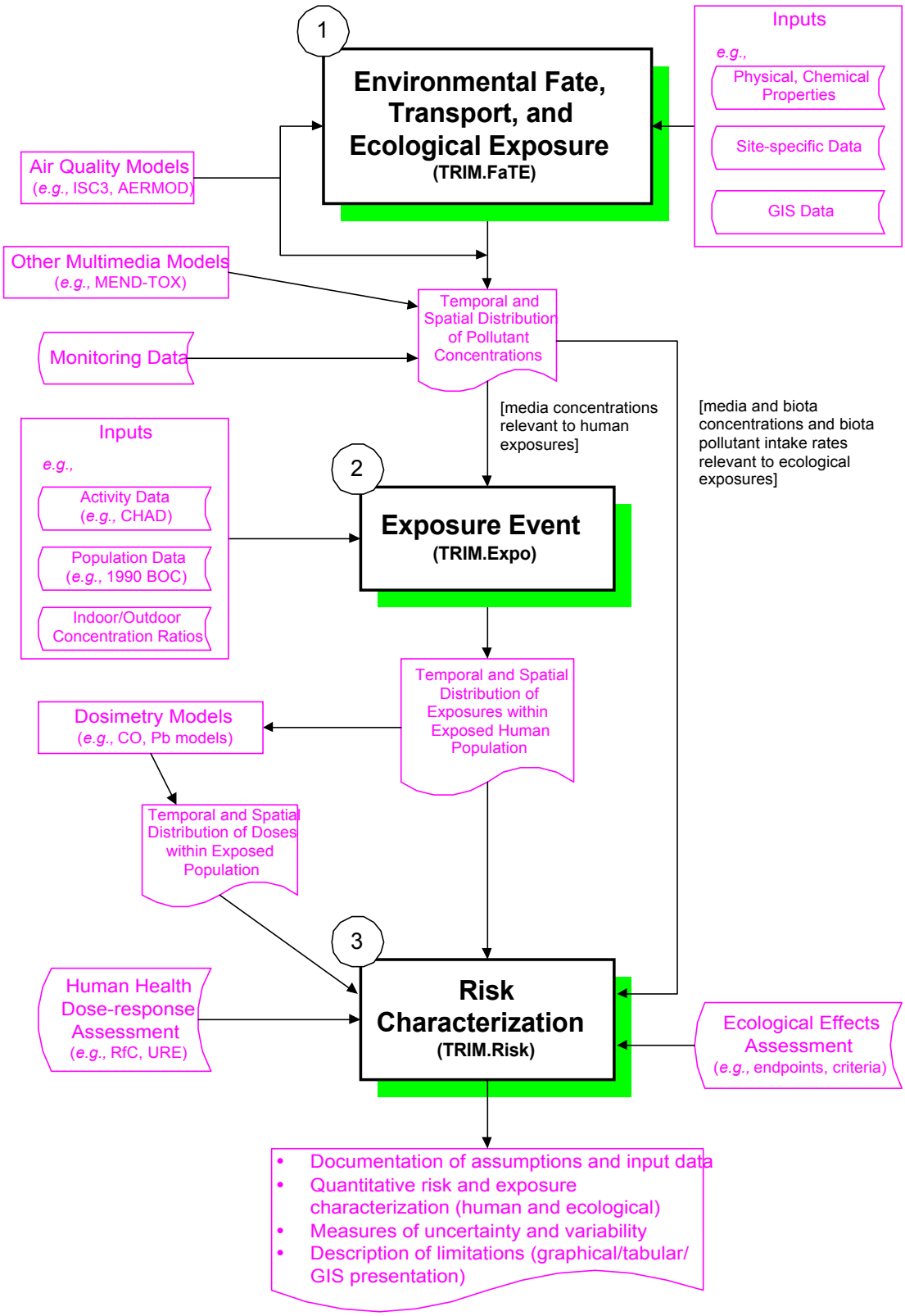
1.2 TRIM DESIGN

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 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.

Figure 1-1
Conceptual Design of TRIM



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 of the TRIM Status Report. The approach for handling uncertainty and variability in TRIM is described in Chapter 3 of the TRIM Status Report. 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, of the TRIM Status Report. Chapter 10 of the TRIM Status Report discusses the computer framework that is being implemented for the TRIM system. In addition, the TRIM.Expo TSD provides more detail on TRIM.Expo.

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.

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.

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.

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

[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.

CHAPTER 1
INTRODUCTION

part of TRIM development activities. Reviews of relevant models existing at the initiation of development activities for each module are described in this document and in the TRIM.Expo TSD. Additionally, OAQPS is closely following several current activities as they relate to TRIM.

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 1999c). 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 1998b). 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 1998d) and the 1994 Agency Task Force on Environmental Regulatory Modeling (U.S. EPA 1994a), internal and external peer

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

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 1998c). In May 1998 in Washington, DC, the Environmental Models Subcommittee (Subcommittee) of the Executive Committee of SAB reviewed the TRIM project. The SAB 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 1998c). The SAB Subcommittee provided specific recommendations related to six specific charge questions. The SAB recommendations are detailed in Chapter 2 of the TRIM Status Report along with brief responses, and changes to TRIM.FaTE based in part on the SAB recommendations are highlighted in Chapter 4 of the TRIM Status 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 of the TRIM Status Report. The development of TRIM.Expo is discussed in Chapter 8, and the conceptual plan for TRIM.Risk is described in Chapter 9 of the TRIM Status Report. In addition, the TRIM.Expo TSD provides more details on TRIM.Expo.

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.

CHAPTER 1
INTRODUCTION

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.*, 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 1998d) 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.

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 user 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.

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.

[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.

CHAPTER 1
INTRODUCTION

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.

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 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 1986)). 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 1998e), 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. INTRODUCTION TO TRIM.FaTE

Implementation of the TRIM system began with development of the TRIM Environmental Fate, Transport, and Ecological Exposure module (TRIM.FaTE), a flexible multimedia fate and transport model designed to estimate pollutant concentrations in various environmental compartments (*i.e.*, media and organisms). These media and biota concentrations, as well as estimates of pollutant intake by organisms, provide measures of ecological exposure in various biota on a temporal and spatial scale. The media and biota concentrations also provide temporally and spatially varying inputs for a human exposure model such as TRIM.Expo, which can model population cohorts through space and time.

Prior to and during the development of TRIM.FaTE, EPA has reviewed the features of existing multimedia models and approaches in order to build on, rather than duplicate, previous efforts. In these reviews, the Agency focused on how existing models address the following characteristics desired for TRIM.FaTE:

- Ability to address varying time steps (of one hour or greater) and provide sufficient spatial detail at varying scales (site-specific to urban scale);
- Conservation of pollutant mass within the system being assessed;
- Transparency, as needed for use in a regulatory context; and
- Performance as a truly coupled multimedia model rather than a set of linked single medium models.

As a result of the Agency's reviews of other models (Section 2.1), OAQPS concluded (as described in Section 2.2) that in order to meet the Office's needs for assessing human health and ecological risks of exposure to criteria and hazardous air pollutants, it is necessary to develop a truly coupled multimedia modeling framework. In developing TRIM.FaTE, the Agency has incorporated several features that improve upon the capabilities of existing models. These key features are summarized in Section 2.3.

2.1 REVIEW OF EXISTING FATE AND TRANSPORT MODELS

In 1996, EPA undertook a review of existing models and approaches as an initial step in the TRIM development effort. The resulting report, entitled *Evaluation of Existing Approaches for Assessing Non-Inhalation Exposure and Risk with Recommendations for Implementing TRIM* (Mosier et al. 1996), examined several multimedia models. Two additional EPA studies conducted in 1997 (IT 1997a, IT 1997b) have updated the 1996 study.

The initial literature searches identified several models/approaches for multimedia, multipathway modeling, including EPA's Indirect Exposure Methodology (IEM), the California Department of Toxic Substance Control's Multimedia Risk Computerized Model (CalTOX), the

Dutch model SimpleBOX, the Integrated Spatial Multimedia Compartmental Model (ISMCM), and the Multimedia Environmental Pollutant Assessment System (MEPAS).

Efforts to assess human exposure from multiple media date back to the 1950s, when the need to assess human exposure to global radioactive fallout led rapidly to a framework that included transport through and transfers among air, soil, surface water, vegetation, and food chains (Wicker and Kirchner 1987). Efforts to apply such a framework to non-radioactive organic and inorganic toxic chemicals have been more recent and have not as yet achieved the level of sophistication that exists in the radioecology field. In response to the need for multimedia models in exposure assessment, a number of multimedia transport and transformation models have been recently developed.

Thibodeaux (1979, 1996) proposed the term "chemodynamics" to describe a set of integrated methods for assessing the cross-media transfers of organic chemicals. The first widely used multimedia compartment modeling approaches for organic chemicals were the "fugacity" models proposed by Mackay (1979, 1991) and Mackay and Paterson (1981, 1982). Cohen and his co-workers applied the concept of multimedia compartment modeling as a screening tool with the Multimedia Compartment Model (MCM) (Cohen and Ryan 1985), followed by the Spatial MCM (SMCM) (Cohen et al. 1990), and more recently with the Integrated SMCM (ISMCM), which allows for non-uniformity in some compartments (van de Water 1995). Another multimedia screening model, called GEOTOX (McKone and Layton 1986), was one of the earliest multimedia models to explicitly address human exposure. The CalTOX program (McKone 1993a, McKone 1993b, McKone 1993c) has been developed for the California EPA as a set of spreadsheet models and spreadsheet data sets to assist in assessing human exposures to toxic substance releases in multiple media. More recently, SimpleBOX (van de Meent 1993, Brandes et al. 1997) has been developed for the National Institute of Public Health and the Environment in the Netherlands to evaluate the environmental fate of chemicals.

A brief summary of key multimedia models evaluated for applicability to the TRIM.FaTE effort follows. Other models reviewed are documented in the background reports referenced in the first paragraph of this section.

- **Indirect Exposure Methodology (IEM)**. The IEM consists of a set of multimedia fate and exposure algorithms developed by EPA's Office of Research and Development that is a significant current Agency methodology for multimedia, multipathway modeling for pollutants for which indirect (*i.e.,* non-inhalation) impacts may be important (*i.e.,* organic and inorganic pollutants that tend to be long-lived, bioaccumulating, non- (or at most semi-) volatile, and more associated with soil and sediment than with water).

An interim document describing this methodology was published in 1990 (U.S. EPA 1990), and a major addendum was issued in 1993 (U.S. EPA 1993).[1] The IEM has undergone extensive scientific review, including review by SAB, which has been useful in focusing efforts in the development of TRIM. The SAB identified several limitations of IEM that are pertinent to its application to the design quals for TRIM (U.S. EPA 1994b). Concurrently with IEM development, EPA has also developed and applied a closely related set of multimedia models in a variety of dioxin assessments (U.S. EPA 1994c; updated document expected in 2000).

Descriptions of fate and transport algorithms, exposure pathways, receptor scenarios, and dose algorithms are presented in the IEM documentation. The IEM includes procedures for estimating the indirect human exposures and health risks that can result from the transfer of emitted air pollutants to soil, vegetation, and water bodies. The methodology addresses exposures via inhalation, food, water, and soil ingestion, and dermal contact.

There appear to be several limitations in the IEM approach relative to the TRIM.FaTE design criteria and OAQPS' needs. For example, IEM, as currently implemented, can be applied only to chemicals that are emitted to the air. This limits its ability to provide assessment of media concentrations resulting from air emissions when other pollutant sources might have a significant impact on the results. However, IEM is an evolving and emerging methodology that moves EPA beyond analyzing the potential effects associated with only one medium (air) and exposure pathway (inhalation) to the consideration of multiple media and exposure pathways. It is crucial in the development of TRIM that a sense of continuity be maintained between IEM and proposed TRIM methodologies.

The IEM was designed to predict long-term, steady-state impacts from continuous sources, not short-term, time series estimates. It consists of a one-way process through a series of linked models or algorithms and requires annual average air concentrations and wet and dry deposition values from air dispersion modeling external to IEM. As a result, IEM cannot provide detailed time-series estimation (*e.g.*, for time steps less than one year) of media concentrations and concomitant exposure, cannot maintain full mass balance, and, because it is not a truly coupled multimedia model, does not have the ability to model "feedback" loops between media or secondary emissions (*e.g.*, re-emission of deposited pollutants). Furthermore, IEM does not provide for the flexibility OAQPS needs in site-specific applications or in estimating population exposures. Significant site-specific adjustment must be made to allow for spatially tracking differences in

[1] Since OAQPS' initial review and consideration of IEM in 1996, the methodology and its documentation have undergone several important changes. A draft revised document addressing SAB and public comments on the 1993 Addendum was released for review in 1998 (U.S. EPA 1998f). The IEM2M was derived from IEM and applied by OAQPS to estimate exposures to mercury for the *Mercury Study Report to Congress* (U.S. EPA 1997). The Agency's Office of Solid Waste and Emergency Response (OSWER) has adapted IEM and compiled detailed information on many of IEM's input parameters and algorithms in the *Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities* (U.S. EPA 1998g), which has been applied to assess exposures and risks for many hazardous waste combustion facilities. The most up-to-date version of the general IEM methodology is scheduled to be published in late 1999 (U.S. EPA 1999d.) The updated documentation no longer refers to the methodology as IEM; it is now referred to as the Multiple Pathways of Exposure (MPE) methodology.

concentrations and exposures. Much of the focus of IEM is on evaluating specific receptor scenarios (*e.g.*, recreational or subsistence fisher) that may be indicative of high-end or average exposures, but the model is not designed to model the range of exposures within a population (*e.g.,* IEM cannot estimate population exposure distributions). More recent advances (Rice et al. 1997) have addressed some of these issues to some degree, but have not been fully implemented.

Therefore, while IEM may meet its own design criteria quite well (*e.g.,* can adequately estimate long-term average exposure media concentrations in the vicinity of an air source for contaminants for which indirect impacts may be important), it does not fully meet the needs of OAQPS for the reasons noted above.

- **California Department of Toxic Substance Control's Multimedia Risk Computerized Model (CalTOX).** First issued in 1993 (McKone 1993a, McKone 1993b, McKone 1993c) and updated in 1995, with continual enhancements underway, CalTOX was developed as a spreadsheet model for California's Department of Toxic Substance Control to assist in human health risk assessments that address contaminated soils and the contamination of adjacent air, surface water, sediment, and ground water. CalTOX consists of two component models: a multimedia transport and transformation (*i.e.*, fate and transport) model, which is based on both conservation of mass and chemical equilibrium; and a multipathway human exposure model that includes ingestion, inhalation, and dermal uptake exposure routes. CalTOX is a fully mass balancing model that includes add-ins to quantify uncertainty and variability.

  The multimedia transport and transformation model is a dynamic model that can be used to assess time-varying concentrations of contaminants introduced initially to soil layers or for contaminants released continuously to air, soil, or water. The CalTOX multimedia model is a seven-compartment regional and dynamic multimedia fugacity model. The seven compartments are: (1) air, (2) surface soil, (3) plants, (4) root-zone soil, (5) the vadose-zone soil below the root zone, (6) surface water, and (7) sediment. The air, surface water, surface soil, plants, and sediment compartments are assumed to be in quasi-steady-state with the root-zone soil, and vadose-zone soil compartments. Contaminant inventories in the root-zone soil and vadose-soil zone are treated as time-varying state variables. Contaminant concentrations in ground water are based on the leachate from the vadose-zone soil.

  The multipathway exposure model encompasses 23 exposure pathways to estimate average daily doses within a human population in the vicinity of a hazardous substances release site. The exposure assessment process consists of relating contaminant concentrations in the multimedia model compartments to contaminant concentrations in the media with which a human population has contact (*e.g.*, personal air, tap water, foods, household dusts/soils). The explicit treatment of differentiating environmental media pollutant concentration and the pollutant concentration to which humans are exposed favorably distinguishes CalTOX from many other exposure models. In addition, all parameter values used as inputs to CalTOX are distributions, described in terms of mean values and a coefficient of variation, rather than point estimates (central tendency or

plausible upper values) such as most other models employ. This stochastic approach allows both sensitivity and uncertainty to be directly incorporated into the model operation.

As indicated in the literature review reports, the CalTOX model appears to be the most promising existing model for application to the TRIM effort. Several of the mathematical concepts and derivations used by the developers of CalTOX can be directly applied to meet the TRIM goals. However, CalTOX does have several limitations that prevent it from being entirely imported into the TRIM approach. These limitations result from the need to go beyond the intended applications for CalTOX; for example, for landscapes in which there is a large ratio of land area to surface water area, for a limited range of chemicals (*e.g.*, non-ionic organic chemicals in a liquid or gaseous state). As a result, the model does not provide adequate flexibility in environmental settings and chemical classes (*e.g.*, volatile metals such as mercury) to be suitable for OAQPS' needs. The most significant of these limitations, in terms of application to TRIM, is the fact that the CalTOX model, as it currently exists, does not allow spatial tracking of a pollutant as is required in the TRIM approach.

- **SimpleBOX**. SimpleBOX is a steady-state, non-equilibrium partitioning, mass balance model (van de Meent 1993, Brandes et al. 1997). It consists of eight compartments, three of which are soils of differing use and properties. It also produces quasi-dynamic (non-steady-state) output by using an external numerical integrator. The model was developed as a regional scale model for the Netherlands, so its default characteristics represent the Netherlands. SimpleBOX uses the classical concentration concept to compute the mass balance (van de Meent 1993). While its goals are comparable to TRIM to the extent that it simulates regional systems, its coarse spatial and temporal complexity and lack of exposure media concentration estimates cause it to fall short of TRIM's goals.

- **Integrated Spatial Multimedia Compartmental Model (ISMCM)**. ISMCM has been under development at the School of Engineering and Applied Science at University of California Los Angeles for approximately 15 years (van de Water 1995). A newer version of ISMCM, called MEND-TOX, is currently under evaluation by the EPA Office of Research and Development's National Exposure Research Laboratory.

  The ISMCM considers all media, biological and non-biological, in one integrated system and includes both spatial and compartmental modules to account for complex transport of pollutants through an ecosystem. Assuming mass conservation, ISMCM is able to predict transport based on a sound mechanistic description of environmental processes, including estimation of intermedia transfer factors.

  One of the limiting factors of the ISMCM system, with regard to use in the TRIM system, is that it is not structured to incorporate uncertainty and variability directly into the model operation. Another of the limitations of the ISMCM model within the context of the goals for TRIM (van de Water 1995) is the fact that the links and compartments (spatial configuration) of this model are predetermined. Thus, ISMCM was apparently not designed from the start with the flexibility to meet the goals of TRIM.

- **Multimedia Environmental Pollutant Assessment System (MEPAS).** MEPAS was developed at the U.S. Department of Energy's (DOE) Pacific Northwest Laboratory to assess risks from mixed (*i.e.*, chemical and radioactive) wastes at DOE facilities. This model consists of single-media transport models linked together under appropriate boundary conditions and considers four primary types of pollutant pathways (ground water, overland, surface water, and atmospheric) in evaluating human exposure. MEPAS also contains an exposure and risk module. The model's ability to estimate multipathway risks for chemicals and radionuclides makes it unique. The nature of its algorithms makes it a screening tool, rather than a detailed assessment tool. The model is updated periodically and the latest version of MEPAS (Version 3.1) contains an uncertainty and variability analysis module (Buck et al. 1995).

  The mathematical design of this model does not include mass balance and could not be integrated into TRIM. As with IEM, MEPAS represents a "linked" model system that utilizes a one-way process through a sequence of models that individually describe a specific environmental process or medium. These types of models are not mass conservative and do not allow for temporal tracking of the pollutants and concomitant exposure necessary to meet the needs of TRIM.

2.2 THE NEED FOR AN IMPROVED FATE AND TRANSPORT MODELING TOOL

Current OAQPS fate and transport models for hazardous and criteria air pollutants do not address multimedia exposures, and current OAQPS HAP models do not adequately estimate temporal and spatial patterns of exposures. Adopting or incorporating existing models into a tool that meets OAQPS' needs represents the most cost-effective approach to developing the tools needed to support regulatory decision-making related to hazardous and criteria air pollutants. Based on the OAQPS review of existing multimedia models and modeling systems (described in Section 2.1), there is no single fate and transport model that meets the needs of OAQPS (outlined in Chapter 1) and that can be adopted as part of TRIM. Most models are limited in the types of media and environmental processes addressed. Simply, no single model can address the broad range of pollutants and environmental fate and transport processes anticipated to be encountered by OAQPS in evaluating risks from hazardous and criteria air pollutants. In addition, it is unlikely that one individual model could be developed to address this wide range of concerns. Therefore, the TRIM framework emphasizes a modular design. The lack of a flexible multimedia fate and transport model was identified as a major limitation and was the focus of the first phase implementation efforts for TRIM.

Existing multimedia models can be divided into two basic categories: "linked" single medium model systems and mass-conserving models. Mass-conserving models can be further classified as fugacity-based, concentration-based, or inventory-based models depending on the choice of state variable (*i.e.*, fugacity, concentration, or inventory). The linked single medium and mass-conserving models each have their own strengths and limitations.

"Linked" single medium modeling systems are composed of several independent single medium models. The linked system typically calculates fate and transport by running a single

medium model (*e.g.*, an atmospheric model) and using the output from each time step as the input for the corresponding time step of another single medium model (*e.g.*, a soil or surface water model). There are several highly sophisticated single media models to choose from when constructing a linked system. However, the linked design does not assure conservation of mass because the dynamic feedback loops and secondary pollutant transfers are not treated in a fully coupled manner. In addition, the level of detail provided by the linked model system is not easily adjusted to suit the needs of different modeling objectives.

Mass-conserving multimedia models were developed to fully account for the distribution of mass within a compartmentalized system. The fugacity type multimedia models were introduced by Mackay (1979, 1991) as screening tools to assess the relative distribution of chemicals in air, water, sediment, and soil. The fugacity concept provides a convenient method for quantifying the multimedia fate of chemicals (Cowen et al. 1995). However, models that use fugacity as the state variable are limited in application only to organic chemicals. Concentration-based models like Simple Box and inventory-based models like CalTOX can technically handle inorganic chemicals, but temporal and spatial resolution is limited by the rigid compartmentalized structure or boxes used to represent the environmental media. Spatial compartmental models (*e.g.*, ISMCM) represent the closest current models to an integrated multimedia system. However, as previously described, ISMCM does not meet the TRIM design criterion for a flexible architecture.

In general, none of the multimedia models existing at the time TRIM development began was sufficiently coupled to account for inherent feedback loops or secondary emissions or releases to specific media, or was able to provide the temporal and spatial resolution critical in estimating exposures. While the degree to which results would differ between existing models and a truly coupled multimedia model is unknown, non-coupled multimedia models have been generally considered to lack scientific credibility. Therefore, OAQPS determined it was necessary to undertake efforts to develop a truly coupled multimedia model.

Another 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. FRAMES-HWIR is a framework system which includes, along with several site-specific databases and processors, a multimedia, multipathway, and multireceptor simulation processor (MMSP) for fate and transport and exposure modeling. MMSP is itself made up of 17 individual modules (*e.g.*, air, watershed, human exposure). FRAMES-HWIR has been developed as part of a focused fast-track (two-year) effort to support a risk based regulation for disposal of hazardous waste (HWIR99). The development plan received peer review in late 1998, and the individual modules have been submitted for peer review upon completion, with the last of those reviews in progress. The FRAMES-HWIR documentation is scheduled for public release and accompanying public review in Fall 1999. OAQPS will be carefully considering the various aspects of FRAMES-HWIR and MMSP – as well as other evolving Agency multimedia modeling methods, including the MPE (formerly IEM) methodology discussed in Section 2.1 – with regard to OAQPS' needs, as well as compatibility with and role in future improvements or evaluations of TRIM.

2.3 NOVEL CAPABILITIES OF TRIM.FaTE

As mentioned earlier, several key characteristics have been identified as essential to the design of TRIM.FaTE:

- Ability to address varying time steps (of one hour or greater) and provide sufficient spatial detail at varying scales (site-specific to urban scale);
- Conservation of pollutant mass within the system being assessed;
- Transparency, as needed for use in a regulatory context; and
- Performance as a truly coupled multimedia model rather than a set of linked single medium models.

To accommodate these characteristics, the Agency developed a new model framework that expanded upon the mass balance and compartmental framework used by CalTOX and the system of equations used in ChemCan[2] and SimpleBOX to produce a modeling system that incorporates a flexible level of spatial and temporal resolution while maintaining a complete multimedia mass balance. Development of the TRIM.FaTE framework required the TRIM team to design several features not available in existing multimedia models. These key features, which are described below, include:

- Implementation as a truly coupled multimedia model framework;
- The adaptability to match a simulation to the spatial and temporal scales needed for a broad range of pollutants and geographical areas;
- The use of a unified approach to mass transfer, based on an algorithm library that allows the user to change mass transfer relationships between compartments without creating a new modeling scenario;
- An accounting of the pollutant mass distributed within, as well as entering and leaving, the environmental system;
- An embedded procedure to characterize uncertainty and variability; and
- The capability to be used as an exposure model for ecological receptors.

[2] ChemCan is a steady-state fugacity balance model, designed for Health Canada, intended to assist in human exposure assessment. The model estimates average concentrations in air, fresh surface water, fish, sediments, soils, vegetation, and marine near-shore waters.

2.3.1 TRULY COUPLED MULTIMEDIA FRAMEWORK

One of the significant distinguishing features of the TRIM.FaTE methodology is the attention paid to possible interactions between media. The transfer of chemical mass between compartments is not restricted to a one-way process, which is common for many "linked" multimedia models. Instead, TRIM.FaTE allows the user to simulate the movement of a chemical in any direction for which transfer can occur. Without this functionality, a multimedia model can never be truly mass conservative and cannot adequately address feedback loops and secondary pollutant movement (*e.g.*, revolatilization and transport). The lack of a full mass balance and the functionality to account for feedback loops and secondary pollutant movement are generally considered significant sources of uncertainty in the application of "linked" models. The use of a truly coupled multimedia framework for TRIM.FaTE can reduce this important area of uncertainty.

2.3.2 SCALABLE COMPLEXITY

The current TRIM.FaTE methodology allows the user a great deal of flexibility in the design of any particular model application, both spatially and temporally. The functionality to account for varying degrees of temporal resolution is common among multimedia models. Conversely, the spatial flexibility provided in TRIM.FaTE is unique among multimedia models because it allows the user to vary the resolution significantly over the modeled region. For example, initially the user may define only a few homogeneous regions for the model area. After inspecting the results of the initial analysis, the user could subdivide those regions where more resolution is desired. This prevents the user from including more resolution than is necessary for a particular application, resulting in more efficiency in modeling. Although some applications of TRIM.FaTE may resemble a simple fugacity-based compartmental model, it also can be scaled to simulate time-series and spatial resolutions that current fugacity-type models could not handle.

2.3.3 FLEXIBLE ALGORITHM LIBRARY

The manner in which the chemical mass transfer algorithms have been implemented in TRIM.FaTE is unique among multimedia models. Rather than storing the equations only in computer code, which is not readable by the user at run time, the equations are stored in a form that allows the user to inspect the equations, variables in the equations, and values for the variables for almost any calculated term *at run time*. It is possible for the user to trace the calculation of almost any of the chemical mass transfers, which can be useful when trying to explore an unexpected result. For most models, the user cannot be sure how faithfully the equations documented have been implemented, or how synchronized the documentation is with the code. With the TRIM.FaTE methodology, these problems can be substantially alleviated.

Another advantage in the algorithm implementation is the potential to choose from a set of algorithms for each of the types of chemical mass transfers. The primary benefit would be in performing sensitivity analyses when there are uncertainties regarding the model approach for some transport or transformation processes. If there were several different algorithms available

for a given process, the user could perform analyses using the different algorithms, thus allowing decision-makers to consider the impact of algorithms selection on predicted values.

2.3.4 FULL MASS BALANCE

One of the design features of TRIM.FaTE that sets it apart from many other multimedia models is that it incorporates a full mass balance. In order to maintain a full mass balance, all environmental media need to be modeled simultaneously, rather than sequentially. This allows the model to properly account for all of the pollutant mass as it moves from within and between media. This approach is in contrast to the methodology used in a set of linked models. With linked models, it is difficult to model the time-fluctuating diffusive transport between the various media. Furthermore, a series of interactions between more than two media is difficult to capture.

With TRIM.FaTE, all of the model compartments are fully coupled such that the exact amount of mass that travels between compartments is accounted for explicitly and continuously. Additionally, diffusion between compartments follows the time-dependent mass in each compartment. As a result, in contrast to many other models, TRIM.FaTE considers time varying concentration for diffusion and thus can provide a more accurate algorithm for diffusive mass transfer among multiple compartments. That is, there is a continuous feedback system adjusting the relative mass exchange among the compartments.

2.3.5 EMBEDDED PROCEDURE FOR UNCERTAINTY AND VARIABILITY ANALYSIS

The overall TRIM model framework has been developed to allow for probabilistic modeling such that variability and uncertainty can be explicitly and separately characterized. This has involved the development of an approach to estimate variability and uncertainty within TRIM, in a manner that allows for: (1) integration among the four TRIM modules; (2) tracking the variability and uncertainty through the modules; and (3) feasible computational processing.

The implementation of this approach for uncertainty analysis is integrated within the TRIM.FaTE module, as opposed to operating as a separate shell around the module. TRIM.FaTE handles some of the calculations internally, and passes information to the uncertainty system during a simulation. This close interfacing of the uncertainty software with the model allows for greater flexibility in terms of what can be tracked and also dramatically reduces the processing time required.

The key features of this approach to variability and uncertainty analysis are joint and separate tracking of variability and uncertainty, characterization of variability and uncertainty of model results with respect to parameter distributions and correlations, and identification of critical parameters and correlations. In addition to providing information to support decision-making, analyses of variability and uncertainty in TRIM will help to guide data and model improvement efforts.

2.3.6 EXPOSURE MODEL FOR ECOLOGICAL RECEPTORS

TRIM.FaTE is also unique in its ability to estimate exposure for ecological receptors. Several measures of ecological exposure are used in exposure-response models: concentrations of chemicals in environmental media; body burdens or tissue levels of chemicals in the organism of concern; and doses to the organism of concern (mass of chemical per mass of organism per unit time). TRIM.FaTE can output chemical mass in all compartments at each time step, thus providing body burden estimates for ecological receptors. TRIM.FaTE is also designed to divide the compartmental chemical mass by the volume or mass of a compartment to estimate concentrations in soil, sediment, water, air, or biota. Additionally, TRIM.FaTE can output chemical intake for organisms of interest at the desired temporal and spatial scale.

Body burdens or tissue concentrations are useful measures of exposure because they integrate exposure from all routes. Dietary exposure is already determined for mammals, birds, and fish by TRIM.FaTE, and exposure to plants from both air and soil is calculated. However, if body burden-response models are not available for particular pollutants, models may be available that relate effects to concentrations in environmental media. These concentrations are available directly from the TRIM.FaTE output as well. Models that relate doses to toxicity may also be used, and doses may be calculated using any averaging time that is equal to or shorter than the length of the TRIM.FaTE simulation.

Given the range of ecological exposure measures directly available from TRIM.FaTE, a user will rarely be limited in the options for exposure-response models that may be used in an ecological risk assessment. Example exceptions are: TRIM.FaTE does not estimate the concentrations of chemicals in vertebrate organs, so models that relate toxicity to organ concentration are not easily implemented; and TRIM.FaTE does not estimate the concentrations of chemicals in potentially sensitive life stages of fish, other than the adult, so using TRIM.FaTE output with models that relate toxicity to concentration in a fingerling may give highly uncertain results.

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3. OVERVIEW OF TRIM.FaTE CONCEPTS AND TERMINOLOGY

The TRIM.FaTE methodology integrates OAQPS' needs and multimedia modeling concepts into a unique model that serves as an integral part of the TRIM system. This chapter provides an overview of the terminology central to the TRIM.FaTE module. An understanding of the terminology and concepts presented in this chapter is crucial to understanding the remainder of this report.

Because the terminology used in the world of environmental modeling can have multiple meanings and implications, it is essential in the initial steps of any model conceptualization that the terminology is clearly defined within the model framework. The terminology for multimedia modeling is particularly complicated because multimedia models are, by nature, multidisciplinary. Thus, terminology can be especially confusing because a single term can have dramatically different meanings in different disciplines. Two general modeling terms are defined, for the purposes of TRIM.FaTE, in the adjacent text box to provide a consistent basis for the discussion in this section and the remainder of the document.

GENERAL MODELING TERMS

Scenario: A specified set of conditions (*e.g.,* spatial, temporal, environmental, source, chemical) used to define a model set-up for a particular simulation or set of simulations

Simulation: A single application of a model to estimate environmental conditions, based on a given scenario and any initial input values needed

The primary objective of the TRIM.FaTE module is to estimate the fate and transport of a chemical pollutant through a modeled environment. Because the term "pollutant" can have various meanings, the modeled unit of chemical mass in TRIM.FaTE is referred to as a chemical. Within the context of TRIM.FaTE, a **chemical** is simply defined as 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. Examples of chemicals that may be modeled in TRIM.FaTE are PAHs, methylmercury, elemental mercury, and benzene.

3.1 SPATIAL TERMINOLOGY

In the TRIM.FaTE module, chemicals are contained within compartments. The term "compartment" is an extension of what is referred to as "medium" in environmental fate and transport modeling literature. The term "medium" was considered too limited in its scope because it generally invokes images of abiotic systems such as soil or air, while TRIM.FaTE includes both abiotic and biotic systems. Therefore, the term compartment was adopted for TRIM.FaTE because it captures the flexibility of the TRIM.FaTE module in that it refers to both abiotic and biotic systems. A **compartment** is defined as a homogeneous unit of space characterized by its physical composition and within which it is assumed, for modeling purposes,

that all chemical mass is homogeneously distributed and is in phase equilibrium. Multiple chemicals can exist within a compartment, and the various phases that compose a compartment (gases, liquids, solids) are assumed to be in equilibrium with respect to chemical partitioning. For example, within an air compartment it can be assumed that the air molecules are in equilibrium with the molecules of water vapor. Compartments can be either biotic, such as a deer compartment, or abiotic, such as a stream compartment. Furthermore, two compartments could have identical compositions and only be distinguished by their location in the modeled environment; they are still separate compartments. It is important to note that biotic compartments do not refer to an individual organism, but instead to the population of that organism within a specified volume.

The term **compartment type** is used to denote a specific kind of compartment, such as an air compartment type or a surface water compartment type. Compartment types are distinguished from each other by the way they exchange chemical mass with other compartment types. Compartments of the same type are distinguished from each other by their location and sometimes also by the values that define their composition at a given location. For example, two different surface soil compartments may have organic carbon contents of 0.015 and 0.01, respectively, but they are both described by the compartment type called "surface soil."

Compartment types are classified as either abiotic or biotic. An abiotic compartment type is a compartment type consisting primarily of a non-living environmental medium (*e.g.*, air, soil) for which TRIM.FaTE calculates chemical masses and concentrations. Abiotic compartment types may also contain biota, such as the microorganisms responsible for chemical transformation. A biotic compartment type is 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. The adjacent text box lists the abiotic compartment types included in TRIM.FaTE. A list of the biotic compartment types included in TRIM.FaTE is provided in Section 3.3.

ABIOTIC COMPARTMENT TYPES IN TRIM.FaTE

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

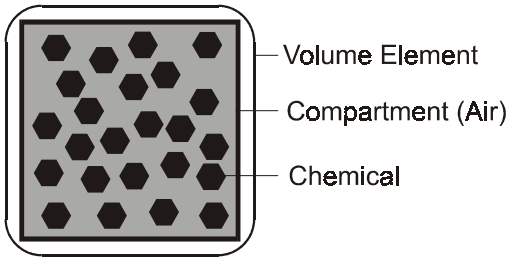
Each compartment is contained within a volume element. A **volume element** is a bounded three-dimensional space that defines the location of one or more compartments. This term is introduced to provide a consistent method for organizing objects that have a natural spatial relationship. Typically, only one type of abiotic compartment is contained within a volume element, although this is not a requirement (*e.g.*, a volume element composed predominantly of a water compartment could also contain a sediment compartment). Volume elements are often identified by this abiotic compartment (*e.g.*, surface soil volume element, ground water volume element) and may contain numerous biotic compartments. All biotic compartments within a volume element are implicitly associated with an abiotic compartment in the volume element (*i.e.*, a fish compartment is implicitly associated with a surface water

compartment), but abiotic compartments do not necessarily have to be associated with any biotic compartments.

The size and shape of volume elements for a given TRIM.FaTE application depends on the needs of the user. For example, if the user is most interested in the range of impacts of a chemical over a given water body, the water body could be divided into a number of volume elements with depth, length, and width. Typically, the higher the desired resolution, the greater the number and the more complicated the shapes of the volume elements.

Figure 3-1 shows the basic spatial relationships between chemicals, compartments, and volume elements. This figure shows that chemicals are contained within compartments, and compartments are contained within volume elements. Figure 3-2 demonstrates how multiple compartments can exist within a single volume element. Because the air compartment is the only abiotic compartment within the volume element in Figure 3-1, this volume element is referred to as the air volume element. Likewise, the volume element in Figure 3-2 is referred to as the water volume element. Figure 3-3 applies the concepts presented in Figures 3-1 and 3-2 by dividing a hypothetical environment into volume elements and compartments.

Figure 3-1
Simple TRIM.FaTE System[a]



[a] Chemicals shown in this figure, and all subsequent similar figures, are units of mass of the same chemical, instead of multiple chemicals.

Figure 3-2
Multiple Compartments within a Single Volume Element

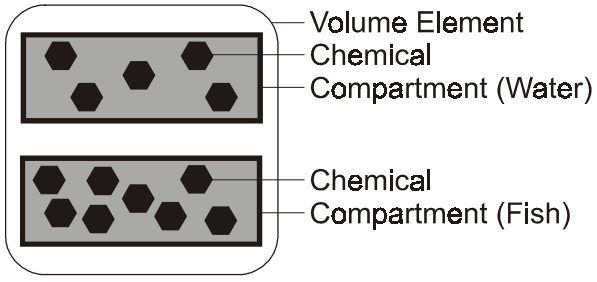
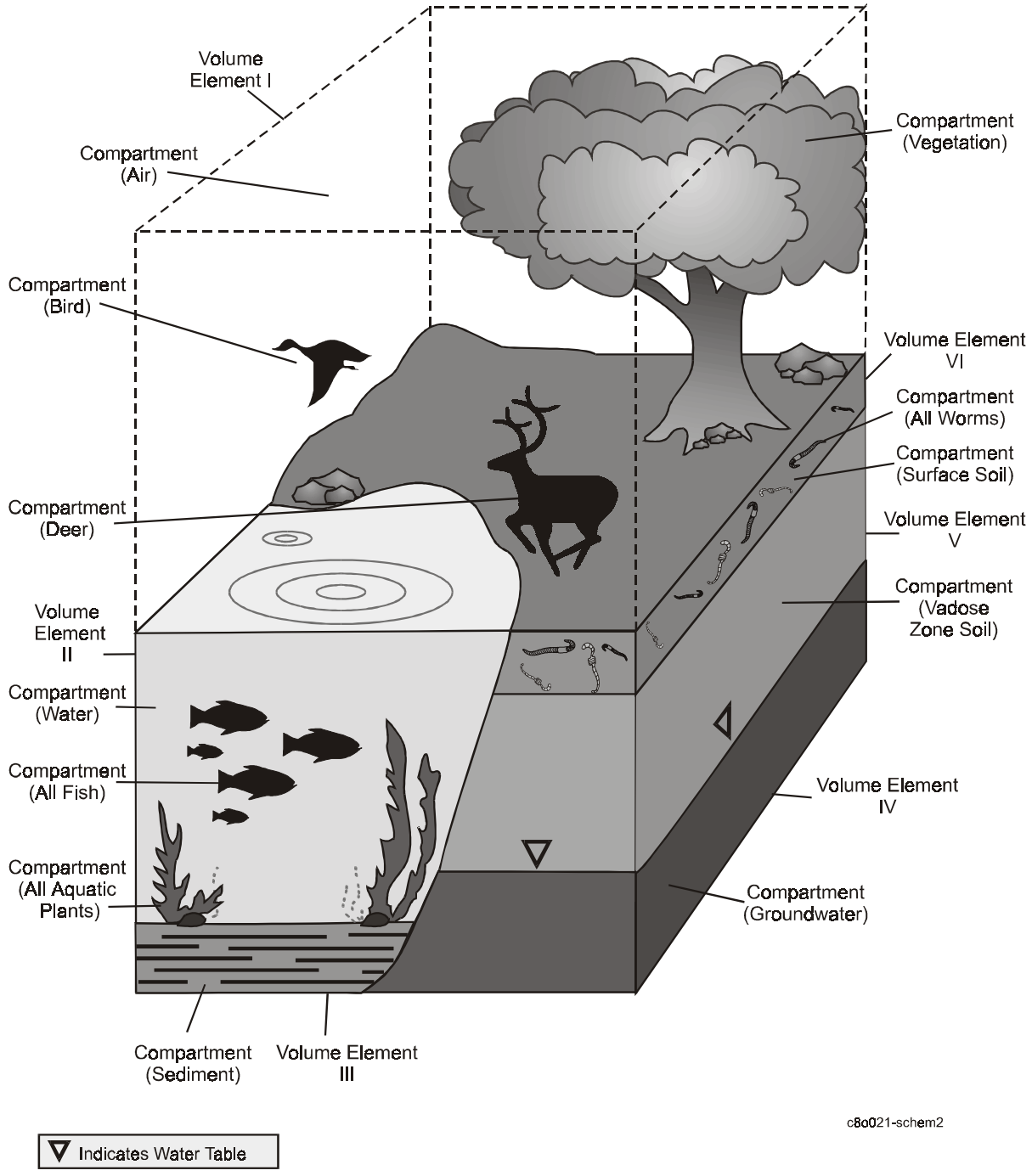


Figure 3-3
"Real Life" Example (Multiple Volume Elements, Multiple Compartments)



3.2 TIME-RELATED TERMINOLOGY

Because TRIM.FaTE is a time-varying model, it is important that the temporal terminology is clearly defined and consistently used. There are three time-related terms that are central to understanding how TRIM.FaTE relates input data, fate and transport calculations, and model outputs: simulation period, simulation time step, and output time step. Definitions of these terms for the purposes of TRIM.FaTE are given below.

For a given TRIM.FaTE simulation, the **simulation period** is the entire length of time for which the model is run and compartment masses and concentrations are calculated – in other words, the time period from the beginning of the simulation until the end. The simulation period, which is usually one or more years, is always greater than or equal to the length of time between the first and last source emissions modeled. Thus, source emissions can occur for either all or part of the simulation period.

For a given model simulation, the **simulation time step** is the time increment at which the model calculates (and re-calculates iteratively throughout the simulation period) a new inventory of compartment masses and concentrations. The simulation time step must be less than or equal to the simulation period – typically, the simulation time step is much less than the simulation period. Within a given simulation time step, the environmental conditions in each compartment are assumed to remain constant.

Because time increments for input data can vary greatly across different model inputs, the simulation time step may change within a simulation depending on how the inputs are changing with time. For example, meteorological data (*e.g.,* wind speeds, precipitation measurements) may be available at hourly increments and source emission rate data may be available at monthly increments. TRIM.FaTE accommodates these different input data increments by assuming that values are constant within a given input data time increment.

When the simulation time step is small relative to the simulation period, it is often useful to reduce the amount of output data by outputting results at periods longer than the simulation time steps. The **output time step**, which is user specified, is defined as a length of time over which the compartment masses and concentrations calculated at each simulation time step are summarized and reported by the model.[1] More than one output time step may be useful for a given TRIM.FaTE simulation (*e.g.,* one year, seventy years). Averaging values over appropriate output time steps also can be useful for inputting output concentrations into exposure models.

Figure 3-4 presents hypothetical values for each of the TRIM.FaTE time-related terms and demonstrates the magnitudes of each term relative to the others.

[1] Even when the smallest output time step is specified as longer than the simulation time step, TRIM.FaTE retains the data calculated for each time step for possible future use, rather than discarding it.

Figure 3-4
Example of TRIM.FaTE Time-related Terminology[a]

simulation period	**30 years**						
output time step	**15 years**				**15 years**		
simulation time step	**2 yrs**	**4 yrs**	**3 yrs**	**6 yrs**	**5 yrs**	**4 yrs**	**6 yrs**

[a] Note that the time periods used in this figure are for illustrative purposes and do not necessarily represent typical time periods used in TRIM.FaTE.

3.3 BIOTIC COMPARTMENT TYPES

Compartment types are determined based on their links with other compartment types. Thus, each biotic compartment type is a different trophic group or has a different route of uptake. Mammalian and avian wildlife, earthworms, fish, benthic invertebrates, macrophytes, and algae are considered different compartment types because they belong to unique trophic groups. The only biotic compartment types that do not have unique links are those that have flexible diets, such as terrestrial omnivores and semiaquatic omnivores that eat a variety of plants, invertebrates, and/or small mammals, depending on the representative species chosen. Plants are divided into four compartment types (leaves, roots, stems, and leaf surfaces) because their routes of exposure are different.

A biotic compartment type in TRIM.FaTE may consist of:

- A trophic group of terrestrial wildlife (*e.g.*, piscivores);
- A trophic group of fish (*e.g.*, carnivores);
- Soil detritivores;
- Benthic invertebrates;
- Algae (phytoplankton);
- Macrophytes;
- All of the leaves of the plant community;
- All of the roots of the plant community;
- All of the stems of the plant community; or
- All of the leaf surfaces of the plant community.

For terrestrial wildlife and fish, one or more species may represent each trophic group. For example, shrews may represent terrestrial insectivores or vermivores (earthworm-eating organisms). These representative species will more clearly represent the whole compartment type when the uncertainty analysis is fully implemented in TRIM.FaTE. A list of biotic compartment types currently in TRIM.FaTE is given in Table 3-1. Parameters for all of the listed representative species are included in TRIM.FaTE.

Major plant community compartment types include: leaves, leaf surfaces, stems, and roots. Particular plant compartments may have different characteristics, depending on whether the vegetation type in the parcel is coniferous forest, deciduous forest, grass/herb fields, agricultural systems, or a hybrid of these types. Woody trunks and roots of trees are not

Table 3-1
Biotic Compartment Types Defined for TRIM.FaTE

Compartment Type (Trophic Functional Group)[a]	Representative Subgroup or Species
Algae	Generalized algal species
Macrophyte	*Elodea densa*
Water column herbivore	Bluegill
Water column omnivore	Channel catfish
Water column carnivore	Largemouth bass
Benthic invertebrate (herbivore)	Mayfly
Benthic omnivore	Channel catfish
Benthic carnivore	Largemouth bass
Terrestrial omnivore	White-footed mouse
Semi-aquatic piscivore	Common loon Mink Belted kingfisher
Semi-aquatic predator/scavenger	Bald eagle
Terrestrial insectivore	Black-capped chickadee
Semi-aquatic herbivore	Mallard
Terrestrial predator/scavenger	Red-tailed hawk Long-tailed weasel
Semi-aquatic insectivore	Tree swallow
Terrestrial herbivore	White-tailed deer Mule deer Black-tailed deer Meadow vole Long-tailed vole
Semi-aquatic omnivore	Raccoon
Terrestrial ground-invertebrate feeder	Short-tailed shrew Trowbridge shrew
Flying insect	Mayfly
Soil detritivore	Earthworm Soil arthropod
Plant leaf	Plant leaf
Plant leaf surface	Plant leaf surface
Plant stem	Plant stem
Plant root	Plant root

[a] Plant parts constitute different compartment types even though they are not different trophic groups.

currently compartment types in TRIM.FaTE because the fate of persistent pollutants in woody components of vegetation is not well understood.

3.4 LINKS

Chemical mass can be transferred between compartments within the same volume element, as well as between compartments in adjacent volume elements. In addition, chemical mass can be transformed within a single compartment. In order to estimate these processes, the relationships, or links, between the compartments must be determined. A **link** is defined as a "connection" that allows the transfer of chemical mass between compartments. Each link is implemented by an algorithm or algorithms that mathematically represent the mass transfer. Figure 3-5 expands on the concepts presented in Figure 3-2 by showing links between compartments in different volume elements. The figure demonstrates that chemicals in the air compartment can be transferred to the water compartment via a link.

Links do not necessarily exist between all adjacent compartments. This concept is demonstrated in Figure 3-6 where chemical mass is transferred between the water and air compartments and between the water and fish compartments, but not between the fish and air compartments. A link may also exist between two chemicals within the same compartment in the form of a transformation process (see Figure 3-7).

Figure 3-5
Two Linked Compartments in Separate Volume Elements

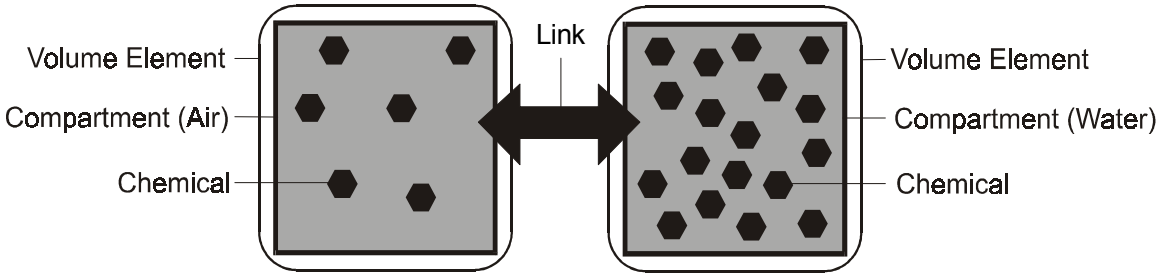


Figure 3-6
Three Linked Compartments in Two Volume Elements

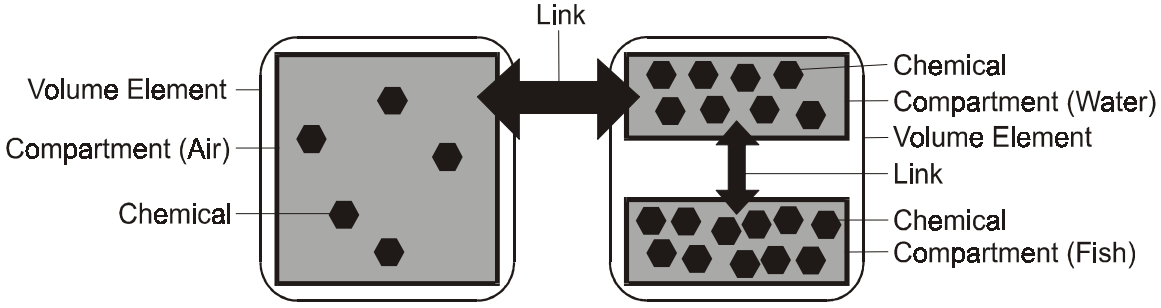
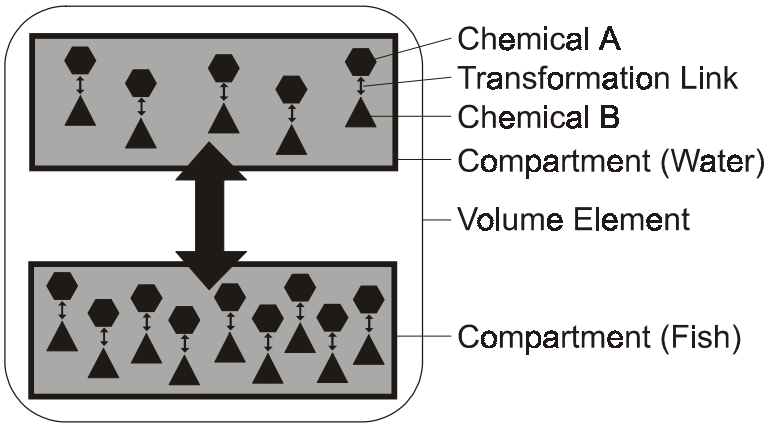


Figure 3-7
Transformation Links Between Chemicals within a Compartment



In the TRIM.FaTE framework, links are a qualitative concept and represent the aggregate of the algorithms and constants used to describe chemical mass transfer among compartments. They can represent relatively simple processes, such as diffusion, or more complicated processes, such as advection. For a given chemical, different links may represent different processes having unique properties. For example, a link between two particular soil compartments may contain information on the advective flow from one soil compartment to another while the shrew-to-soil compartment link would contain information on the ingestion rate of soil by shrews. Figure 3-8 adds the concept of links to a portion of the hypothetical environment presented in Figure 3-3.

3.5 SOURCES

The set of all compartments in a TRIM.FaTE modeling scenario is assumed to contain all of the chemical mass within the system being modeled, excluding sources. A **source** is an external component that introduces chemical mass directly into a compartment. Examples of sources would include the factory emissions of a chemical into an air compartment, the influx of chemical into a river compartment as the result of a spill, or the influx of chemical mass from outside the modeling boundaries into an air compartment as the result of a distant power plant. TRIM.FaTE is designed to accommodate single or multiple source scenarios. Figure 3-9 expands upon Figure 3-6 by adding a source emitting into the air compartment. Figure 3-10 presents the "real life" TRIM.FaTE system shown in Figure 3-8 with the addition of sources.

Figure 3-9
Linked TRIM.FaTE System with Source

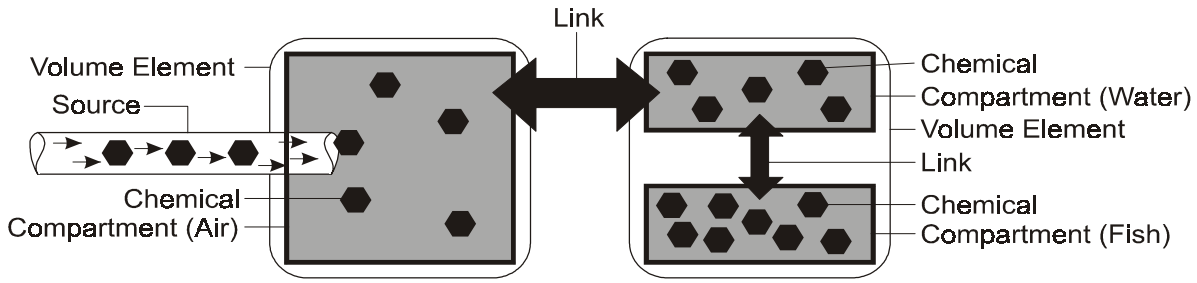


Figure 3-8
"Real Life" TRIM.FaTE System Example with Linked Compartments

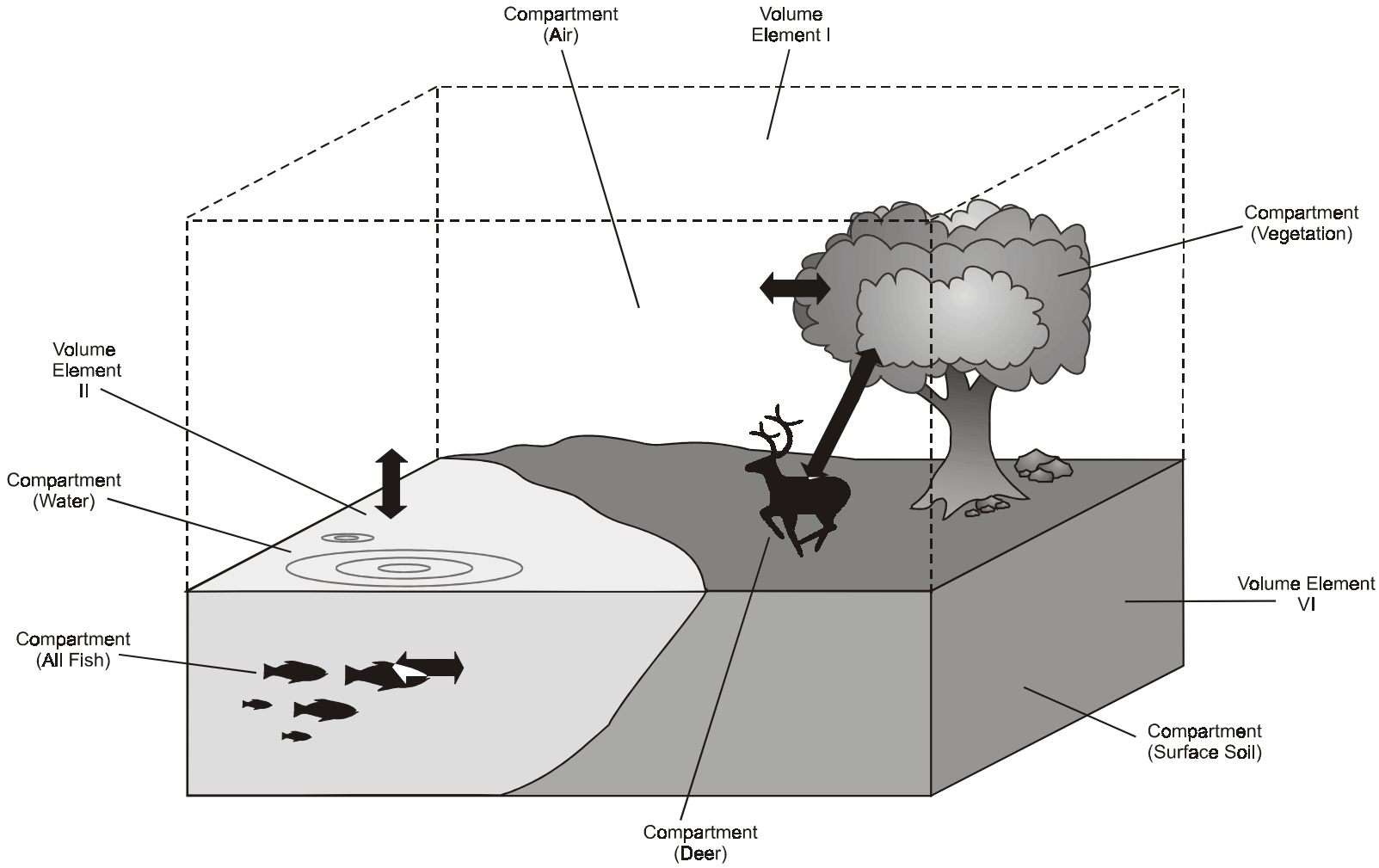
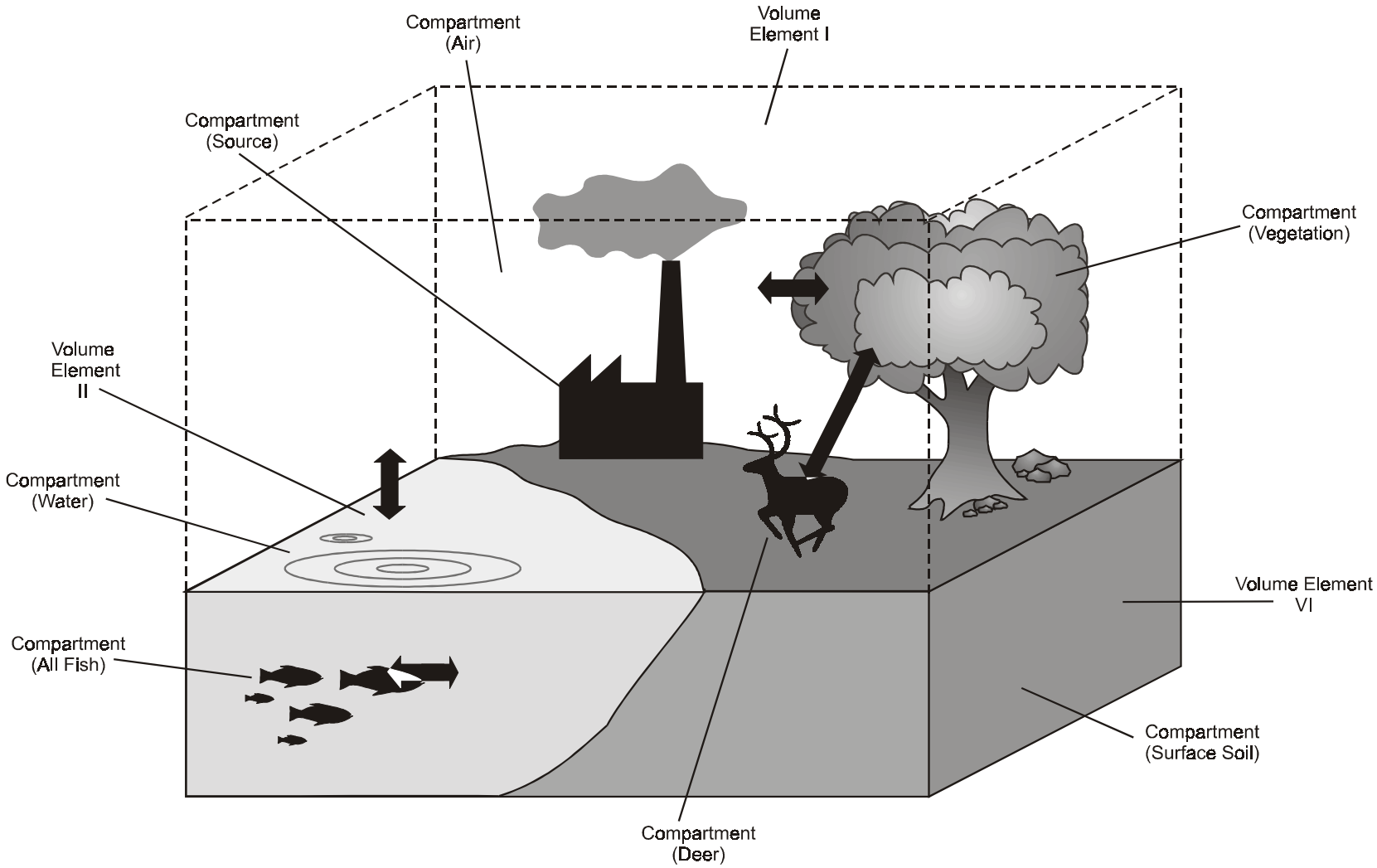


Figure 3-10
"Real Life" TRIM.FaTE System Example with Sources



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4. CONCEPTUAL DESIGN AND MASS BALANCE FRAMEWORK FOR TRIM.FaTE

This chapter, building on the definitions and spatial and temporal concepts discussed in Chapter 3, presents the overall logic implemented in TRIM.FaTE for expressing transport and transformation of chemicals in a multimedia environment. Specifically, this chapter discusses and illustrates the mass balance approach and describes the processes simulated in TRIM.FaTE. The actual algorithms used to implement the approach are documented in Volume II.

4.1 CONCEPTUAL DESIGN

TRIM.FaTE calculates, given an initial mass inventory and mass inputs over time from one or more sources, the mass of one or more chemicals being modeled in each compartment in the modeled system for each simulation time step. With the volume and estimated chemical mass of each compartment, TRIM.FaTE can then calculate the concentration of each chemical in each compartment at each time step.

The development of TRIM.FaTE began with a conceptual diagram of the relationships and processes that affect chemical transport within the environment. The current version of this diagram is shown in Figure 4-1. In this figure, biotic compartments are represented by rectangles and abiotic compartments are represented by ovals. The various lines illustrate the potential chemical transfers between each of the components of the ecosystem.

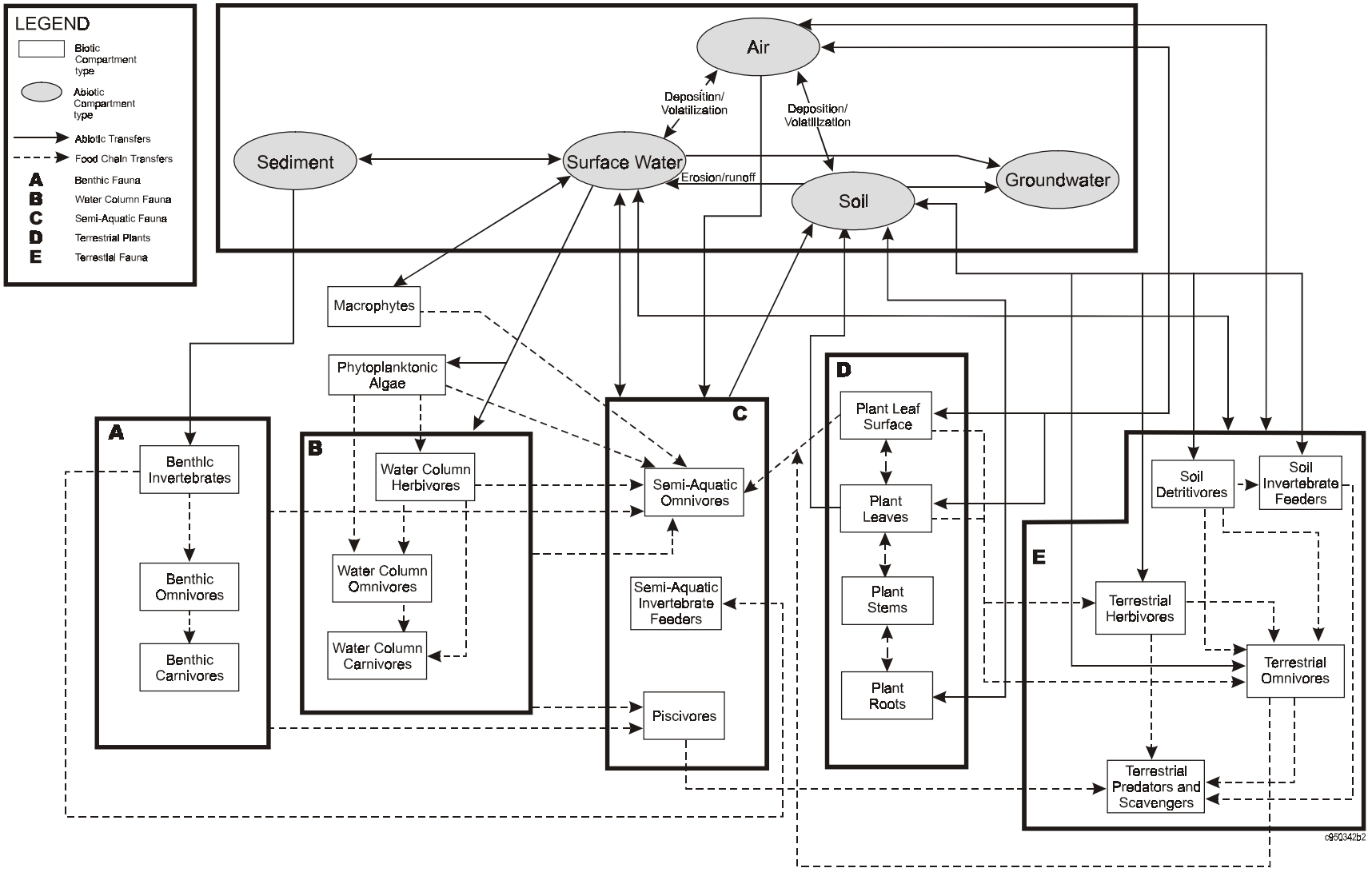
4.2 GOVERNING MASS BALANCE EQUATIONS

TRIM.FaTE has been developed with an emphasis on conserving chemical mass. This means that the entire quantity of a chemical input to the system is tracked throughout the system being modeled. When applied to a specific compartment (*e.g.*, soil, or a mouse population), this implies that, over a given time period, the amount of the chemical in the compartment at the end of the period is equal to the amount of the chemical in the compartment at the beginning of the period, plus the gains of the chemical that occurred during the time period, minus the chemical that was lost from the compartment during the time period.

To date, the mass balance approach has been implemented primarily for first-order linear processes. Therefore, this discussion is limited to algorithms of this type. It is important to note that higher order non-linear methods can also be implemented within this structure.

First-order transfers between compartments are described by transfer factors, referred to as T-factors. In most cases, T-factors are in units of inverse time. Technically, the units of a T-factor depend on the sending and receiving chemicals, as what is actually being preserved across the exchange is the amount of "core" chemical present in all transforming chemicals. The T-factor is the instantaneous flux of this "core" compound per amount of the compound in the sending compartment. The definition of the "core" compound depends on the particular chemicals being considered (*e.g.,* for the test case the core compound is an Hg atom).

Figure 4-1
Conceptual Diagram for TRIM.FaTE[a]



[a] Chemical transformation processes are not depicted but may occur in all compartment types. Transformation products may be tracked in TRIM.FaTE or transferred out of compartments to sinks.

In most cases, it is expected that the molecular weights of the inter-transforming chemicals will be similar, and so preservation of the "core" compound will be essentially equivalent to preservation of mass. Significant differences between the preservation of "core" compound and the preservation of mass occur only if the sending and receiving chemicals have very different molecular weights. This has not been the case to date, but may occur as the model is applied to other transforming chemicals.

The preservation of "core" compound and the preservation of mass would be identical if the time-dependent masses of the reaction products were estimated simultaneously for each chemical of interest. Given the current computation and logistical demands of modeling transformation in many compartments, this is not seen as a practical general solution.

A simplification of a first-order transfer process is shown in the top part of Figure 4-2 for a system of one chemical, two compartments, and two transformation sinks, where transformation is treated as an irreversible loss. Denoting by $N_a(t)$ and $N_b(t)$ the mass of chemical in compartments *a* and *b*, respectively (in units of *mass*), it can be seen that:

$$\textit{Chemical gains for compartment } a = S_a + T_{ba}N_b \quad (1)$$

$$\textit{Chemical losses for compartment } a = T_{ab}N_a + R_aN_a \quad (2)$$

and

$$\textit{Chemical gains for compartment } b = T_{ab}N_a \quad (3)$$

$$\textit{Chemical losses for compartment } b = T_{ba}N_b + R_bN_b \quad (4)$$

where:

N_a = mass of chemical in compartment a, units of *mass*

N_b = mass of chemical in compartment b, units of *mass*

S_a = chemical source outputting to compartment *a*, units of *mass/time*

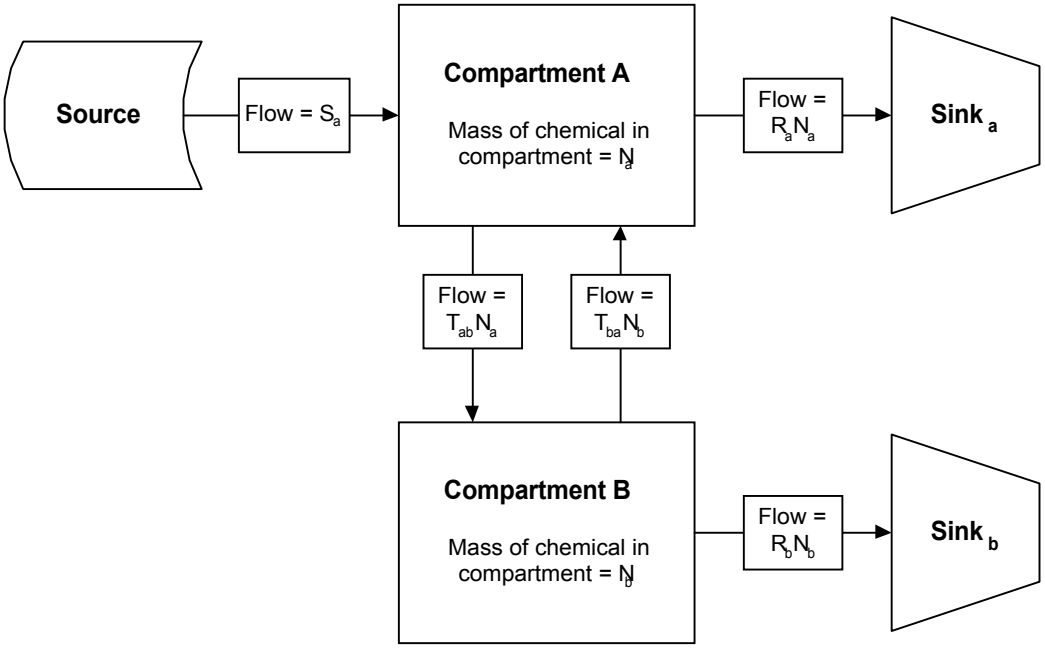
T_{ab} = transfer factor for movement of chemical from compartment *a* to compartment *b* during simulation time step, units of */time*

T_{ba} = transfer factor for movement of chemical from compartment *b* to compartment *a* during simulation time step, units of */time*

R_a = reaction loss of chemical in compartment *a*, units of */time*

R_b = reaction loss of chemical in compartment *b*, units of */time*.

Figure 4-2
Example of First-order Transfer Processes for Two Compartments, One Chemical
(Transformation Treated as Irreversible Sink)



$$\begin{bmatrix} dN_a/dt \\ dN_b/dt \\ dSink_a/dt \\ dSink_b/dt \end{bmatrix} = \begin{bmatrix} -(T_{ab}+R_a) & T_{ba} & 0 & 0 \\ T_{ab} & -(T_{ba}+R_b) & 0 & 0 \\ R_a & 0 & 0 & 0 \\ 0 & R_b & 0 & 0 \end{bmatrix} \begin{bmatrix} N_a \\ N_b \\ Sink_a \\ Sink_b \end{bmatrix} + \begin{bmatrix} S_a \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (5)$$

The constraint that mass balance must be preserved means that, over any time interval, the change in mass in a compartment is equal to the gains minus the losses in mass over the time interval. The instantaneous change in mass with respect to time is the derivative with respect to time, denoted by *dN/dt*. Thus, the mass balance constraint, when applied to the simple system discussed here, yields a system of two linked differential equations:

$$\frac{dN_a}{dt} = S_a + T_{ba}N_b - (R_a + T_{ab})N_a \quad (6)$$

$$\frac{dN_b}{dt} = T_{ab}N_a - (R_b + T_{ba})N_b \quad (7)$$

Additional terms are needed to properly account for the chemical mass. In particular, the fate of the chemicals after reacting must be tracked. For this reason, two additional compartments are added to the system, and serve as the repository of the chemicals after reaction. These are referred to as "sinks," since after the chemical is transferred into these compartments, it no longer moves to any other compartments. While the chemical would continue to move in its altered form throughout the system, this movement is not of interest in this example. Denoting by $Sink_a$ and $Sink_b$, the mass in the reaction sinks for compartments *a* and *b*, respectively, the complete system is:

$$\frac{dN_a}{dt} = S_a + T_{ba}N_b - (R_a + T_{ab})N_a \quad (8)$$

$$\frac{dN_b}{dt} = T_{ab}N_a - (R_b + T_{ba})N_b \quad (9)$$

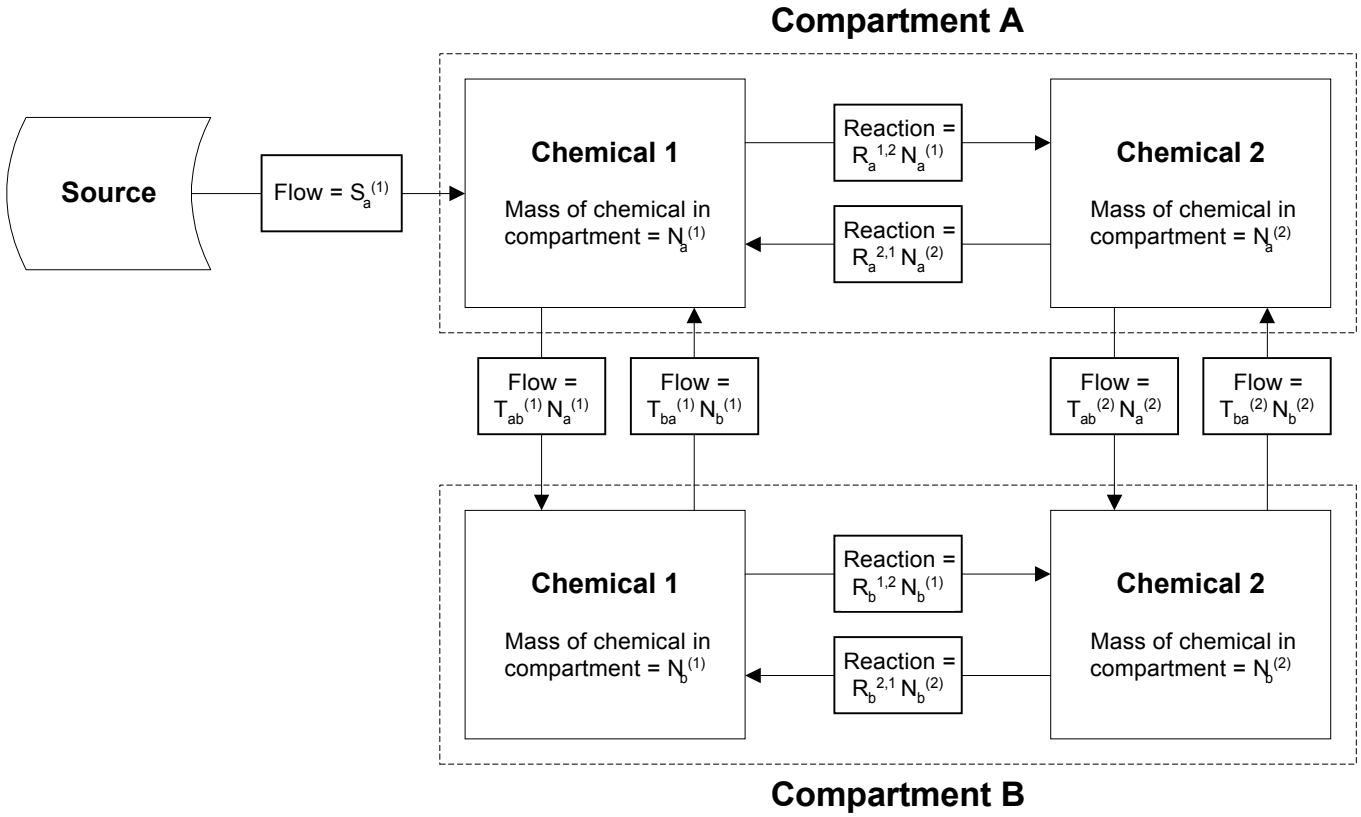
$$\frac{dSink_a}{dt} = R_aN_a \quad (10)$$

$$\frac{dSink_b}{dt} = R_bN_b \quad (11)$$

This system of equations is shown in matrix form in Equation (5) at the bottom of Figure 4-2.

If the fate of the transformed chemical is of interest, and the necessary algorithms and input data are available for the transformed chemical, then the mass balance approach can be modified accordingly. Figure 4-3 shows a generalization of the previous example, including the matrix form of the system [Equation (12)], to the case where the transformed chemical is modeled in addition to the chemical being transferred. In this case, transfer factors are added for the transformed chemical to account for additional possible transfers.

Figure 4-3
Example of First-order Transfer Processes for Two Compartments, Two Chemicals
(Chemicals 1 and 2 in Reversible Transformation Process; Transformation Products Tracked)



$$\begin{bmatrix} dN_a^{(1)}/dt \\ dN_b^{(1)}/dt \\ dN_a^{(2)}/dt \\ dN_b^{(2)}/dt \end{bmatrix} = \begin{bmatrix} -(T_{ab}^{(1)}+R_a^{1,2}) & T_{ba}^{(1)} & R_a^{2,1} & 0 \\ T_{ab}^{(1)} & -(T_{ba}^{(1)}+R_b^{1,2}) & 0 & R_b^{2,1} \\ R_a^{1,2} & 0 & -(T_{ab}^{(2)}+R_a^{2,1}) & T_{ba}^{(2)} \\ 0 & R_b^{1,2} & T_{ab}^{(2)} & -(T_{ba}^{(2)}+R_b^{2,1}) \end{bmatrix} \begin{bmatrix} N_a^{(1)} \\ N_b^{(1)} \\ N_a^{(2)} \\ N_b^{(2)} \end{bmatrix} + \begin{bmatrix} S_a^{(1)} \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (12)$$

Applying this same approach to a general system with M compartments (including all sinks), and allowing the transfer factors and source terms to depend on time as well, results in a system of linked differential equations of the form:

$$\frac{d}{dt}\vec{N} = A(t)\vec{N}(t) + \vec{s}(t), \quad \vec{N}(t_0) = \vec{N}_0 \tag{13}$$

where:

$\vec{N}(t)$ = an M-dimensional vector whose ith entry is the mass in the ith compartment

A(t) = an M x M time-dependent matrix

$\vec{s}(t)$ = an M-dimensional vector accounting for the source terms in each compartment.

The matrix A(t) is referred to as the *transition matrix* for the system. This term is borrowed from Markov theory (Schneider and Barker 1989), although the model is not strictly a Markov process. The vector $\vec{s}(t)$ accounts for pollutant sources located within specific compartments. The vector $\vec{N}_0$ is the initial distribution of mass among the compartments.

4.3 PHASES

There are multiple environmental phases within many of the compartments in TRIM.FaTE. The most common phases are liquid, gas, and solid, which are assumed to be at chemical equilibrium within a compartment in this model unless otherwise specified. Other phases may include biotic phases (*e.g.*, algae in surface water). The adjacent text box lists the phases currently implemented in TRIM.FaTE for each medium.

PHASES CURRENTLY IMPLEMENTED IN TRIM.FaTE (listed by medium)

Air
- vapor
- suspended particulate

Soil
- soil pore water
- vapor
- soil solids

Surface water
- suspended solids
- water
- algae

Sediment
- sediment pore water
- sediment solids

In any compartment, the total amount of chemical present is made up of the sum of the amounts in the different phases. Because chemical equilibrium among phases is assumed, the ratios of the concentrations in the individual phases are constant for a given chemical. The fraction of the chemical that is in each phase in a compartment can easily be calculated. The chemical mass in each phase is tracked in TRIM.FaTE because transfer factors are sometimes phase dependent (*i.e.,* the transfer factor for particle deposition from air is dependent on chemical mass in the particle

phase of air). The mathematical details related to implementation of phases in TRIM.FaTE are presented in Chapter 2 of Volume II of the TRIM.FaTE TSD (U.S. EPA 1999d).

4.4 FATE, TRANSFORMATION, AND TRANSPORT PROCESSES

In TRIM.FaTE, the following processes are addressed and implemented as first-order processes for the modeling of the transfer and transformation of chemicals.

- Advective processes;
- Diffusive processes;
- Dispersive processes;
- Biotic processes; and
- Reaction and transformation.

More detailed explanation of the mathematical representation of these processes and documentation of all of the currently implemented algorithms are presented in Volume II of the TRIM.FaTE TSD (U.S. EPA 1999d).

4.4.1 ADVECTIVE PROCESSES

An advective process is one in which a chemical is transported within a given medium that is moving from one compartment to another. Mackay (1991) refers to this as a "piggyback" process, in which a chemical is "piggybacking" on material that is moving from one place to another for reasons unrelated to the presence of the chemical. Advective processes are modeled using first-order methods in TRIM.FaTE. Mathematically, all that is required to calculate the advective flux is the velocity of the moving phase and the amount of the chemical that is in the moving phase. Examples of advective processes considered for transport of a chemical are: erosion from a surface soil compartment to a surface water compartment, runoff from a surface soil compartment to a surface water compartment, and advective transport from one air compartment to another due to the wind field.

4.4.2 DIFFUSIVE PROCESSES

In a diffusive process, a chemical is transported from one compartment to another as a result of the magnitude and direction of the concentration differences between the two compartments at the interface between the two locations. Examples of diffusive processes considered include exchange between air compartments and soil or surface water compartments, exchange between benthic sediment compartments and surface water compartments, and exchange between air compartments. Models for diffusion frequently use non-first-order methods; however, these are often approximated with first-order methods. All diffusive processes are currently modeled in TRIM.FaTE using first-order methods. Diffusion rates are based on the compartment concentrations at the beginning of each simulation time step.

4.4.3 DISPERSION

Dispersion refers to the "spreading out" of a chemical during advective transport, and may result in movement perpendicular to the direction of advective flow. In TRIM.FaTE, dispersion is explicitly addressed (as a first-order process) in transfers between surface water compartment types. For surface water dispersion, the methods in the Water Quality Analysis Simulation Program (WASP) water transport model are used (Ambrose et al. 1995).

4.4.4 BIOTIC PROCESSES

The transport of chemicals to biota (*i.e.,* into biotic compartments) consists of diffusive and advective processes, though the latter term is rarely used by biologists. Chemicals diffuse into plant leaves from air; chemicals deposit onto plant leaves with particles in air, an advective process. The uptake of chemicals from soil or water in soil by plant roots or earthworms is treated as diffusion, though water carries the chemical into the plant (advection). Similarly, chemicals are assumed to enter algae, macrophytes, and benthic invertebrates by diffusion. The major advective process for animals is food intake by fish, birds, and mammals.

The only transport process within biota that is included in TRIM.FaTE is transport between roots and leaves through the plant stem in xylem and phloem fluids. The distribution of chemicals among organs in fish and wildlife is not a feature of TRIM.FaTE.

4.4.5 REACTION AND TRANSFORMATION

Reaction and transformation processes include biodegradation, photolysis, hydrolysis, oxidation/reduction, and biotic metabolism. These are processes that transform a chemical species into another chemical species. Reaction and transformation are modeled in TRIM.FaTE as reversible reactions using first-order reaction/transformation rates (or, equivalently, transformation half-lives). The first-order transformation rates may incorporate more than one of the processes involved. Depending on the algorithm and compartments involved, the mass of chemical transformed may be either lost from the system (*i.e.*, transferred to a sink), or tracked as a different chemical.

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5. APPLICATION OF TRIM.FaTE

This chapter describes the application of the concepts presented in Chapters 3 and 4 by briefly explaining each of the main steps necessary to set up and perform a simulation with TRIM.FaTE. It explains the methods associated with key steps in the modeling process, provides a general sense of the level of effort associated with performing a TRIM.FaTE simulation, and summarizes the inputs and outputs of the model. This chapter is not intended to be a "user's guide" to the model. OAQPS recognizes the importance of developing detailed user's guidance material for TRIM.FaTE that will assist users in defining the spatial and temporal modeling resolution, compartments and linkages, as well as parameters and initial conditions. Such material will be developed during the next phase of TRIM development activities. The intended purpose of this chapter, however, is simply to provide an understanding of how TRIM.FaTE works by explaining in general terms how it is applied to model the fate and transport of air emissions from one or multiple sources.

5.1 STRUCTURE OF A TRIM.FaTE SIMULATION

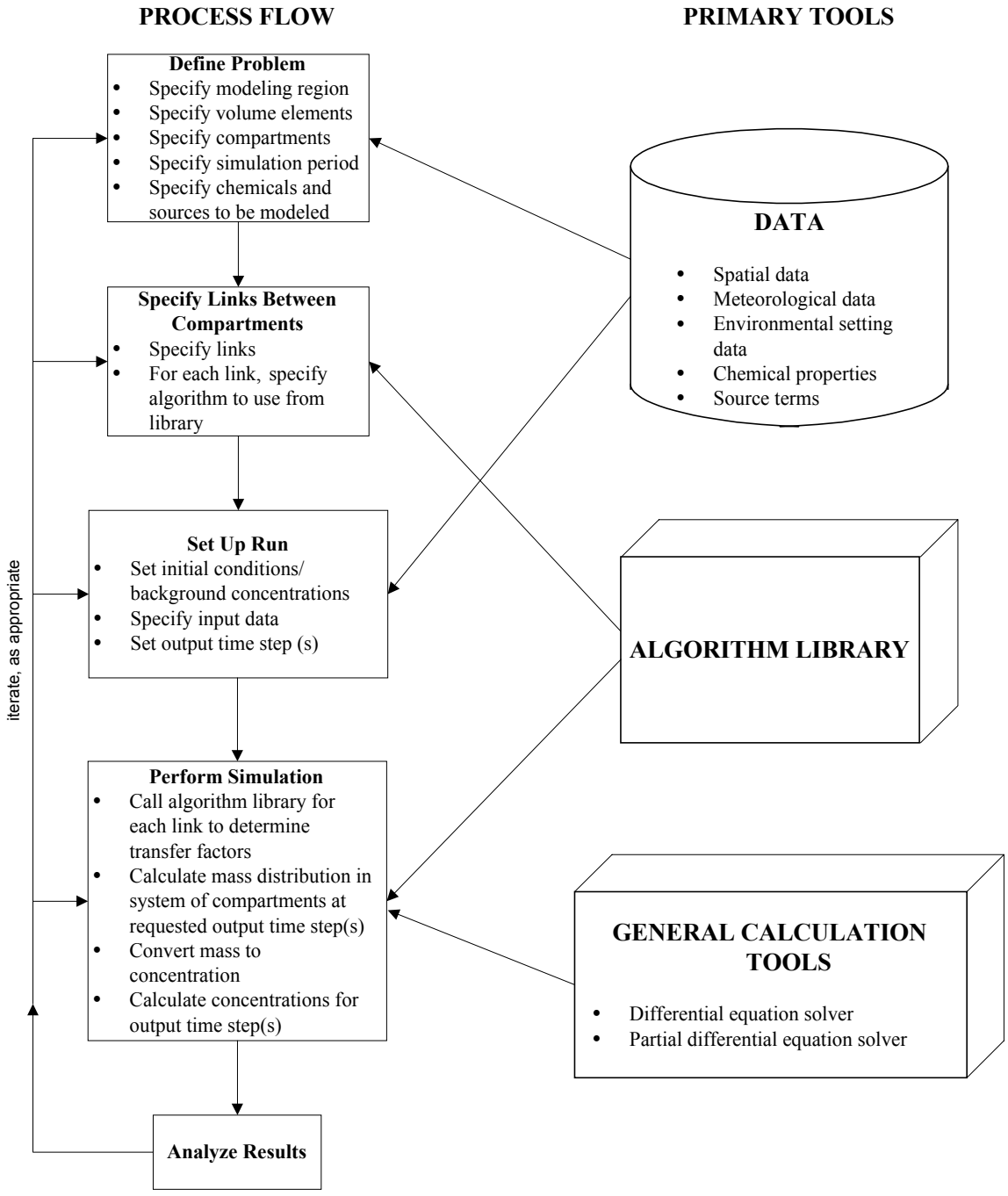
One of the strengths of TRIM.FaTE is that it is designed to be an iterative and flexible model. When the modeling process begins, there is a general sequence that typically is followed. After the initial step, however, there is no fixed order in which the modeling steps are necessarily performed (although some steps must be completed before others begin). This process is shown in Figure 5-1. The boxes on the left side of the figure represent a partitioning of the modeling sequence into five broad areas. These areas include: basic problem definition, specification of links, simulation setup, simulation implementation, and analysis of results. The particular division into five such areas is somewhat arbitrary, and in an actual application the progression may not be quite as linear as that shown in the figure. However, all of these steps are necessary. The vertical arrows between these boxes represent the typical order of events in the modeling process. The arrows on the left side of the boxes indicate the iteration that may be necessary or desired.

The shapes under the heading “Primary Tools” represent the main tools used in the modeling process. The arrows from these shapes to the flow boxes indicate where in the modeling process these tools would be used. To focus on key aspects of the TRIM.FaTE approach, only selected tools are shown. There are other tools that may be necessary that are not included in this figure. Such tools include pre-/post-processing software, which may automate some aspects of the process, uncertainty and variability analysis software, and general user interface software.

5.2 PROBLEM DEFINITION

The first step in the TRIM.FaTE modeling process is a clear statement of the problem definition. Through the formulation of this problem definition , the chemical(s) and source(s) to be modeled, the initial spatial features of the ecosystem to be modeled, and the simulation period

Figure 5-1
TRIM.FaTE Modeling Sequence



are determined. Using the nomenclature presented in Chapter 3, the volume elements and compartments within the volume elements are specified.

5.2.1 DETERMINING SCALE AND SPATIAL RESOLUTION

A **parcel** is a planar (*i.e.,* two-dimensional) geographical area used to subdivide the modeling region. Parcels, which can be virtually any size or shape, are the basis for defining volume elements and do not change for a given scenario. There can be separate parcels for air and for the land surface (surface soil or surface water).

This section introduces the considerations for defining the overall modeling scale and the level of spatial complexity (*i.e.*, location, size, shape, and number of parcels) in a TRIM.FaTE analysis. After the initial scenario is constructed and a simulation has been completed, the preliminary results need to be evaluated to confirm that an appropriate level of resolution has been used. An example of a general approach for determining appropriate scale and spatial resolution as well as suggestions for defining compartments are included in Appendix C. At some point, EPA may consider automating the process of determining spatial resolution to enhance user consistency.

5.2.1.1 Specifying the Modeling Region

The first step in determining the scale and spatial resolution of a TRIM.FaTE scenario is to determine the modeling region (*i.e.,* spatial boundaries of the analysis). In this step, the user specifies the extent of the area to be modeled. A user should consider factors such as mobility of the modeled chemical(s), location of source(s), and background concentrations of the chemical(s). In regions where the predominant wind direction is variable, the modeling region may be defined to include and extend beyond the region of interest to account for the possibility of pollutant mass leaving and re-entering the system.

5.2.1.2 Specifying Parcels

The next step in determining the scale and spatial resolution of a TRIM.FaTE scenario is to specify the modeling parcels. Parcels are planar geographical areas of any size or shape that are the basis for defining volume elements and do not change for a given scenario. The higher the number of parcels in a given scenario, the higher the spatial resolution. However, more parcels generally correspond to greater resource requirements, both in terms of input data collection and model completion time.

Beyond resource considerations, there are three principal technical considerations for determining the parcels for a TRIM.FaTE scenario: the likely pattern of transport and transformation of each chemical of concern (*i.e.,* where significant concentration gradients are likely to be), locations of natural boundaries, and locations of the targets. The target is defined as a receptor, either human or ecological, or landscape component (*e.g.*, lake, wetland, agricultural plot) of interest.

For the chemical(s) of interest , the three most important factors for determining the appropriate modeling scale and resolution are the atmospheric transport of chemical mass, rapidity of chemical transport, and degradation of the chemical(s) in the environment. Understanding the atmospheric transport of the chemical(s) of interest is useful in developing both the modeling scale and spatial resolution. Because air pollutants travel more rapidly in air than any other medium, insight into atmospheric transport can provide the user with a general idea of the extent of chemical transport and thus can be useful in determining the modeling scale. Furthermore, this information can provide the user with a general picture of the path of chemical transport, helping the user determine where higher spatial resolution may be beneficial.

Information about the mobility and degradation of the chemical(s) of interest, when combined with land use data, can provide additional insight into the transport in media other than air. It can be helpful in refining the scale of the scenario as well as providing additional input to help determine the spatial resolution of the scenario.

Natural boundaries are also an important consideration in developing parcels. These natural boundaries may include areas such as an air shed that can be identified by a combination of geographic and meteorologic conditions or a watershed or valley. An air shed can include large valleys such as the Sacramento Valley (CA) where, due to inversion layers and diurnal wind patterns, the air mass is confined and well mixed throughout the area for a large portion of the time. Air shed boundaries can also include smaller valleys when meteorological conditions produce long residence time for the air mass in the bounded region. Air shed boundaries are useful in providing information about the scale of the model region (*i.e.*, external boundaries of the system).

Watersheds are also useful in determining the scale of the system as well as the size and location of parcels within the system, especially if the concentration in a particular lake or wetland is of interest. Watershed boundaries can be identified or approximated from topographical maps by tracing ridgelines and noting the origin and direction of flow for streams and rivers. The size and location of a watershed can influence the transfer of chemical to water bodies within the basin.

Another important consideration in developing parcels is the location of the target(s). The location of the target(s) is important because it allows the user to focus the analysis on the area(s) of interest, thus allowing resolution to be coarse in areas that are not expected to affect the chemical concentrations near the targets and resolution to be finer in the areas that may have an impact on the targets. Evaluations to determine the extent to which these nonessential area(s) can be simplified without significantly changing the model outcome are ongoing.

The illustrative approach to specifying parcels described in Appendix C generates a starting point for any given analysis objective for which TRIM.FaTE is designed. The approach is intended to impart some consistency and transparency into the scenario setup process. Additionally, after a scale has been chosen, one must determine if that scale is appropriate when compared to other sources of model uncertainty.

5.2.1.3 Determining Volume Elements

After the parcels have been determined for a scenario, the volume elements corresponding to those parcels are specified. This step involves determining the appropriate number of volume elements and specifying the appropriate depth for each one. Whereas parcels only represent the modeling region in two dimensions, volume elements add the component of depth, thus representing the modeling region in three dimensions (the location and two-dimensional planar shape of a volume element corresponds exactly to the relevant parcel). The volume elements are determined from a general knowledge of mixing heights in air, average depth of water bodies or approximate levels of stratification, and typical demarcations in the soil horizon. The development of volume elements represents the final step in specifying the spatial resolution of the modeling region.

5.2.1.4 Determining Compartments

Abiotic

Abiotic compartment types are determined by the predominant abiotic medium in the volume element within which they are contained. At least one abiotic compartment must be contained within each volume element and, although not typically utilized, the model framework does support multiple abiotic compartments within a volume element. In most cases, the determination of abiotic compartments is an implied step because they are simply defined by the predominant abiotic media within the volume element. For example, if a given volume element is composed predominantly of surface soil, a surface soil compartment would be included in the volume element.

Biotic

Of the available biotic compartment types, the user is only required to run the model with those that significantly influence the overall mass balance of the chemical in TRIM.FaTE. In applying the model to PAHs, for example, the plant biomass significantly influences the mass balance in the system. Thus, it would not be appropriate to run a PAH application of the model without the plant compartment types, even if the particular application was only interested in the concentrations in abiotic compartments. A user can choose to exclude terrestrial or aquatic biotic compartment types from the analysis if they are not large reservoirs or significant sinks for chemical mass. The only vertebrate or invertebrate compartment types in TRIM.FaTE that are required for model runs are those that are part of the food chain for a trophic group of concern.

A user can perform a TRIM.FaTE assessment for a whole trophic group if a representative species is chosen, particularly if distributions of input parameters are used. In addition, a user can choose particular animal species of concern (*e.g.*, threatened or endangered populations) and parameterize the model for those species.

5.2.2 DETERMINING SOURCE(S) AND CHEMICAL(S) TO BE MODELED

In determining the sources and chemicals to be modeled, the user must consider the objective of the modeling exercise and the effects endpoints of concern. The user would need to assess the modeling region and determine the sources and chemicals that can be expected to have an impact on the endpoints of concern. The user must then decide, given the resource constraints of the analysis, which sources and chemicals should be included in the modeling analysis. Ideally, this would be part of the problem definition process performed earlier in the analysis because the chemical(s) and location of the source(s) influences how the parcels are initially layed out.

5.2.3 DETERMINING SIMULATION PERIOD

After determining the sources and chemicals to be modeled, the user must determine the appropriate simulation period by considering the modeling objective, the lifetime of the modeled source(s), the persistence and, in some cases, mobility of the modeled chemical(s), and the effects endpoints of concern. In addition, the user should again consider the resource limitations when determining the simulation period because the selected simulation period directly affects the necessary computing time.

5.3 DETERMINING LINKS/ALGORITHMS

The second step shown in Figure 5-1 is to specify the links between all adjacent compartments specified for a given scenario (the compartment types currently available in TRIM.FaTE are listed in Chapter 3). The system of links is one of the most critical components of TRIM.FaTE. This component is critical because the links determine how the processes that drive chemical transfer and transformation will be approximated in TRIM.FaTE. By specifying a link between two adjacent compartments, it is assumed that some method exists by which to estimate the transfer of chemical through the link. If more than one method is already available in the algorithm library, then it is necessary to specify which of the algorithms to use. If an algorithm is not in the algorithm library, then it must be "added" so that it can be accessed by the underlying software. Methods for adding additional algorithms to the library will be included in a future version of the model. Table 5-1 presents the currently implemented links between abiotic compartment types, and Table 5-2 presents the currently implemented links between biotic compartment types and abiotic compartment types, and between biotic compartment types.

TRIM.FaTE also has the flexibility to use model results from single-medium models (*e.g.*, ISC) in place some of the internal links and algorithms. In this case, the output from the external model would replace the calculations of fate and transport within the specific medium. A description of how external models can be integrated with TRIM.FaTE is presented in Appendix B.

Table 5-1
Links and Processes Addressed for Abiotic Compartment Types

Links Between Compartment Types		Processes Addressed
Receiving	**Sending**	
Air	Air	Bulk Advection
	Surface Soil	Diffusion Resuspension
	Surface Water	Diffusion
Surface Soil	Surface Soil	Diffusion Erosion Runoff
	Root Zone Soil	Diffusion
	Air	Diffusion Dry Deposition Wet Deposition
Root Zone Soil	Root Zone Soil	Diffusion Percolation
	Surface Soil	Diffusion Percolation
	Vadose Zone Soil	Diffusion
Vadose Zone Soil	Vadose Zone Soil	Diffusion Percolation
	Root Zone Soil	Diffusion Percolation
Surface Water	Surface Water	Bulk Advection Dispersion
	Surface Soil	Erosion Runoff
	Air	Dry Deposition Wet Deposition Diffusion
	Sediment	Resuspension Pore Water Diffusion
Sediment	Surface Water	Abiotic Solids Settling 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 5-2
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] Litterfall [b]
	Leaf	Litterfall [b]
	Terrestrial Ground-Invertebrate Feeder	Excretion [a]
	Terrestrial Vertebrate Herbivore	
	Terrestrial Omnivore	
	Terrestrial Insectivore	
	Semiaquatic Omnivore	
	Predator/Scavenger	
	Semiaquatic Insectivore	
	Semiaquatic Herbivore	
	Semiaquatic Piscivore	
Leaf	Leaf Surface Air Stem	Uptake [a]
Air	Leaf	Diffusion/Advection
Root	Root Zone Soil	Uptake [a]
Stem	Root Zone Soil (Water Phase) 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 Surface Soil	Diet [b]
	Air	Inhalation [b]
Terrestrial Vertebrate Herbivore	Leaf Leaf Surface Surface Soil	Diet [b]
	Air	Inhalation [b]

Links Between Compartment Types		Processes Addressed
Receiving	**Sending**	
Terrestrial Omnivore	Leaf Leaf Surface Soil Detritivore Surface Soil	Diet [b]
	Air	Inhalation [b]
Terrestrial Insectivore	Soil Detritivore	Diet [b]
	Air	Inhalation [b]
Semiaquatic Omnivore	Benthic Invertebrate Soil Detritivore Herbivorous Fish Omnivorous Fish Carnivorous Fish Surface Soil	Diet [b]
	Air	Inhalation [b]
Predator/Scavenger	Terrestrial Vertebrate Herbivore Terrestrial Omnivore Terrestrial Insectivore Soil Detritivore Benthic Invertebrate (Insect)	Diet [b]
Semiaquatic Insectivore	Benthic Invertebrate (Insect)	Diet [b]
Semiaquatic Herbivore	Benthic Invertebrate Leaf	Diet [b]
Semiaquatic Piscivore	Terrestrial Omnivore Terrestrial Herbivore Terrestrial Insectivore Herbivorous Fish Omnivorous Fish 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]

Links Between Compartment Types		Processes Addressed
Receiving	**Sending**	
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.

5.4 SIMULATION SETUP

The third step shown in Figure 5-1 is the preparation of a simulation after the volume elements, compartments, and links have been specified. This involves specifying the chemical properties of each modeled chemical, the initial distribution of chemical mass in the compartments, the data for each modeled source, all environmental setting data needed by the selected algorithms, and the output time step(s) of interest. The role that each of these inputs plays in estimating the fate and transport of chemical mass is briefly explained in this section. A complete list of all the inputs for the currently implemented algorithms is presented in Appendix D.

5.4.1 CHEMICAL PROPERTIES

To estimate the fate and transport of chemical mass through the system, the relevant properties for each modeled chemical must be specified. The list of chemical properties that are necessary for a given simulation varies depending on the chemical (*e.g.*, organic chemicals differ from metals) and the media and biota modeled. Several examples of abiotic and biotic chemical properties are listed in the adjacent text box.

ILLUSTRATIVE EXAMPLES OF ABIOTIC CHEMICAL PROPERTIES

- half life (in each environmental medium)
- Henry's Law constant
- melting point
- molecular weight

ILLUSTRATIVE EXAMPLES OF BIOTIC CHEMICAL PROPERTIES

- half life (for each modeled species)
- accumulation factor (for modeled animal species)
- bioaccumulation rate (for modeled plant species)
- elimination rate (for modeled animal species)

5.4.2 INITIAL CONDITIONS

For each compartment in a scenario, the user must specify the initial conditions, *i.e.,* the initial inventory of chemical mass. Default values of zero may be assumed in some compartments for pollutants that have a relatively short half-life or if the objective of the simulation is to assess the effects of a source (or sources) in the absence of background, but it is important to have estimates of initial conditions if the pollutant is persistent and the objective is to assess "cumulative" exposures, or if results of the analysis are to be compared with monitoring and measurement data.

5.4.3 SOURCE DATA

Source data must be specified for each source modeled in the scenario. Conceptually, there is no limit on the number of different sources that can be modeled. The adjacent text box lists the variables that must be defined for each source.

SOURCE INPUTS

- source location
- emission height
- emission rate (for each chemical)
- particle size (for each chemical)
- gas or liquid (for each chemical)

5.4.4 ENVIRONMENTAL SETTING DATA

Whereas initial conditions and source data specify the location and influx of chemical mass in the system, environmental setting data are needed to estimate the fate and transport of

that mass throughout the modeled system. There are two general types of data necessary to define the links between compartments in TRIM.FaTE: meteorological data and other environmental setting data. The level of desired refinement in the simulation dictates the appropriate data (*i.e.,* ranging from site-specific data to default values). Each general type of input data is briefly described below.

5.4.4.1 Meteorological Data

METEOROLOGICAL INPUTS
- horizontal wind speed
- horizontal wind direction
- air temperature
- precipitation
- frost date
- mixing height
- atmospheric stability class
- day/night

Meteorological data provide the input data necessary for many of the transport-related algorithms. For example, the advection algorithms in air rely on wind data, the deposition algorithms in air rely on precipitation data, and the erosion algorithms rely on precipitation data. Meteorological data can be entered as point estimates or distributions, depending on the goal of the analysis and the availability of data. Concurrent, meteorological data are needed for each calculation time step. Preprocessors should be used to convert the meteorological data to the time increments equivalent to the calculation time step. The meteorological inputs needed for TRIM.FaTE are listed in the adjacent text box.

5.4.4.2 Other Environmental Setting Data

ILLUSTRATIVE EXAMPLES OF ABIOTIC ENVIRONMENTAL SETTING DATA
- atmospheric dust load (for air compartment type)
- soil density (for all soil compartment types)
- current flow velocity (for surface water compartment type)

ILLUSTRATIVE EXAMPLES OF BIOTIC ENVIRONMENTAL SETTING DATA
- population per area (for all animal compartment types)
- biomass per area (for all plant compartment types)
- food ingestion rate (for all animal compartment types)

Other environmental setting data define the characteristics of the biotic and abiotic compartment types that are needed to estimate the transport and transformation of chemical mass in the system. These data may depend on the characteristics of one or both compartments in a link. For example, atmospheric dust load only depends on the characteristics of the air compartment, whereas the erosion flow rate between a soil compartment and a water compartment may depend on the characteristics of both the soil and water. Input data can be entered as point estimates or distributions, depending on the goal of the analysis and the availability of data. The adjacent text box presents some examples of both biotic and abiotic environmental setting data that may be necessary for a TRIM.FaTE simulation.

5.4.5 OUTPUT TIME STEPS

The final input necessary to begin a TRIM.FaTE simulation is the output time step(s). This determines the interval at which the mass and/or concentration in each compartment will be reported as an output. Post-processors may be used to aggregate these results over longer

averaging periods. For example, the results using an output time step of one hour may be averaged to produce the daily (and/or monthly and/or annual) concentrations and/or mass of the pollutant in each compartment.

5.5 SIMULATION IMPLEMENTATION AND ANALYSIS OF RESULTS

The next step is the actual running of the model, where the movement of the chemical(s) through the compartments is simulated for each calculation time step for the specified simulation period. The exact manner in which this is performed depends on the algorithms selected. For each link, a call is made to the algorithm library to determine the transfer factors that indicate the potential exchange of chemical mass. If all algorithms involve only first-order processes, then movement of the chemical will be simulated with a system of linked differential equations, the solution of which would be found using a differential equation solver (*e.g.,* LSODE). For more complicated algorithms, other tools would be necessary (*e.g.*, a method of solving partial differential equations).

The basic TRIM.FaTE outputs are described in the adjacent text box. The concentration estimates in the biotic compartments can be used to estimate ecological risks (see Section 2.3.6). The concentration estimates in the abiotic and biotic compartments can be output to an exposure model (*e.g.,* TRIM.Expo) to estimate human exposure.

TYPES OF OUTPUTS

TRIM.FaTE provides several different types of output to a user. The main TRIM.FaTE output is the mass and concentration in each compartment at each output time step. TRIM.FaTE can also output all algorithms used, all input values, and transfer factors for each transfer of mass, as well as certain intermediate calculated values, such as fluxes, that can be used for evaluating the performance of the model.

After the completion of a simulation, the user must interpret the model output. This can be a daunting task because of the quantity of output data TRIM.FaTE produces. For example, for an analysis that models the fate and transport of three chemicals in 30 compartments for 30 years, with a simulation time step of one hour, the model would produce over 23 million mass/concentration values (3 x 30 x 30 x 8,760). If the user wanted to also examine the intermediate model calculations, the output data set could grow even larger. Because output data from a multimedia fate and transport model can be used in many ways, such as permitting and development of regulations, different users will have different needs for the model's output. Automated post-processors can be used to present the output in forms that are useful to the decision-makers, such as the maximum concentration in the modeling region or in specific compartments, the average concentration in an environmental medium or species of wildlife, and long-term time trends of environmental concentrations.

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6. TREATMENT OF UNCERTAINTY AND VARIABILITY

This chapter summarizes the approach for assessing uncertainty and variability in TRIM.FaTE, which follows the general approach for TRIM as described in Chapter 3 of the TRIM Status Report. Additional background on how this method was selected is provided in Appendix B of the TRIM Status Report. The following text box presents definitions for the key terms used in this chapter to explain the uncertainty and variability analysis framework for TRIM.FaTE.

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 peoples' 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 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 analysis

Sensitivity analyses assess the effect of changes in individual model input parameters on model predictions. This is usually done by varying one parameter at a time and recording the associated changes in model response. One primary objective of a sensitivity analysis is to rank the input parameters on the basis of their influence on or contribution to the variability in the model output.

Uncertainty analysis

Uncertainty analysis involves the propagation of uncertainties and natural variability in a model's inputs to calculate the uncertainty and variability in the model outputs. It can also involve an analysis of the uncertainties resulting from model formulation. The contributions of the uncertainty and variability of each model input to the uncertainty and variability of the model predictions are explicitly quantified.

The EPA chose a staged approach for analysis of uncertainty and variability. 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 6-1 illustrates this staged approach for the TRIM.FaTE module and how the functional parts fit together. The first tests for both stages of analysis have been conducted using a TRIM.FaTE test case based on an actual site.

6.1 SENSITIVITY AND SCREENING ANALYSES

Sensitivity and screening analyses comprise the first stage of the overall analysis of uncertainty and variability of the TRIM.FaTE model. The sensitivity analysis provides a quantitative characterization of the sensitivity of the model results to variations in the model input parameters. The screening analysis is essentially a ranking of sensitivity results. The purpose of the screening analysis is to make a first-order determination of the most influential parameters, those that will need to be included in the detailed uncertainty analysis.

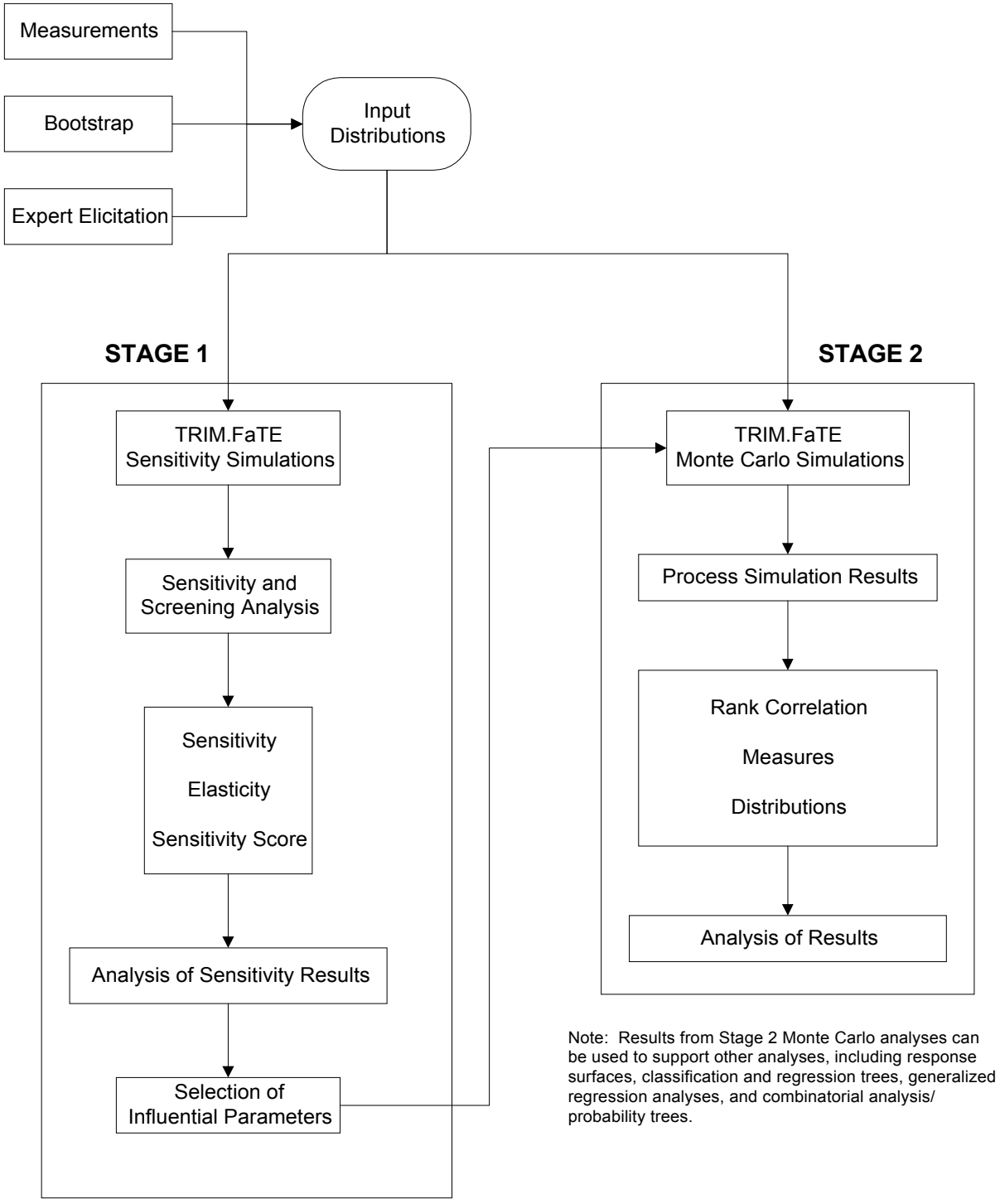
Several simulations of the TRIM.FaTE model are performed, with the parameters being varied singly and in pairs, and the model results are summarized to show the sensitivity to parameters and to identify the most influential parameters. Nominal values for all parameters need to be specified to provide a base model run for which the sensitivity analysis is performed.

The results of a sensitivity analysis are applicable to a particular location and for the range of conditions simulated, and may not apply to conditions outside of this. To broaden the applicability of the sensitivity analysis, the sensitivity analysis can be performed for a number of different "nominal" base simulations representing distinct modeling regimes (for example, summer and winter, or Maine and Louisiana locations).

In addition to the base simulation with parameters at nominal values, sensitivity simulations are performed with each individual parameter varied by Δp, keeping all other parameters at their nominal values, where Δp is a small fixed percentage (*e.g.*, one to ten percent) of the nominal parameter value, or where Δp is a small fixed percentage of a measure of the spread of values the parameter typically addresses. One can use the standard deviation or a range of percentiles, for example, the range from the 1^{st} to the 99^{th} percentile. A simulation for each parameter is required for this locally linear analysis. Thus, 2,000 simulations are needed to examine 2,000 parameters.

Varying parameters by $\pm\Delta p$ instead of $+\Delta p$ doubles the number of simulations, but allows one to calculate the local non-linearity of the effect of varying a parameter on the model results. These are reported as second order terms in the sensitivity measures to show the extent of local nonlinearity for parameters. Non-local non-linearities are quantified by increasing Δp to be in the range of 10 to 100 percent of the nominal values or spread of the parameters.

Figure 6-1
Uncertainty and Variability Analysis Framework
(Illustrated for TRIM.FaTE Module)



Sensitivity analyses of pairs and other combinations of parameters can also be performed. The purpose of varying parameters in pairs (or other combinations) is to identify synergistic sensitivity effects, where the joint variation of parameters is more (or less) influential than the combined influence of varying the parameters individually. An additional simulation for each pair of parameters is required to do this, which greatly increases the number of simulations performed. On the order of two million additional simulations would be needed to conduct an all-pairs analysis for 2,000 parameters. However, if there is prior information or knowledge about which parameters may be synergistic, these parameters should be jointly varied.

The results of these simulations are processed to produce measures of the importance of the parameters in the sense of how the model results change when the parameters are changed. The measures of parameter sensitivity and ranking identified to be computed for screening analyses are the *sensitivity,* the *nominal range sensitivity,* the *elasticity*, and the *sensitivity score*. We define these measures following Morgan and Henrion (1990).

The *sensitivity* of a model output to a parameter is the rate of change of the output with respect to changes in the parameter. Denoting the parameter as p and the model output as y, the sensitivity (at a particular value p^0 of p) is conventionally defined as the partial derivative $\partial y/\partial p$, evaluated at p^0. This measure describes how the model responds to small changes in the parameter p for values of p that are close to p^0, and is referred to as a "local" measure.

We calculate the sensitivity by:

$$Sensitivity = \frac{y(p^0+\Delta p) - y(p^0)}{\Delta p} = \frac{\Delta y}{\Delta p} \tag{14}$$

where Δp is a small change in the parameter value and:

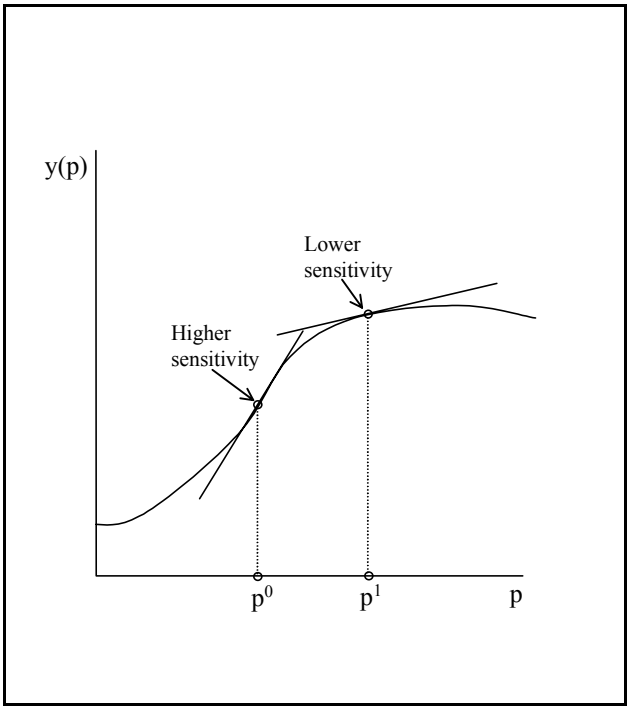
$$\Delta y = y(p^0+\Delta p) - y(p^0) \tag{15}$$

The *nominal range sensitivity* is used to assess changes in the model outputs resulting from large variations in input parameters. The effects on model outputs of varying each input parameter from the low end to the high end of the range of values for the parameter, are calculated in essentially the same way as the (local) sensitivity:

$$Nominal\ Range\ Sensitivity = \frac{y(p_{high}) - y(p_{low})}{p_{high} - p_{low}} \tag{16}$$

The sensitivity can be interpreted as the slope of the tangent to the response surface y(p) at the point p^0 (Figure 6-2). Note that the calculated value of the sensitivity depends both on the nominal parameter value p^0 and the amount of change Δp. As long as Δp is small, and the model is well behaved (bounded derivatives) in the local neighborhood of p^0, the effect of changing Δp should be very small. However, the sensitivity to a parameter can be quite different at different values p^0 of the parameter. It can be useful to vary both of these to see how the sensitivity depends on them.

Figure 6-2
Illustration of Sensitivity in One Dimension



The *elasticity* is defined as the ratio of the relative change in the model output y to a specified relative change in a parameter p.

$$Elasticity = \frac{\Delta y}{y^0} \Big/ \frac{\Delta p}{p^0} \tag{17}$$

where $\Delta p/p^0$ is a fixed relative change. For example, if the specified parameter change is one percent ($\Delta p/p^0 = 0.01$), then the elasticity is the percent change in y due to a one percent change in the parameter p, evaluated at a particular value p^0 of p.

The *sensitivity score* is the elasticity weighted by a normalized measure of the variability of the parameter which takes the form of a normalized range or normalized standard deviation of

the parameter. The sensitivity score for the model input parameter p with respect to the model output y is defined as:

$$Sensitivity\ Score = \frac{\Delta y}{\Delta p} \cdot \frac{\sigma}{\mu} \cdot \frac{p^o}{y^o} \quad (18)$$

where:

$\Delta y/\Delta p$ = change in output y per change in input p
σ/μ = coefficient of variation of p (standard deviation/mean)
p^o/y^o = ratio of nominal values of the input and output

Other normalized measures of the variation of the parameter can be used in place of the coefficient of variation, *e.g.*, the range of p divided by the mean.

The sensitivity score was used with an early TRIM.FaTE Prototype using one percent relative changes, for each input parameter, running the model, and then weighting the Δy's by estimated standard deviations of the parameters to obtain normalized changes (U.S. EPA 1998d). The analysis for that particular scenario identified 20 parameters with relatively large sensitivity scores, out of 400 input parameters. Note that sensitivity analyses are scenario-specific and parameters identified as influential for one scenario can be different for another scenario.

6.2 THE MONTE CARLO APPROACH FOR UNCERTAINTY AND VARIABILITY ANALYSES

A Monte Carlo approach with Latin Hypercube Sampling (LHS) was selected to be the core method for characterizing and analyzing the uncertainty and variability of the TRIM.FaTE outputs, with respect to the model inputs and parameters. The primary advantages of Monte Carlo methods for this type of analysis are the generality with which they can be applied, the lack of assumptions required, and their computational efficiency. Particular strengths of a Monte Carlo approach relevant to TRIM uncertainty and variability analyses include the following:

- Monte Carlo (MC) can be used to analyze many parameters.
- MC handles different ways of specifying parameter distributions.
- MC treats correlations and dependencies.
- MC allows for tracking the propagation of uncertainty and variability through model components at any level.
- MC gives estimates of confidence bounds for the estimates of the output distributions.
- MC allows precision to be increased easily by performing additional iterations.

- LHS is an efficient sampling scheme, reducing the number of simulations required. (MC with LHS has computational complexity linear with the number of parameters or model inputs that are being analyzed.)

- MC handles complex algorithms in the model without increased difficulty.

- MC is flexible and will accommodate future additional analyses without major restructuring.

- MC output is compatible with a number of methods for specific analyses of uncertainty and variability, including response surfaces, regression models, classification and regression trees (CART), ranking methods, and combinatorial analysis.

- MC is widely used, is generally accepted in the scientific community, and can be explained to a lay audience.

A significant limitation results from the fact that the analysis of uncertainty and variability requires estimates of the distributions of parameters, reflecting both the uncertainty and the variability of the parameters. Of lesser importance, estimates of dependencies (correlations) between parameters would enable a more detailed analysis to be performed. However, information on the distribution of parameters is unavailable for most parameters. When a parameter distribution has been developed, it is rarely separated into components of uncertainty and variability. This limitation of the Monte Carlo approach can be addressed over time by developing distributions for parameters the model is most sensitive to. Distributions are not needed for all parameters.

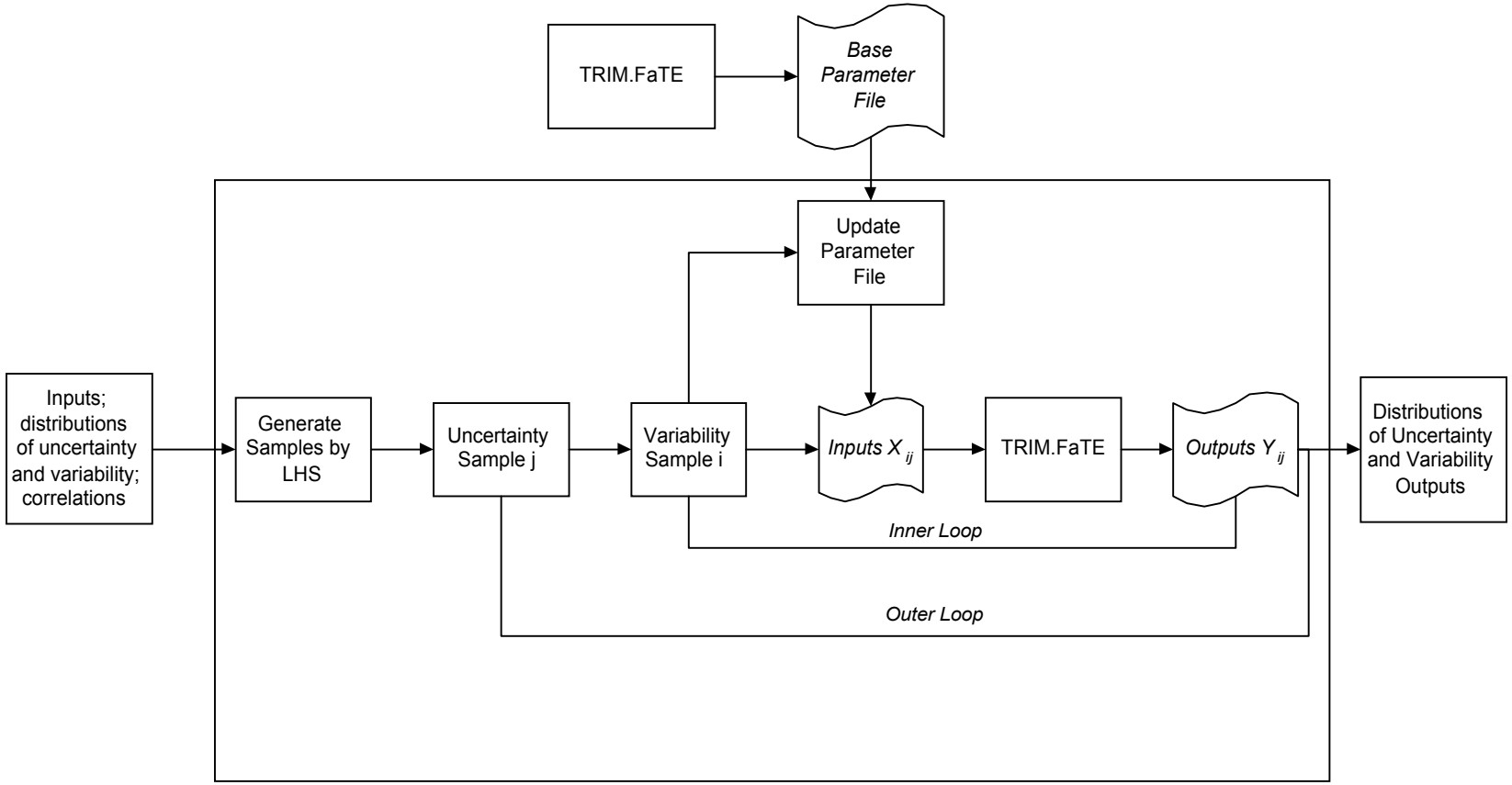
The implementation of this approach for uncertainty and variability analysis is integrated with the TRIM.FaTE model to some extent, as opposed to operating as a separate shell around the model. TRIM.FaTE handles some of the iterations internally, and passes information to the uncertainty system during a simulation. This close interfacing of the uncertainty software with the model allows for greater flexibility in terms of what can be tracked and also reduces the overall processing time.

6.2.1 TWO-STAGE MONTE CARLO DESIGN

Joint uncertainty and variability Monte Carlo simulations are generated based on sampling from an uncertainty distribution and a variability distribution for each parameter, with the uncertainty distributions sampled in an outer loop and the variability distributions sampled in an inner loop. For each uncertainty realization (outer loop sample) there is a specified distribution of variability (for each parameter) from which several samples are drawn to represent variability in the inner loop. These several samples represent one variability realization. Figure 6-3 illustrates the structure of this two-stage Monte Carlo design.

As an example, suppose there are N_u samples drawn from the uncertainty distributions, and that for each uncertainty sample there are N_v variability samples. The cumulative

Figure 6-3
Two-stage Monte Carlo Approach



distribution function (of a model output) representing variability for that uncertainty sample can be estimated from these N_v variability samples and statistics can be calculated (mean, percentiles, variance, etc.). For each of these statistics, we have N_u values, corresponding to the N_u uncertainty samples. These then are used to calculate a cumulative distribution function for each statistic, representing the uncertainty distribution for that statistic.

6.2.2 DISTRIBUTIONS OF INPUT PARAMETERS

The Monte Carlo approach requires specification of probability distributions for each parameter being analyzed for its role in the overall uncertainty of the model. The distributions can be specified in any of several standard ways, including sets of data points (discrete distributions), nonparametric probability distribution functions (PDFs) or cumulative distribution functions (CDFs), and parametric PDFs or CDFs (analytic functions). For discrete distributions some additional information about the underlying distribution needs to be provided so that appropriate samples are selected from the distribution (*e.g.*, whether values between data points are realizable).

Distributions for parameter variability and for parameter uncertainty are required for those parameters to be analyzed; we do not use "default" distributions where there is no information. Parameters without any specification of distributions are treated as if they are known exactly.

6.2.3 LATIN HYPERCUBE SAMPLING

There are four sampling techniques that are widely used in Monte Carlo methods for generating random samples from parameter distributions: simple random sampling, Latin hypercube sampling (LHS), midpoint LHS, and importance sampling. Randomness is an important feature of these methods for sampling, since it allows one to directly estimate the precision of the statistics estimated using the Monte Carlo approach.

The sampling technique selected for TRIM is LHS, which employs a stratified random sampling without replacement scheme, which is very efficient for sampling, especially for multiparameter models (Iman and Shortencarier 1984, Iman and Helton 1987). Importance sampling strategies also will be used in conjunction with LHS to obtain better coverage of distribution tails or extreme values. The strata for LHS are chosen to be intervals partitioning the range of each parameter, in such a way that the parameter has equal probability of realization within each interval. Then a sample is selected randomly from each of the intervals. To illustrate this, say there are k intervals used for each parameter. A random sample is selected from within each interval, and this is repeated for each parameter, yielding k samples for each parameter. Then k multivariate samples are constructed by randomly pairing up the samples for each parameter. These k sets of parameter values (each set containing a value for each parameter) are referred to as the Latin hypercube sample.

If there are correlations among the parameters, there is a technique for sampling within the LHS framework so that the sample reflects the correlations (Iman and Conover 1982, Iman et al. 1985). This treatment of correlation is based on rank-order correlation (Kendall and Gibbons

1990) and has desirable properties. It can be used with any distribution and with any sampling scheme, and it does not change the marginal distributions of the parameters.

6.2.4 TREATMENT OF TAILS OF DISTRIBUTIONS

As noted above, for certain influential parameters an importance sampling technique will be incorporated to obtain adequate sampling coverage of extreme values of these parameters. Importance sampling refers to a class of sampling techniques that takes into account the areas of a distribution that are important to the analysis, providing enhanced detail in these areas. Importance sampling is often used when increased accuracy in one or both tails of a distribution is desired.

6.2.5 TRACKING INFORMATION BETWEEN MODULES

There are two levels at which tracking of information related to uncertainty analysis occurs; the first is from one TRIM module to the next, and the second is within each TRIM module.

The information passed from one TRIM module to the next (*e.g.*, from TRIM.FaTE to TRIM.Expo) needs to provide enough detail to allow for continuation of the Monte Carlo propagation of uncertainty and variability in the next module. Information on the joint distributions of a TRIM module's inputs and outputs is required to do this, for both uncertainty and variability.

There is some flexibility as to how this information is summarized or condensed. For example, each TRIM module could pass the complete distributions for all of the output variables and parameters tracked in the uncertainty analysis. At the other end of the spectrum, the module could pass only the means, variances, and correlations of the distributions, for a selected subset of the parameters and outputs.

At this time, an intermediate approach has been implemented for passing information from TRIM.FaTE to TRIM.Expo, which will be revised if necessary. The distributional information is somewhat condensed, while passing enough information about the uncertainty and variability distributions to allow them to be adequately sampled for the Monte Carlo analysis within the next module. For the uncertainty and variability distributions of each parameter and each output, TRIM.FaTE calculates and passes 101 percentiles (minimum, maximum, and every percent) as well as some additional percentiles at the tails (how many is to be determined). Features of the joint distributional structure are summarized in a correlation matrix of correlations between all pairs of parameters and outputs. Although this is a strong condensation of the joint distributional structure, it is likely to be adequate relative to the lack of information that is likely to be available to estimate parameter correlations in the first place.

6.2.6 COMPUTATIONAL RESOURCES

Although the Monte Carlo technique is very efficient, Monte Carlo simulations of TRIM.FaTE require substantial computer processing time, especially when treating more than a

few parameters. The available computational resources can be a limiting factor in the scope of the analysis performed. The more detailed analyses may have to restrict their scope to small numbers of parameters being jointly varied, for example.

Computer processing time for both the uncertainty propagation and tracking and the TRIM.FaTE model depends on the definition of the TRIM.FaTE modeling scenario, in terms of the numbers of compartments, time steps, length of simulation, chemicals, and so forth. It also depends on the number of parameters and number of model outputs analyzed, the sizes of the Monte Carlo samples (which relates to the number of simulations), and the level of detail of the analysis.

6.2.7 SPATIAL AND TEMPORAL RESOLUTION AND AGGREGATION

Estimation of the effects of spatial and temporal aggregation on uncertainty and variability will be accomplished by sensitivity analyses of Monte Carlo results. For analysis of spatial aggregation, EPA will set up a small number (three to five) of TRIM.FaTE scenarios with increasing levels of spatial resolution (decreasing levels of aggregation), and run the same set of simple Monte Carlo simulations for each scenario. Comparison of the Monte Carlo results for the scenarios will show the impact of the aggregation on uncertainty and variability for the scenarios modeled. Similarly, the effects on model output uncertainty of temporal aggregation will be assessed by comparing uncertainty results from scenarios with and without seasonal aggregation. Initial efforts have included evaluation of the effects of explicitly modeling seasonal variability, and treatment of other temporal scales can be evaluated similarly.

6.2.8 SPECIFICATION OF PROBABILITY DISTRIBUTIONS AND CORRELATIONS OF MODEL INPUTS

The need for distributions for the input parameters is discussed above. Implementation of this Monte Carlo approach employs a data file that specifies the distributions of uncertainty and variability for each parameter. For each parameter this file contains the distribution name *(e.g.*, lognormal) and the parameters or data that complete the specification of the distribution. There needs to be a set of distributions for variability and a set of distributions for uncertainty for each parameter.

The Monte Carlo method can also handle the joint distributions of the dependent parameters. However, information to estimate full joint distributions is not presently available. In addition to the marginal distributions, the current implementation only requires the correlation structure of the set of parameters, which is specified by $(N^2-N)/2$ estimates of pairwise rank correlations for the set of N parameters.

There are often physical constraints on values of parameters and intermediate quantities in the model; for example, mass is always non-negative. These can have implications for how parameter distributions are set. The specified distributional forms should satisfy the physical constraints as well as reflect the distributions indicated by the available data.

6.3 PRESENTATION OF UNCERTAINTY RESULTS

When a model has many inputs and is complex, as TRIM.FaTE is, the analyst will make use of methods that are simple and give a first-order picture of uncertainty, as well as more complex methods giving a more refined, detailed analysis of uncertainty. There are several ways to form summary measures and present the uncertainty and variability of a modeling system. Loosely speaking, "measures" are low-dimensional statistics (one or a small number of descriptive statistics), for example, the sensitivity score or the 10^{th}, 50^{th}, and 90^{th} percentiles of a distribution. In addition to measures, ways of presenting the results include graphs of distributions, tree diagrams, other graphs, and tables of statistics.

In presenting results, the objectives of the uncertainty and variability analysis should be clearly stated, and it should be shown how the objectives were met (or not met). It is best to use a reasonable number of significant digits when reporting results, lest the audience be misled as to the accuracy of the results (the use of fewer digits also improves readability). The key results should be presented clearly and not obscured by concomitantly reporting several less-comprehensible statistics. If it is necessary to report extensive statistics, they can be documented in an appendix. Tables and figures need to be labeled clearly and completely, so they can more or less stand alone, reducing misleading impressions if seen out of the context of a report.

The uncertainty results from TRIM.FaTE will be presented in a tiered style, with three tiers of increasing detail and complexity. The first tier is designed to be meaningful to a wide audience, including the public, decision-makers, and risk analysts, and will present the main findings in easily understandable charts, tables, and descriptive text.

The first tier results will be derived from the more comprehensive second tier results. The second tier will present more detailed results requiring the user to have some familiarity with risk analysis statistics, such as probability distribution functions (PDFs), cumulative distribution functions (CDFs), and graphs of results. For example, a tier 1 table might present the probability that a predicted risk exceeds a given risk cutoff level, for three cutoff values. A corresponding tier 2 graph would plot the curve of exceedance probabilities for a range of cutoff values. To assist in interpretation of PDFs and CDFs, the PDF and CDF of a distribution (or family of distributions) will always be presented as a pair of graphs, one above the other, with the same horizontal scales. The mean of the distribution as well as other relevant points (*e.g.*, the 95^{th} percentile; the deterministically predicted point value) will be indicated on both graphs. The second tier will also include an overview of the distributions of uncertainty and variability of the input parameters and an explanation of dependencies and correlations of both the input parameters and the model results.

The third presentation tier will have the most detailed graphs and tables, and will usually be referred to for details supporting specific pieces of the analysis. These results can be lengthy, and will be relegated to an appendix. Also part of the third tier, another appendix will be prepared which documents the probability distribution of each input parameters. This document will include a discussion of the data used to estimate the distributions, how much data were used, representativeness of the data, whether the distributions characterize uncertainty, variability or

both, and how the distributions were estimated from the data. Graphs comparing the fitted distributions and measured data will be presented along with goodness of fit statistics.

There are a number of first-order measures of the importance, or influence on modeled results, of model input parameters, which are quite straightforward to compute. These sensitivity/screening measures (sensitivity, sensitivity score, elasticity) are important in the context of selecting parameters for detailed analysis of uncertainty and variability, and are described above in Section 6.1. In addition to these, the results of the TRIM.FaTE uncertainty and variability analysis are described using distributions, dependencies, and joint distributions and confidence bounds. Specifically, the core presentation will include the following:

Measures, Graphs, and Tables

- Sensitivity
- Sensitivity score
- Elasticity
- Probability density functions
- Cumulative distribution functions
- Confidence intervals
- Tables of statistics
- Rank order correlation
- Ranking groups of parameters
- Correlation matrix
- Scatter plots, scatter plot matrix

These items are described in the remainder of this section.

Probability density functions can be depicted by smoothed histograms. Care must be taken when using histograms in order to avoid inaccurate representations of peaks and valleys (caused by too tight a spline fit on histograms with too many bins), to keep the area under the distribution equal to 1.0, and to avoid over-smoothing, which suppresses features of the distribution.

Cumulative distribution function graphs lack the intuitive appeal of graphs of the probability distribution function, but don't have the difficulties of smoothing that probability distribution function graphs do. The cumulative distribution function can be generated directly from the data points. Probabilities of exceeding given values or of being within a given range can be read off graphs of the cumulative distribution function or the probability distribution function. Overlays of distributions can be informative using either of these graphs.

Confidence bands and vertical confidence intervals on graphs of probability distribution functions and cumulative distribution functions provide information about the uncertainty of the distributions. Vertical confidence intervals ("whiskers") tend to be easier to interpret visually than bands. These graphs are effective for presenting uncertainty and variability together, where the distribution of variability is graphed with bands or intervals representing the spread of the uncertainty distributions.

Tables of selected statistics provide another useful way to present summaries of distributions. Descriptive statistics such as percentiles, means, standard deviations, and coefficients of variation can concisely describe several distributions in a single table. Table 6-1 shows how six statistics summarizing a distribution can be presented to describe a family of distributions.

Table 6-1
Example Table Summarizing Distributions

Stratification Variable	Variability of the Concentration of Arsenic in Soil (μg/m^3)					
	Mean	1st %ile	10th %ile	Median	90th %ile	99th %ile
Location 1						
Location 2						
Location 3						

Tables presenting uncertainty results in relation to cutoff values of concentrations, exposure, or risk are useful to decision-makers using the results of TRIM modeling. These tables aim to present in more directly meaningful ways the information presented in PDFs and CDFs, which can be difficult to interpret if one is not familiar with their use. For example, the likelihood that a pollutant concentration in a media or specific location is greater than a fixed concentration cutoff, with a given level of confidence, can be tabulated for a series of cutoff values (Table 6-2). This type of table will be presented taking into account only the variability of input parameters, and also taking into account both variability and uncertainty of the parameters. Another type of table, useful for assessing data requirements, tabulates the effectiveness of reducing the uncertainty in parameter values towards reducing the uncertainty in model results to acceptable values. Different users of the model and different types of decisions influenced by the model results will have differing requirements as to how much uncertainty is acceptable. Combinations of parameter uncertainty reductions which result in bringing model uncertainty down to a specified level can be tabulated. If the cost of collecting additional data is taken into account, then least-cost options addressing this can be presented.

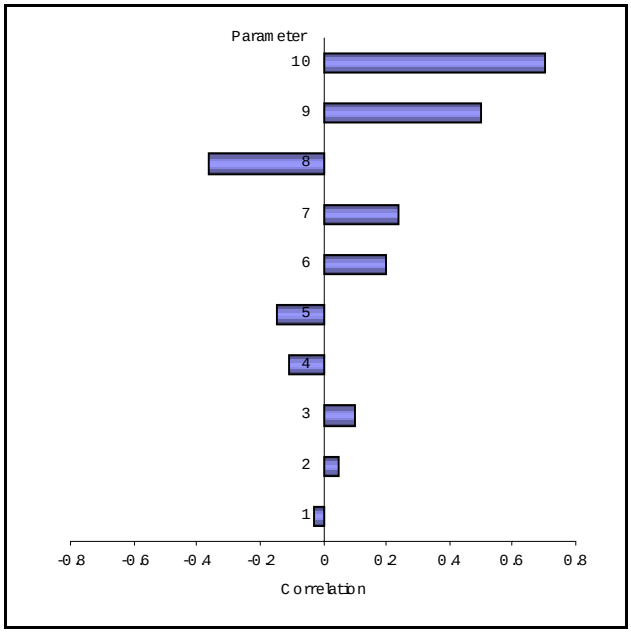
Table 6-2
Likelihood that the Concentration of Lead in Catfish Exceeds Concentration Cutoff Values

The concentration cutoff value Y_c	Probability the concentration will exceed Y_c (%)
0.1	12
1.0	0.013
10.0	4.1×10^{-6}
100.0	2×10^{-7}

Correlation measures such as Spearman's rank order correlation, Kendall's tau-b, and Pearson's product-moment correlation of model outputs with inputs are useful for identifying influential parameters. Spearman's rank order correlation and Kendall's tau-b are based on ranks. Rank correlation methods have the advantages of robustness to outliers and availability of distribution-free tests. A good account of rank order correlation methods is given by Kendall and Gibbons (1990). The Pearson correlation makes the restrictive assumption that the model input/output relationships are linear (rank order correlation does not), but it does provide information about how uncertainty in a parameter contributes linearly to uncertainty in the outputs.

Correlations for several parameters can be graphed as a *tornado chart*, where the x-axis is the correlation (between parameters and a specific model output variable) and the y-axis is categorical, listing the parameters (Figure 6-4). Horizontal bars extend out from the y-axis, with the length of the bars equal to the correlation. The y-axis parameters are ordered from highest correlation at the top to lowest at the bottom. It is useful to include vertical bands indicating where correlations are not statistically different from zero (at a specified confidence level and sample size). Inspection of a tornado chart can show three classes of parameters: independent parameters (changing the parameter within the range does not change the model results), parameters with small influence (parameter changes do not affect the results much), and influential parameters (results change significantly).

Figure 6-4
Tornado Chart



Ranking groups of parameters, in addition to ranking individual parameters, is a way of ranking that takes into account strong correlations between parameters. Parameters are grouped that are highly correlated with each other, are influential parameters when looked at individually, but are not influential when the effects of any other parameter in the group are already accounted for (small partial correlation). Canonical correlation (Mardia et al. 1979) can be used to identify the parameter groups.

Correlation matrices provide a way to compactly present the correlations among a set of variables (inputs, outputs, or both) as a matrix of the correlations between pairs of variables. Table 6-3 illustrates a correlation matrix for three variables A, B and C. The notation $\rho(A,B)$ indicates the correlation between variables A and B. The correlation $\rho(A,B)$ is the same as $\rho(B,A)$, hence the correlation matrix is symmetric and only half of the matrix needs to be filled. For correlations between parameters and model outputs or between different model outputs, the Pearson correlations are calculated as well as the rank order correlations.

Table 6-3
Correlation Matrix

Variable	A	B	C
A	1		
B	$\rho(A,B)$	1	
C	$\rho(A,C)$	$\rho(B,C)$	1

Scatter plots visually illustrate correlations between parameters and also indicate other features of the relationships between parameters, such as non-linearity, regions with more or less scatter or correlation, points that drive the correlation, and potential outliers. A *scatter plot matrix* for illustrating correlations between parameters is similar to the correlation matrix but with a scatter plot instead of a number in each "table cell." This is cumbersome for more than a few parameters and is more effectively used with subsets of parameters that exhibit significant correlation.

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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).

Advective Process — A process by which a chemical can be transported within a given medium that is moving from one compartment to another.

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.

Compartment — A homogeneous unit of space characterized by its physical composition 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.

Diffusive Process — A process by which a chemical is transported from one compartment to another as a result of the magnitude and direction of the concentration differences between two compartments at the interface between the two locations.

Dispersion — The "spreading out" of a chemical during advective transport. May result in movement of the chemical perpendicular to the direction of advective flow.

Fugacity — A measure of the tendency of a substance to escape by some chemical process from the phase in which it exists.

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.
Model Evaluation	The broad range of review, analysis, and testing activities designed to examine and build consensus about a model's performance.
Modeling Region	The region of space through which the transport and transformation of the modeled chemical(s) is estimated.
Output Time Step	A length of time over which the compartment masses and concentrations calculated at each simulation time step are summarized and reported by the model.
Parameter	A model input that defines a variable in an algorithm (*e.g.*, emission rate, half-life, biomass).
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.
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.
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.
Simulation Period	The entire length of time for which the model is run and compartment masses and concentrations are calculated – in other words, the time period from the beginning of the simulation until the end.
Simulation Time Step	The time increment at which the model calculates (and re-calculates iteratively throughout the simulation period) a new inventory of compartment masses and concentrations.
Source	An external component that introduces chemical mass directly into a compartment.

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.

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APPENDIX B
Integrating External Models or Measured Data into TRIM.FaTE

At some point, it may be desirable to use either measured data or the output of other models with the TRIM.FaTE model. In either case, there are two basic forms that the data can take: (1) fluxes into certain compartments (*e.g.*, deposition rates), or (2) calculated/specified concentrations or chemical mass in certain compartments. The first case is the simpler of the two, as it requires only adding additional source terms to the affected compartments. The second case has more of an impact on the system of equations used in the modeling, and is the focus of this Appendix.

B.1 Compromises that Must be Made in Order to Use Externally Derived Compartment Concentrations

The incorporation of externally derived compartment concentrations into *any* multimedia model dictates that compromises be made with regard to preserving chemical mass balance. The basic problem is the loss of chemical mass from the compartments that send a chemical to the compartment for which an externally derived compartment concentration is used. Since the receiving compartment will not receive the chemical, it is effectively lost from the system. The only way to avoid this loss of chemical mass is to modify all of the links to the "constant" compartments so that this exchange does not take place (*e.g.*, disable resuspension from surface soil to the air domain if the results of an air model are to be used).

While we will know mathematically how much mass has been lost through these processes, the chemical lost will not be allowed to participate in any further exchanges with other compartments. Whether this is acceptable or not depends on the attitude of the user, but this compromise is unavoidable if they are to use externally derived compartment concentrations.

B.2 Implementation Details in the Case of First-order Transfers – Case of Constant Inputs

In this section, explicit details are provided for incorporating externally derived compartment concentrations for selected compartments in the case where these concentrations are constant for the time period of interest. The general case where the values from externally derived compartment concentrations change with time can be addressed by sequentially using this method over the different intervals over which the values from the externally derived compartment concentrations are constant.

For a given time interval in which the parameters are constant with time, the system of differential equations to be solved is:

$$\frac{d\vec{N}}{dt} = A\,\vec{N} + \vec{s} \tag{1}$$

where $\vec{N}$ is the vector of the mass of chemical(s) in each compartment, given by:

$$\vec{N} = \begin{bmatrix} n_1(t) \\ n_2(t) \\ \vdots \\ n_m(t) \end{bmatrix} \tag{2}$$

where $n_i(t)$ is the mass of a particular chemical in a compartment/chemical pair, m is the total number of compartment/chemical pairs; A is the matrix of transfer factors describing transport between compartment/chemical pairs:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1m} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2m} \\ \vdots & & & & \\ a_{m1} & a_{m2} & a_{m3} & \dots & a_{mm} \end{bmatrix} \tag{3}$$

and $\vec{s}$ is the vector of sources terms for each chemical in each compartment.

The fact that chemical mass balance is preserved implies that the matrix A satisfies two basic conditions:

$$a_{ij} \geq 0, \text{ if } i \neq j \text{ and } a_{ii} \leq 0 \tag{4}$$

$$a_{jj} = -\sum_{i=1, i\neq j}^{m} a_{ij} \tag{5}$$

Using externally derived compartment concentrations is equivalent to fixing the concentration/chemical mass in some compartments. This can be done by solving a reduced system of differential equations, using constant values for the applicable terms $n_i(t)$. This can be conceptualized as using "virtual sources" for the relevant compartment/chemical pairs, with each (time-dependent) virtual source set so that the mass of chemical is constant.

For example, if there is only one chemical being considered, and we want the concentration/mass to be fixed in the first compartment, say $n_1(t)=M_1$, then $dn_1/dt=0$, and the original system becomes:

$$\frac{d}{dt}\begin{bmatrix} M_1 \\ n_2(t) \\ \vdots \\ n_m(t) \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1m} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2m} \\ \vdots & & & & \\ a_{m1} & a_{m2} & a_{m3} & \dots & a_{mm} \end{bmatrix} \begin{bmatrix} M_1 \\ n_2(t) \\ \vdots \\ n_m(t) \end{bmatrix} + \begin{bmatrix} s_1 \\ s_2 \\ \vdots \\ s_m \end{bmatrix} \tag{6}$$

Since the derivative of a constant is zero, examining the first row of the above system shows that:

$$0 = \sum_{i=1}^{m} n_i(t)\, a_{1i} + s_1(t) \tag{7}$$

i.e., the virtual source $s_1(t)$ in the first compartment is given by:

$$\begin{aligned} s_1(t) &= -\sum_{i=1}^{m} n_i(t)\, a_{1i} \\ &= -Ma_{11} - \sum_{i=2}^{m} n_i(t)\, a_{1i} \end{aligned} \tag{8}$$

The terms $n_i(t)$ for $i>1$ can be determined by solving the system of differential equations obtained by eliminating the first row, and using $n_1(t)=M$:

$$\begin{aligned} \frac{d}{dt}\begin{bmatrix} n_2(t) \\ \vdots \\ n_m(t) \end{bmatrix} &= \begin{bmatrix} a_{21} & a_{22} & a_{23} & \dots & a_{2m} \\ \vdots & & & & \\ a_{m1} & a_{m2} & a_{m3} & \dots & a_{mm} \end{bmatrix} \begin{bmatrix} M \\ n_2(t) \\ \vdots \\ n_m(t) \end{bmatrix} + \begin{bmatrix} s_2 \\ \vdots \\ s_m \end{bmatrix} \\ &= \begin{bmatrix} a_{22} & a_{23} & \dots & a_{2m} \\ \vdots & & & \\ a_{m2} & a_{m3} & \dots & a_{mm} \end{bmatrix} \begin{bmatrix} n_2(t) \\ \vdots \\ n_m(t) \end{bmatrix} + \begin{bmatrix} s_2 + Ma_{21} \\ \vdots \\ s_m + Ma_{m1} \end{bmatrix} \end{aligned} \tag{9}$$

This system of differential equations is of the same form as the original equation, and can be solved using the same solver used for the original equation. However, it can also be rewritten as a system of the same size as the original system by adding the differential equation $dn_1/dt=0$, $n_1(0)=M$; this results in the system (with initial condition):

$$\frac{d}{dt}\begin{bmatrix} n_1(t) \\ n_2(t) \\ \vdots \\ n_m(t) \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & \dots & 0 \\ 0 & a_{22} & a_{23} & \dots & a_{2m} \\ \vdots & & & & \\ 0 & a_{m2} & a_{m3} & \dots & a_{mm} \end{bmatrix} \begin{bmatrix} n_1(t) \\ n_2(t) \\ \vdots \\ n_m(t) \end{bmatrix} + \begin{bmatrix} 0 \\ s_2 + Ma_{21} \\ \vdots \\ s_m + Ma_{m1} \end{bmatrix}, \quad \begin{bmatrix} n_1(0) \\ n_2(0) \\ \vdots \\ n_m(0) \end{bmatrix} = \begin{bmatrix} M \\ n_2(0) \\ \vdots \\ n_m(0) \end{bmatrix} \tag{10}$$

Note that the mass lost from the system to the compartments which are to be held constant is accounted for, as condition (5) is still satisfied for the diagonal elements of the matrix in equation (10), where the coefficients a_{ij} are used in the sum.

When more than one of the n_i's is constant, this same method can be used. In general, if the kth compartment/chemical pair is to be constant (say with value M_k), then one puts zeros in the kth row and kth column, and adds the term $M_k\, a_{nk}$ to the nth row of the source term vector. This is done for every compartment/chemical pair which is to be constant. For example, applied to equation (2), one would obtain the following:

$$\frac{d}{dt}\begin{bmatrix} n_1(t) \\ n_2(t) \\ \vdots \\ n_{k-1}(t) \\ n_k(t) \\ n_{k+1}(t) \\ \vdots \\ n_m(t) \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & \dots & 0 & 0 & 0 & \dots & 0 \\ 0 & a_{22} & a_{23} & \dots & a_{2,k-1} & 0 & a_{2,k+1} & \dots & a_{2m} \\ \vdots & & & & & & & & \\ 0 & a_{k-1,2} & a_{k-1,3} & \dots & a_{k-1,k-1} & 0 & a_{k-1,k+1} & \dots & a_{k-1,m} \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 & \dots & 0 \\ 0 & a_{k+1,2} & a_{k+1,3} & \dots & a_{k+1,k-1} & 0 & a_{k+1,k+1} & \dots & a_{k+1,m} \\ \vdots & & & & & & & & \\ 0 & a_{m2} & a_{m3} & \dots & a_{m,k-1} & 0 & a_{m,k+1} & \dots & a_{mm} \end{bmatrix} \begin{bmatrix} n_1(t) \\ n_2(t) \\ \vdots \\ n_{k-1}(t) \\ n_k(t) \\ n_{k+1}(t) \\ \vdots \\ n_m(t) \end{bmatrix} + \begin{bmatrix} 0 \\ s_2 + Ma_{21} + M_k a_{2,k} \\ \vdots \\ s_{k-1} + Ma_{k-1,1} + M_k a_{k-1,k} \\ 0 \\ s_{k+1} + Ma_{k+1,1} + M_k a_{k+1,k} \\ \vdots \\ s_m + Ma_{m1} + M_k a_{m,k} \end{bmatrix}, \quad \begin{bmatrix} n_1(0) \\ n_2(0) \\ \vdots \\ n_{k-1}(0) \\ n_k(0) \\ n_{k+1}(0) \\ \vdots \\ n_m(0) \end{bmatrix} = \begin{bmatrix} M \\ n_2(0) \\ \vdots \\ n_{k-1}(0) \\ M_k \\ n_{k+1}(0) \\ \vdots \\ n_m(0) \end{bmatrix} \tag{11}$$

The method described in this section fits seamlessly into the general process of calculating transition matrices and source terms prior to calling LSODE. In general, one uses all zeros for any row that is to be constant, adds the extra flux terms to the source term vector, and calls LSODE as is done normally.

APPENDIX C
DETERMINING APPROPRIATE SCALE AND SPATIAL RESOLUTION

This appendix is an example of a detailed approach for defining the level of spatial complexity (*i.e.*, location, size, and number of parcels) in a TRIM.FaTE analysis. There are many factors that influence scenario complexity, including the characteristics of the pollutant, the environmental setting, the exposed population, the impact of interest, the available data, and available computer resources. A clear analysis objective offers a starting point for setting up the scenario with an appropriate level of complexity. The TRIM.FaTE modeling framework uses a system where the analysis objective is classified into one of three basic types. For each type of objective, a series of questions can be used to identify the natural and artificial boundaries of the system. A preliminary decision tree is developed for each objective type to assist the user in determining which boundary or set of boundaries is appropriate for a given modeling objective. The decision trees are used to provide a standard approach for setting up a simulation.

After the initial scenario is constructed and a simulation has been completed, the preliminary results need to be evaluated to confirm that the most appropriate scale has been used. The methodology for determining appropriate scale and spatial resolution as well as suggestions for defining compartments are included in this chapter.

There are several questions that need to be answered before the appropriate level of scenario complexity can be determined. As with any modeling exercise, the first and foremost step in a TRIM.FaTE analysis is to clearly state the objective of the analysis. The objective should identify the chemical(s) of concern, the exposed population (individual, species, population, cohort, or environmental compartment), and the health endpoint (chronic or acute) to be assessed. The exposed population, either human or ecological, or landscape component (*e.g.*, lake, wetland, agricultural plot), is referred as the **target**. This section presents a tiered approach that incorporates all of these objectives to define the appropriate scale and resolution of a given TRIM.FaTE scenario.

For the chemical(s) of concern, the two most important factors for determining the appropriate modeling scale are how rapidly the chemical moves and how rapidly the chemical degrades in the environment. The range of mobility for each target of interest also needs to be considered. In addition to providing information about modeling scale, the mobility characteristics of the target help determine the appropriate level of resolution of the scenario. Finally, the endpoint being assessed will provide important information about both temporal and spatial scale of the scenario.

The approach described in the following section generates a starting point for any given analysis objective for which TRIM.FaTE is designed, and is intended to impart some consistency and transparency into the scenario set up process. Additionally, once a scale has been chosen, one must determine if that scale is appropriate when compared to other sources of model uncertainty.

C.1 CLASSIFICATION OF THE ANALYSIS OBJECTIVE

The methodology for the set up of a scenario will depend largely on the mobility of the target. The mobility of each exposed population is categorized into one of three general classes: mobile, bounded, and stationary. Each class is described in the following sections and summarized in Table C-1. Depending on which category best describes the target of interest, the user is referred to one of three binary decision trees that are described in Section C.2. The decision trees provide a series of questions that help the user determine the appropriate set of boundaries and parcels in the analysis. Information on the different boundary types is provided in Section C.2.

Table C-1
Classification of Modeling Objectives Based on Target of Interest

Target Class	Description	Rationale and Example
Mobile	Highly mobile cohorts, individuals, animals or organisms	Concentration in air resulting from point source will decline with distance traveled from source. If a child goes to school near a source but lives farther from the source and plays in a park somewhere else then one would want to maximize resolution within the model system.
Bounded	Animals with a limited range or habitat	Red tailed hawks or land mammals in a limited or bounded habitat that is a fixed distance from the source. Concentrations or environmental conditions may vary across the habitat/range but highly resolved concentration gradients between the source and the study area are not necessary.
Stationary	Fixed location in space that may be influenced by its surroundings but does not move relative to source	Forest, pond, agricultural plot, wetlands. Consider chemical transfer from adjacent areas (watershed, air parcel).

C.1.1 MOBILE EXPOSED POPULATIONS

The first target class is referred to as **mobile**. This class includes humans and large animals that are highly mobile and can freely move about the region impacted by the source(s). Mobile targets require maximum resolution when estimating concentration, especially for areas where the highest exposure is likely to occur or with a high likelihood of occupancy by the target (schools, residential areas, wintering grounds). Each scenario focused on mobile targets should be designed to provide maximum possible resolution, given the constraints of limited computing resources, model uncertainty, and measurement imprecision.

C.1.2 BOUNDED EXPOSED POPULATIONS

The second target class is referred to as **bounded**. This class includes targets that are expected to have some limits, either natural or artificial, on their habitat or mobility range. For example, red tailed hawks that hunt and live in a specific orchard or fish confined to a certain lake or pond would be included in this class. The scale and resolution of a given scenario should be selected to provide the desired level of detail within the bounded region. Areas outside the bounded region can be simplified to include only the information that influences transport of chemical into the region of interest. For example, if one region has a high quantity of vegetation and the chemical has a high degradation rate in vegetation, this would be considered separately because it influences the mass balance. The bounded area where the target(s) reside may or may not be well mixed (*i.e.*, the concentration across the area does not change significantly). If the range is not expected to be well mixed, more spatial resolution within the range can be included, provided it can be justified under the constraints of model uncertainty. If the range is well mixed then additional spatial resolution is not necessary.

C.1.3 STATIONARY EXPOSED POPULATIONS

The third target class is referred to as **stationary**. This class includes all immobile targets such as lakes, forests, agricultural plots, or wetlands. Stationary targets also require little resolution between the source and the target. Only information that relates the point source to the location of interest is necessary. Such information might include adjacent air parcels and drainage areas from which water (runoff) and soil (erosion) are transferred to the stationary target.

When more than one target is considered in the analysis, the scenario should be set up to satisfy the target that requires the most resolution. For example, if a study was interested in both the exposure received by a cohort of humans (mobile target) and the maximum concentration in a local pond (stationary target), the setup should follow the procedure described in the decision tree for the mobile target. The concentration in the pond will likely be estimated in the process of characterizing the various human exposure pathways. Thus, the "high resolution" system based on the mobile target should provide an adequate level of detail for estimating the concentration in the pond. If the concentration in the pond were not determined by the system for the mobile target, the user could either add additional parcels to the scenario to account for the pond or set up an additional analysis based on the stationary target.

C.2 PARCEL BOUNDARY TYPES

The decision trees for each of the target classes use existing information about boundaries of the modeling system to facilitate the set up of a scenario. There are several types of these boundaries that can be used independently or in concert. For simplicity, three classes of boundaries are defined: natural boundaries, physiochemical boundaries, and population boundaries. Each of the boundary types is summarized below along with a description of how they are used to define system boundaries and parcels. The boundary types are summarized in Table C-2. These simple classifications allow the boundary types to be easily referenced from the binary decision trees.

Table C-2
Boundary Types Coded for Use in Decision Trees

CODE	BOUNDARY TYPE
1	**Natural**
1a	Air shed
1b	Water shed
1c	Lakes and rivers
1d	Homogeneous land use/cover regions
2	**Physiochemical**
2a	Characteristic travel distance
2b	Dispersion modeling
2max	External boundary capturing 90 % of chemical mass (system boundary)
3	**Population**
3a	Semi-mobile (range)
3b	Immobile (location)

C.2.1 NATURAL BOUNDARIES

Natural boundaries include air sheds, watersheds, water bodies and homogeneous land use and land cover regions. When specifying natural boundaries one can refer to satellite images, topographical maps, or GIS coverage databases.

An air shed can include large valleys such as the Sacramento valley (CA) where, due to inversion layers and diurnal wind patterns, the air mass is confined and well mixed throughout the area for a large portion of the time. Air shed boundaries can also include smaller valleys when meteorological conditions produce long residence time for the air mass in the bounded region. Air shed boundaries are useful in providing information about the scale of the model region (*i.e.*, external boundaries of the system).

Watersheds are also useful in determining the scale of the system as well as the size and location of parcels within the system, especially if the concentration in a particular lake or wetland is of interest. Watershed boundaries can be identified or approximated from topographical maps by tracing ridgelines and noting the origin and direction of flow for streams and rivers. The size and location of a watershed can influence the transfer of chemical to water bodies within the basin.

Locations and sizes of water bodies and information describing land use and land cover patterns can also indicate important boundaries in the system. If the analysis objective includes estimating the impact of a source on a particular water body, agricultural plot, or forest, these boundaries can be incorporated into the scenario setup.

C.2.2 PHYSICOCHEMICAL BOUNDARIES

Physicochemical boundaries are based on the characteristic travel distance and direction of the chemical of interest. Physicochemical boundaries can help define both internal parcels and system scale. Physiochemical boundaries can be applied to water bodies, such as rivers and streams, if advection and diffusion in water is the dominant pathway by which a chemical travels through the environment, but the default translocation pathway for most chemicals will be advection in the air.

When determining the scale of the external system boundaries, the user needs to determine the range over which the contaminant is likely to spread and if it is necessary for the model system to capture this range for the user to be able to answer the desired question. For example, chemicals that are highly mobile in the environment will move far from the source. One might want to include this entire range, for example, if they want to determine the total number of people exposed to the chemical. If the goal is to determine the exposure to a nearby population, a smaller system might be appropriate. In this case, a background concentration will need to be used to account for pollutant mass flowing back into the system when there is a change in the wind direction. For chemicals that rapidly deposit to the land surface, it is often easier to model the range over which the chemical is likely to spread and thus is desirable to model the full range of the chemical.

Travel distance (based on the chemical-specific deposition velocity), local weather data (*e.g.*, wind speed/direction, rainfall data, temperature), and approximate landscape characteristics (*e.g.*, locations of water, forest, and bare soil) are used to provide an estimate of the distance that a chemical will travel from the source. Ideally, one needs to account for the travel distance in each of the four major directions (*i.e.*, north, south, east, and west) to account for variations resulting from land use and changing weather patterns. The travel distance can be used to estimate changes in atmospheric concentration, thus providing the maximum resolution that can still be considered statistically significant (can be detected given the uncertainty in model predictions and imprecision in environmental measurements). Characteristic travel distance can be used to construct polygons that incorporate advection, dispersion, and physical loss of chemical from the atmosphere.

If the objective is to track the movement and fate of the pollutant over its lifetime then one would want to calculate the distance over which 90 percent of the pollution had been removed from the air by reactions and dry deposition.

The size of a grid cell can then be determined by calculating the length over which X percent of the mass of the chemical species with the shortest characteristic distance is lost. One would want to base this on both atmospheric reactions and the most rapid depositional processes (*i.e.,* assume both wet and dry deposition). The selection of a factor of X = 50 is dependent on

the precision of the model output and relevant measurements and will likely result in grid cells that are smaller than necessary. The following equation can be used to approximate the distance, L, for any specified percent reduction:

$$L = -\ln((100 - \%\ \text{reduction}) / 100) * \text{characteristic length}$$

where:

% reduction = the specified percent change in chemical mass along a path of length L

The characteristic travel distance for a chemical in the environment can be calculate using the chemical's estimated residence time in the atmosphere along with speed and direction of the moving phase. The characteristic travel distance in the atmosphere can be calculated finding the distance at which the concentration has reached 36 percent of the initial concentration (Bennett et al. 1998). This can be calculated as:

$$\text{characteristic length} = 0.23 * \text{wind velocity/loss rate}$$

where:

characteristic length	=	distance at which 63 percent of the mass in the air cell has been removed
wind velocity	=	average wind velocity (m/d)
loss rate	=	loss rate from the atmosphere from transformation and depositional processes (1/d)

The 0.23 term approximates the effects of dispersion but dispersion and diffusion are not explicitly modeled in the above calculation. Gifford and Hanna (1973) have shown that the yearly average concentration in a simple box model is proportional to the source strength in mass per unit area divided by the wind speed. McKone (1993a,1993b,1993c) has used the Gifford and Hanna work with Benarie (1980) to derive the proportionality constant in this relationship. Multiplying the unidirectional wind velocity by 0.23 accounts for is the changing direction of the wind; in other words, if you averaged the wind in one direction it would be about 23 percent of the wind speed at any time. This factor may underestimate the characteristic travel distance in locations with persistent wind flow in one direction, and as a result, may result in finer grid spacing.

For transformation losses, the loss rate is equal to the reaction rate in the atmosphere which, for first order reactions, is given by 0.693 divided by the half life in the atmosphere. For deposition losses, the loss rate is equal to the deposition velocity divided by the mixing height.

$$\text{loss rate} = (0.693/\text{half life} + \text{deposition velocity/mixing height})$$

where:

half life	=	reaction half life of the chemical in the atmosphere (d)
deposition velocity	=	total deposition velocity including wet and dry deposition to soil, water, and vegetation (m/d)
mixing height	=	mixing height of the atmosphere (*i.e.,* the height over which pollutants can be assumed evenly mixed) (m)

The atmospheric mixing height is a function of climatic conditions and can be calculated from meteorological data. When determining the characteristic travel distance for a chemical, one may want to make a calculation for each season since the average weather (mixing height, precipitation, mean winds, etc.) may vary significantly. The reaction rates and deposition velocities are chemical specific.

Air dispersion models can also be used to locate system boundaries. By plotting x-y spatial coordinates along with air concentration (z), a map or map-overlay can be generated and used in the same way that a topographical map is used for identifying natural boundaries. The key to using dispersion models or characteristic travel distance for estimating boundaries is deciding what change in concentration can be considered significant. Even if the model gave perfect information, variation in field measurements and imprecision in analytical equipment would likely require a 10 percent to 50 percent change in concentration before the concentration difference between two places on a map could be considered statistically significant (Eiceman et al. 1993). This coefficient of variation increases as the environmental concentration approaches the experimental detection limit of the equipment.

However, it can be safely assumed that multimedia models do not give perfect information. An international group of expert model developers and model users recently concluded that a reasonable estimate (admittedly subjective) of model accuracy for multimedia pollutants was a factor of three. This factor is expected to increased by an additional factor of two each time the pollutant crossed a compartmental interface (Cowen et al. 1995). Thus, as the pollutant moves away from the source through adjacent compartments in TRIM.FaTE, the distance across each compartment should be increased (*i.e.*, reduce resolution with increased distance from source). This characteristic is intuitive in that at some distance from the source, the pollutant will become a regional or global pollutant and one will no longer be able to directly link the pollutant back to the original source.

C.2.3 POPULATION BOUNDARIES

Population mobility boundaries take into account additional information about the habitat of the target and the different locations in which the target is likely to be during an exposure event. Population mobility boundaries are comparable to natural boundaries except that no physical boundary would be visible on a map. Population boundaries can be used to justify increased complexity of a landscape parcel within a natural boundary or within the range of a bounded target (as described in previous sections). For example, an antelope may spend most of its life foraging in the high desert sage around a munitions storage facility. No natural boundaries exist and physicochemical boundaries may provide more resolution than is

appropriate. If the seasonal foraging area of the antelope can be identified, this information can be used to construct parcels that encompass the animal's range for each season. If that range is large, physicochemical boundaries can be used to increase resolution (more parcels) within the boundaries as necessary.

C.3 REVISITING THE INITIAL MODEL SETUP

This section addresses methods for identifying necessary changes in grid spacing and changes to the external system boundary after an initial TRIM.FaTE simulation and a basic uncertainty analysis have been completed. It is important to determine if any changes to the grid spacing are necessary once an initial run has been completed, keeping in mind the analysis objective, the type of target, and the variance in model results.

If the uncertainty of the concentrations within a compartment is greater than the difference in concentration between adjacent compartments, using a finer grid scale will not increase the information that can be obtained from the model. On the other hand, if the uncertainty is less than the difference in concentration between compartments providing a situation where there is a statistically significant difference in concentration between adjacent compartments of similar composition, then a finer grid size may be appropriate. When considering combining adjacent parcels it is important to also examine environmental characteristics of each parcel. An obvious example where adjacent parcels would not want to be combined is adjacent air parcels over land and water. If the water body is large, then the atmospheric mixing height would be different and as a result, the parcels should not be combined.

For instance, a user might find that the initial simulation did not include a large enough region, and the simulations result in a significant portion of chemical mass leaving one of the system boundaries. In this case, the user might want to consider increasing the scale, if warranted by the model objectives, and completing a new simulation. The user would need to consider whether or not there is a potential exposed population downwind from the site. If there is a sensitive ecosystem, farmland, or marine-harvesting region just outside the suggested model range, the user might want to extend the range to include this area as the chemical may bioaccumulate in the food chain, causing a significant exposure. Also, the user would want to evaluate whether or not the mass leaving the system will result in concentrations above the background level. If not, the user might not want to expand the region. If the region was expanded and no gain in useful information was realized, those parcels could always be removed for future simulations.

C.4 SETTING UP THE MODELING REGION

This section builds upon the principles important to selecting the scenario scale, as presented in Sections C.1 through C.3, and addresses the details of defining parcels, volume elements, and compartments.

C.4.1 DETERMINING PARCELS

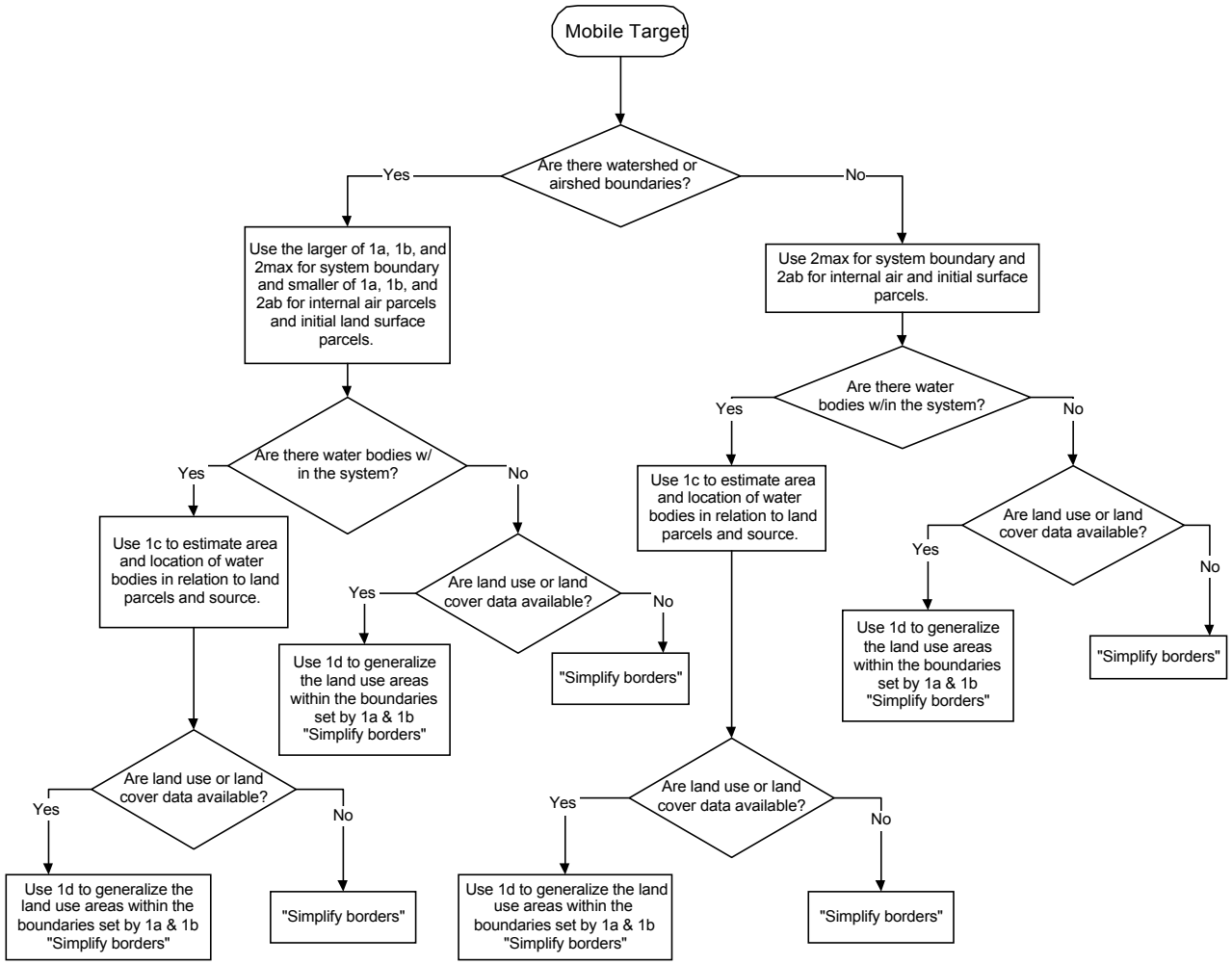
To guide the development of parcels for a given model scenario, a series of decision trees are presented, each for a different model objective. By following the decision tree, appropriate parcels can be determined. After the analysis objective is defined, the dominant target class and chemical(s) of concern can be identified. The target class is then used to select the appropriate decision tree to aid in defining parcels. Refer to Figure C-1 for a mobile target, Figure C-2 for a bounded target, and Figure C-3 for a stationary target. By following the decision tree down a yes/no path, the important boundary types are identified in the order of significance until an adequate level of complexity is attained. The boundary types are listed and coded in Table C-2.

The general pattern within the decision trees consists of a starting point indicated by an oval containing the target class at the top of the page. Following the decision tree, one will come to a diamond that contains a simple question that is answered either yes or no. This may lead to another question or to an action indicated by a rectangle. The action boxes direct the user to one or more of the coded boundary types listed in Table C-2. For mobile targets, the air parcels are defined first. For the bounded and stationary targets, the land surface parcels are defined first followed by the air parcels. When all parcels are defined (no more questions remain on the tree) the process moves to the simplification stage. This stage includes final smoothing of boundary lines, combining adjacent parcels with similar composition, and adding additional parcels around the perimeter of the system.

After the preliminary map of the parcels has been completed based on the decision tree, some slight modifications may need to be made to the map of parcels. Conceptual filtering (also known as best judgment) can be used to transform the curved lines into simple connected polygons while conserving the area and approximate location relative to the source and adjacent parcels. The horizontal area of an air or water basin can be can be estimated using a planimeter by tracing the boundary several times and calculating the average area. The area can then be used to estimate the parcel size. Alternatively, one can simply use a clear ruler and best judgment to straighten the lines. Boundaries based on airsheds can be simplified in the same manner.

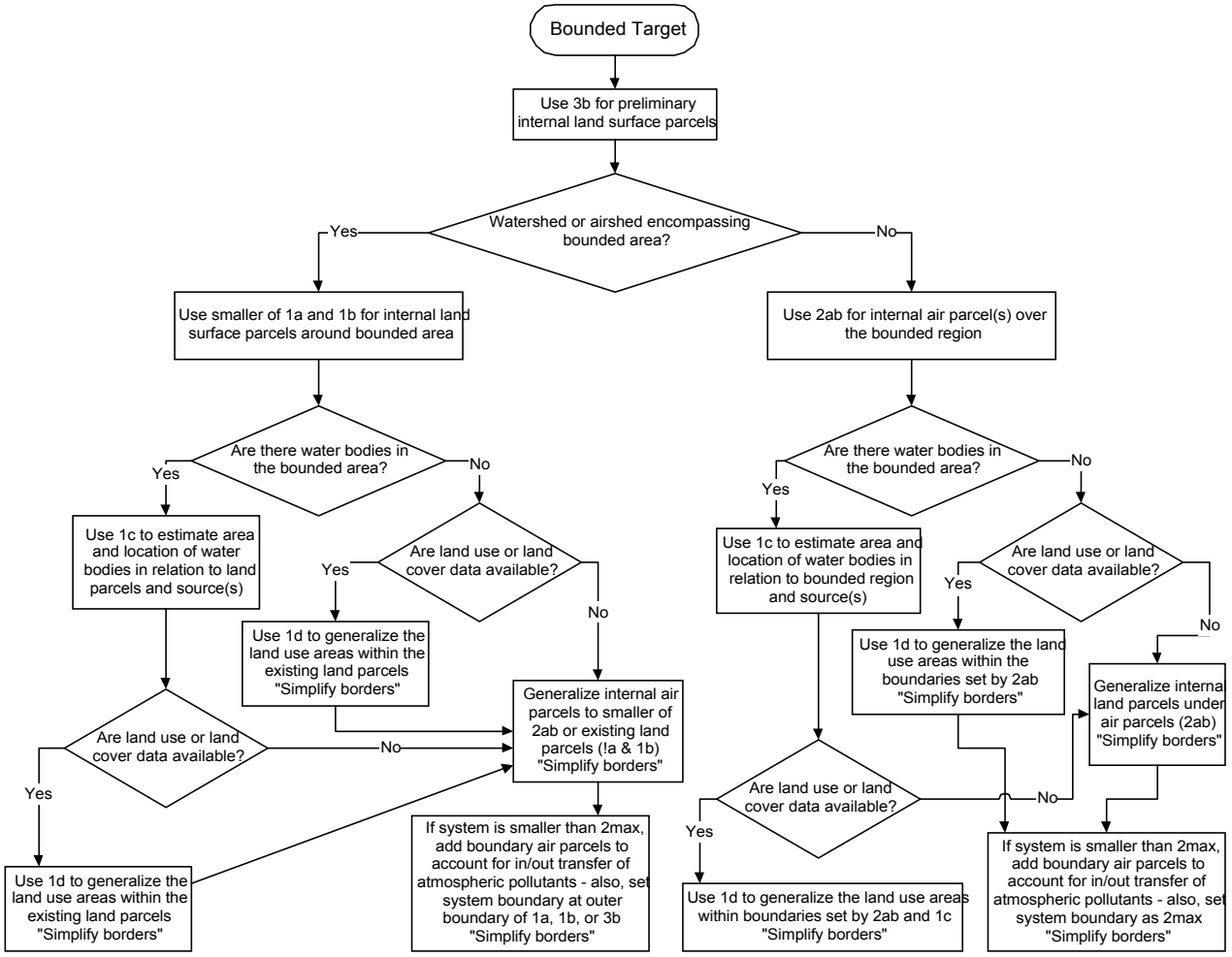
Although the major land types (*e.g.*, forests, urban areas) generally should be considered separately, the actual boundaries of the landscape types may need to be modified to fit the grid structure. In order to capture differences in landscape regions, the land under an air parcel can be split into multiple parcels. This can be an advantage for including rivers and lakes that are narrow or small relative to the air parcel size (differences in atmospheric mixing height over land and water can be ignored if the water body is small). Also, one could include various land uses in a single land parcel if transport differences across various land uses are not significant (*e.g.*, a land parcel may include 90 percent conifer forest and 10 percent deciduous forest). In this case, a hybrid parcel containing a fraction of each cover would be created.

Figure C-1
Mobile Target - Binary Decision Tree for Setting Up Model Region[a]



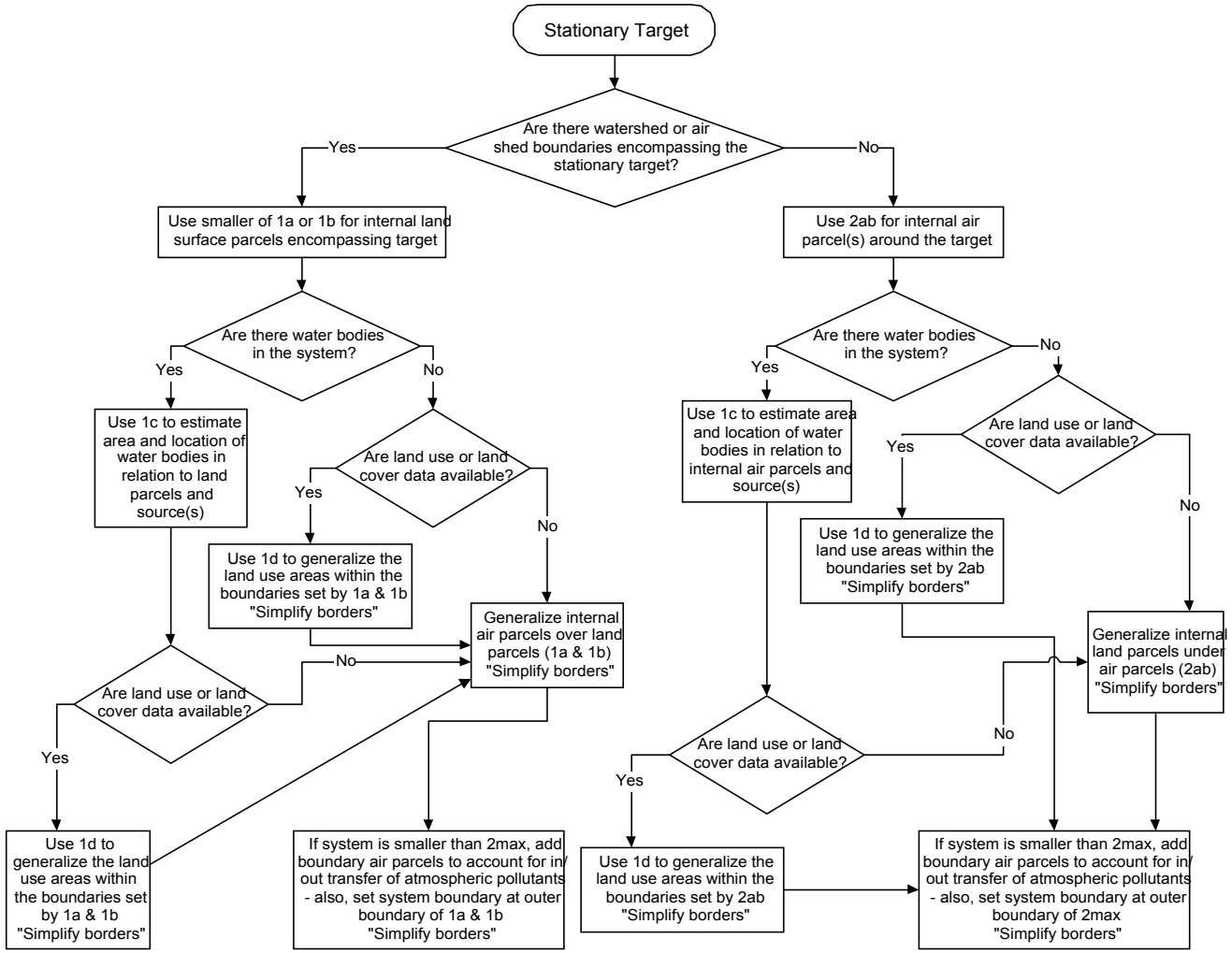
[a] Codes refer to the boundary types referenced in Table C-2.

Figure C-2
Bounded Target - Binary Decision Tree for Setting Up Model Region[a]



[a] Codes refer to the boundary types referenced in Table C-2.

Figure C-3
Stationary Target - Binary Decision Tree for Setting Up Model Region[a]



[a] Codes refer to the boundary types referenced in Table C-2.

C.4.2 DETERMINING VOLUME ELEMENTS

After the parcels have been determined, the volume elements are specified. This step involves determining the appropriate number of volume elements and specifying the appropriate depth for each one. Whereas parcels only represent the modeling region in two dimensions, volume elements add the component of depth, thus representing the modeling region in three dimensions. The development of volume elements represents the final step in specifying the spatial resolution of the modeling region.

If the parcel represents a surface water area, surface water and sediment volume elements may need to be defined. The appropriate depth of the surface water volume element can be determined, for example, based on the average depth of the surface water within that region. An upper and lower water volume element may be appropriate if, for example, the water body is very deep or if different types of fish and other aquatic animals live at different depths. The level of refinement (*i.e.,* number of volume elements used to represent) for a surface water body also depends on the level of detail necessary to answer the modeling questions.

If the parcel represents a land area, the number, depth, and type of soil volume elements will need to be determined. For instance, if the region is in the forest, the soil is unlikely to be tilled and thus the number and depth of soil volume elements would be determined based on the depth the chemical is likely to penetrate. The number of modeled soil layers depends on the desired level of detail and objective of the scenario, but typically three soil layers (represented as volume elements) are considered. For a given land parcel, there is generally a thin volume element composed predominantly of surface soil, reflecting the depth of soil likely to be incidentally ingested by wildlife. The root zone soil layer, represented by a separate volume element, would typically be immediately below the surface soil layer and would reflect the depth to which plant roots are likely to be in contact with the modeled chemical(s). The vadose zone would then extend from the bottom of the root zone soil layer to the ground water surface. If the chemical is likely to penetrate deeply into the soil, a volume element composed predominantly of ground water may also be included.

If the parcel represents air, the number and depth of air volume elements needs to be determined. The boundaries of air parcels do not necessarily have to coincide with the boundaries of the surface water and soil parcels, although to limit the computer resources required for a simulation, the parcel boundaries may be made identical. The number of vertical layers (represented as volume elements) modeled for each air parcel is determined based on the desired level of detail and the modeling objective. For example, if the modeled source has a high release height and only one volume element is modeled, the results are likely to overestimate the deposition of the chemical close to the source. In this case, it would be advantageous to model multiple volume elements representing multiple vertical layers. In contrast, it may be appropriate to model a source with a low release height with one vertical layer.

C.4.3 DETERMINING COMPARTMENTS

Abiotic

Abiotic compartments are determined by the predominant abiotic medium in the volume element within which they are contained. At least one abiotic compartment must be contained within each volume element and, although not typically utilized, the model framework does support multiple abiotic compartments within a volume element. In most cases, the determination of abiotic compartments is an implied step because they are simply defined by the predominant abiotic media within the volume element. For example, if a given volume element is composed predominantly of surface soil, a surface soil compartment would be included in the volume element.

Biotic

The transport of chemicals to biota consists of diffusive and advective processes, through the latter term is rarely used by biologists. Chemicals diffuse into plant leaves from air; chemicals deposit onto plant leaves with particles in air, an advective process. The uptake of chemicals from soil or soil water by plant roots or earthworms is treated as diffusion, though water carries the chemical into the plant (advection). Similarly, chemicals are assumed to enter algae, macrophytes and benthic invertebrates by diffusion. The major advective process is food intake by fish, birds and mammals.

The only transport process within biota that is included in TRIM.FaTE is transport through the plant stem in xylem and phloem fluids. The distribution of chemicals among organs in individual wildlife is not a feature of TRIM.FaTE.

C.5 REFERENCES

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APPENDIX D
TRIM.FaTE Inputs

Input Parameter	Units
SOURCE DATA (for each source)	
Location of source	UTM coordinates (x,y)
Height of emission source	m
Emission rate (for each chemical)	g / s
Particle size	mm
BACKGROUND DATA (for each modeled chemical)	
Background concentration in each compartment	Soil and air: ng / m^3 Water: ng / l
METEOROLOGICAL DATA	
Horizontal wind speed	m / s
Horizontal wind direction	degrees
Vertical wind speed	m / s
Air temperature	°K
Precipitation	m / day
Mixing height	m
Relative humidity	unitless
SPATIAL DATA	
Corners of each volume element (VE)	UTM coordinates
Height of each air VE	m
Surface soil depth (for each surface soil VE)	m
Root zone depth (for each root zone VE)	m
Vadose zone depth (for each vadose zone VE)	m
Ground water layer depth (for each aquifer layer VE)	m
Surface water depth (for each surface water VE)	m
Sediment layer depth (for each sediment layer VE)	m
ABIOTIC ENVIRONMENTAL SETTING DATA	
Air (assume same for all air compartments)	
Atmospheric dust load	kg[dust] / m^3[air]
Dust density	kg[dust] / m^3[dust]
Dry deposition velocity of air particulates	m / day
Washout ratio	[mass chem/volume rain] / mass chem/volume air]
Surface area per volume of particles	m^2[area] / m^3[particles]
Junge_C	m-Pa
Density of air	g / cm^3
Fraction organic matter on particulates	unitless
Diffusion coefficient of water in air	m^2 / d
Boundary layer thickness in air above soil	m
Surface Soil (assumed same for all surface soil compartments)	
Land use type	unitless

Input Parameter	Units
Water content	volume[water] / volume[compartment]
Air content	volume[air] / volume[compartment]
Soil material density	kg[soil] / m^3[soil]
Organic carbon fraction	unitless
Air soil boundary thickness	m
Default depth of runoff water	m
Fraction of area available for vertical diffusion	m^2[area available] / m^2[total]
Fraction of area available for erosion	m^2[area available] / m^2[total]
Fraction of area available for runoff	m^2[area available] / m^2[total]
Root Zone (assumed same for all root zone compartments)	
Water content	volume[water] / volume[compartment]
Air content	volume[air] / volume[compartment]
Soil material density	kg[soil] / m^3[soil]
Organic carbon fraction	unitless
Vadose Zone (assumed same for all vadose zone compartments)	
Water content	volume[water] / volume[compartment]
Air content	volume[air] / volume[compartment]
Soil material density	kg[soil] / m^3[soil]
Organic carbon fraction	unitless
Ground Water (assumed same for all ground water compartments)	
Porosity	volume[total pore space] / volume[compartment]
Air content	volume[air] / volume[compartment]
Solid material density in aquifer	kg[soil] / m^3[soil]
Organic carbon fraction	unitless
Surface Water (depends on water body type - values provided have been developed for an initial simple water body scenario)	
Flush rate	flushes/year
Suspended sediment concentration	kg[sediment] / m^3[water column]
Evaporation of water	m^3[water] / m^2[area]-day
Current velocity	m / s
Organic carbon fraction in suspended sediments	unitless
Suspended sediment density	kg[sediment] / m^3[sediment]
Boundary layer thickness above sediment	m
Drag coefficient for water body	unitless
Viscous sublayer thickness	m
pH	unitless
Chloride concentration	mg / L
Sediment (depends on associated water body type)	
Organic carbon fraction	unitless
Solid material density in sediment	kg[sediment] / m^3[sediment]
Porosity of the sediment zone	volume[total pore space] / volume[sediment compartment]
Benthic solids concentration	kg[sediment] / m^3[sediment compartment]

Input Parameter	Units
ABIOTIC CHEMICAL-SPECIFIC DATA (for each chemical)	
General to all media	
Molecular weight	g / mol
Octanol-water partition coefficient (K_{ow})	L[water] / L[octanol]
Melting point	°K
Water solubility	mol / m^3
Henry's Law constant	Pa-m^3 / mol
Diffusion coefficient in pure air	m^2 / day
Diffusion coefficient in pure water	m^2 / day
Organic carbon partition coefficient	L[water] / kg[carbon]
Surface Soil	
Methylation rate constant for Hg(2) to MHg	1 / day
Demethylation rate constant for MHg to Hg(2)	1 / day
Reduction rate constant for Hg(2) to Hg(0)	1 / day
Oxidation rate constant for Hg(0) to Hg(2)	1 / day
Root Zone	
Methylation rate constant for Hg(2) to MHg	1 / day
Demethylation rate constant for MHg to Hg(2)	1 / day
Reduction rate constant for Hg(2) to Hg(0)	1 / day
Oxidation rate constant for Hg(0) to Hg(2)	1 / day
Vadose Zone	
Methylation rate constant for Hg(2) to MHg	1 / day
Demethylation rate constant for MHg to Hg(2)	1 / day
Reduction rate constant for Hg(2) to Hg(0)	1 / day
Oxidation rate constant for Hg(0) to Hg(2)	1 / day
Ground Water	
Methylation rate constant for Hg(2) to MHg	1 / day
Demethylation rate constant for MHg to Hg(2)	1 / day
Reduction rate constant for Hg(2) to Hg(0)	1 / day
Oxidation rate constant for Hg(0) to Hg(2)	1 / day
Surface Water	
Methylation rate constant for Hg(2) to MHg	1 / day
Demethylation rate constant for MHg to Hg(2)	1 / day
Reduction rate constant for Hg(2) to Hg(0)	1 / day
Oxidation rate constant for Hg(0) to Hg(2)	1 / day
Sediment	
Methylation rate constant for Hg(2) to MHg	1 / day
Demethylation rate constant for MHg to Hg(2)	1 / day
Reduction rate constant for Hg(2) to Hg(0)	1 / day
Oxidation rate constant for Hg(0) to Hg(2)	1 / day
ABIOTIC FLOW DATA	
Total erosion rate from soil	kg[soil] / m^2[area]-day
Erosion rates between soil and soil	kg[soil] / m^2[area]-day
Erosion rates between soil and surface water	kg[soil] / m^2[area]-day
Total runoff rate from soil	m^3[water] / m^2[area]-day
Runoff rates between soil and soil	m^3[water] / m^2[area]-day

Input Parameter	Units
Runoff rates between soil and surface water	m^3[water] / m^2[area]-day
Percolation rates between soil and soil	m^3[water] / m^2[area]-day
Surface water flow between surface water compartments	m^3[water] / m^2[area]-day
Recharge from ground water to surface water	m^3[water] / m^2[area]-day
Horizontal water flow rate in ground water	m^3[water] / m^2[area]-day
Deposition of suspended sediment in the water column to the sediment bed	kg[sediment] / m^2[area]-day
Resuspension of sediment from the sediment bed to the water column	kg[sediment] / m^2[area]-day
Burial rate of sediment in the sediment bed	kg[sediment] / m^2[area]-day
BIOTIC ENVIRONMENTAL SETTING DATA (for each relevant compartment)	
ANIMALS - AQUATIC	
Water Column Carnivore - Bass	
Body weight (BW)	kg
Fraction lipid weight	unitless
Biomass per area	km / m^2
Population per area	# / m^2
Ventilation rate	ml / min / kg
Fraction of food diet comprised of fish omnivore	unitless
Fraction of food diet comprised of fish herbivore	unitless
Fraction of food diet comprised of fish carnivore	unitless
Fraction of food diet comprised of fish mayfly nymph	unitless
Water Column Herbivore - Bluegill	
Body weight (BW)	kg
Fraction lipid weight	unitless
Biomass per area	km / m^2
Population per area	# / m^2
Ventilation rate	ml / min / kg
Fraction of food diet comprised of phytoplankton (algae)	unitless
Fraction of food diet comprised of macrophyte	unitless
Fraction of diet_mayfly	unitless
Water Column Omnivore - Channel Catfish	
Body weight (BW)	kg
Fraction lipid weight	unitless
Biomass per area	km / m^2
Population per area	# / m^2
Ventilation rate	ml / min / kg
Fraction of food diet comprised of macrophyte	unitless
Fraction of food diet comprised of mayfly nymph	unitless
Fraction of food diet comprised of omnivore	unitless
Fraction of food diet comprised of fish herbivores	unitless
Benthic Omnivore	
Body weight (BW)	kg
Fraction lipid weight	unitless
Biomass per area	kg / m^2
Population per area	# / m^2

Input Parameter	Units
Ventilation rate	ml / min / kg
Fraction of diet comprised of benthic invertebrates	unitless
Benthic Carnivore	
Body weight (BW)	kg
Fraction lipid weight	unitless
Biomass per area	kg / m^2
Population per area	# / m^2
Ventilation rate	ml / min / kg
Fraction of diet comprised of benthic omnivores	unitless
Benthic Invertebrate-Mayfly	
Body weight (BW)	kg
Biomass per area	kg / m^2
Total biomass of invertebrates per area	kg / m^2
PLANTS - AQUATIC	
Macrophyte	
Biomass per area	kg / m^2
Density of macrophytes	kg / m^3
Phytoplankton - Algae	
Diameter of algae	mm
Average cell density (per vol cell, not water)	g / mm^3
Algae growth rate	1 / day
Algae density in water column	g[algae] / L[water]
Algae carbon content (fraction)	unitless
Algae water content (fraction)	unitless
ANIMALS - TERRESTRIAL	
Soil Detritivore - Earthworm	
Density per soil area, deciduous forest	kg[worm] / m^2 [area]
Density per soil area, coniferous forest	kg[worm] / m^2 [area]
Density per soil area, grass/herb	kg[worm] / m^2 [area]
Density per soil area, agriculture	kg[worm] / m^2 [area]
Density	kg[worm] / L[volume]
Water content of worm	mass fraction
Soil Detritivore - Soil Arthropod	
Body weight (BW)	kg
Biomass per area	kg / m^2
Terrestrial Ground-Invertebrate Feeder - Black-capped Chickadee	
Body weight (BW)	kg
Population per area	# / m^2
Soil ingestion rate	kg[soil] / kg BW-day
Water_a	unitless
Water_b	unitless
Inhalation_a	unitless
Inhalation_b	unitless
Food ingestion rate	kg[food] / kg BW-day
Fraction of food diet comprised of plants	unitless
Fraction of food diet comprised of benthic invertebrates	unitless
Fraction excretion to soil	unitless

Input Parameter	Units
Fraction excretion to water	unitless
Semiaquatic Piscivore - Kingfisher	
Body weight (BW)	kg
Population per area	# / m^2
Soil ingestion rate	kg[soil] / kg BW-day
Water_a	unitless
Water_b	unitless
Inhalation_a	unitless
Inhalation_b	unitless
Food ingestion rate	kg[food] / kg BW-day
Fraction of food comprised of water column herbivore	unitless
Fraction of food comprised of water column omnivore	unitless
Fraction of food comprised of benthic omnivore	unitless
Fraction excretion to soil	unitless
Fraction excretion to water	unitless
Semiaquatic Predator/Scavenger - Bald eagle	
Body weight (BW)	kg
Population per area	# / m^2
Soil ingestion rate	kg[soil] / kg BW-day
Water_a	unitless
Water_b	unitless
Inhalation_a	unitless
Inhalation_b	unitless
Food ingestion rate	kg[food] / kg BW-day
Fraction of food diet comprised of mouse	unitless
Fraction of food diet comprised of chickadee	unitless
Fraction of food diet comprised of water column herbivore	unitless
Fraction of food diet comprised of water column omnivore	unitless
Fraction of food diet comprised of water column carnivore	unitless
Fraction of food diet comprised of benthic omnivore	unitless
Fraction of food diet comprised of benthic carnivore	unitless
Fraction excretion to soil	unitless
Fraction excretion to water	unitless
Semiaquatic Piscivore - Common Loon	
Body weight (BW)	kg
Population per area	# / m^2
Soil ingestion rate	kg[soil] / kg BW-day
Water_a	unitless
Water_b	unitless
Inhalation_a	unitless
Inhalation_b	unitless
Food ingestion rate	kg[food] / kg BW-day
Fraction of diet comprised of water column herbivore	unitless
Fraction excretion to soil	unitless
Fraction excretion to water	unitless
Semiaquatic Omnivore - Mallard	
Body weight (BW)	kg

Input Parameter	Units
Population per area	# / m^2
Soil ingestion rate	kg[soil] / kg BW-day
Water_a	unitless
Water_b	unitless
Inhalation_a	unitless
Inhalation_b	unitless
Food ingestion rate	kg[food] / kg BW-day
Fraction of food diet comprised of plant	unitless
Fraction of food diet comprised of benthic invertebrate	unitless
Fraction excretion to soil	unitless
Fraction excretion to water	unitless
Terrestrial Predator/Scavenger - Red-tailed Hawk	
Body weight (BW)	kg
Population per area	# / m^2
Soil ingestion rate	kg[soil] / kg BW-day
Water_a	unitless
Water_b	unitless
Inhalation_a	unitless
Inhalation_b	unitless
Food ingestion rate	kg[food] / kg BW-day
Fraction of food diet comprised of soil arthropod	unitless
Fraction of food diet comprised of chickadee	unitless
Fraction of food diet comprised of mouse	unitless
Fraction of food diet comprised of short tailed shrew	unitless
Fraction of food diet comprised of vole	unitless
Fraction excretion to soil	unitless
Fraction excretion to water	unitless
Terrestrial Insectivore - Tree Swallow	
Body weight (BW)	kg
Population per area	# / m^2
Soil ingestion rate	kg[soil] / kg BW-day
Water_a	unitless
Water_b	unitless
Inhalation_a	unitless
Inhalation_b	unitless
Food ingestion rate	kg[food] / kg BW-day
Fraction of food diet comprised of benthic invertebrate	unitless
Fraction excretion to soil	unitless
Fraction excretion to water	unitless
Terrestrial Herbivore - Meadow Vole	
Body weight (BW)	kg
Population per area	# / m^2
Soil ingestion rate	kg[soil] / kg BW-day
Water_a	unitless
Water_b	unitless
Inhalation_a	unitless
Inhalation_b	unitless

Input Parameter	Units
Food ingestion rate	kg[food] / kg BW-day
Fraction of food diet comprised of plant	unitless
Fraction excretion to soil	unitless
Fraction excretion to water	unitless
Terrestrial Herbivore - Long-tailed Vole	
Body weight (BW)	kg
Population per area	# / m^2
Soil ingestion rate	kg[soil] / kg BW-day
Water_a	unitless
Water_b	unitless
Inhalation_a	unitless
Inhalation_b	unitless
Food ingestion rate	kg[food] / kg BW-day
Fraction of food diet comprised of plant	unitless
Fraction excretion to soil	unitless
Fraction excretion to water	unitless
Terrestrial Predator/Scavenger - Long-tailed Weasel	
Body weight (BW)	kg
Population per area	# / m^2
Soil ingestion rate	kg[soil] / kg BW-day
Water_a	unitless
Water_b	unitless
Inhalation_a	unitless
Inhalation_b	unitless
Food ingestion rate	kg[food] / kg BW-day
Fraction of food diet comprised of mouse	unitless
Fraction of food diet comprised of vole	unitless
Fraction of food diet comprised of shrew	unitless
Fraction excretion to soil	unitless
Fraction excretion to water	unitless
Semiaquatic Omnivore - Mink	
Body weight (BW)	kg
Population per area	# / m^2
Soil ingestion rate	kg[soil] / kg BW-day
Water_a	unitless
Water_b	unitless
Inhalation_a	unitless
Inhalation_b	unitless
Food ingestion rate	kg[food] / kg BW-day
Fraction of food diet comprised of mouse	unitless
Fraction of food diet comprised of vole	unitless
Fraction of diet comprised of water column herbivore	unitless
Fraction of diet comprised of water column omnivore	unitless
Fraction of diet comprised of benthic omnivore	unitless
Fraction of food diet comprised of benthic invertebrate	unitless
Fraction of food diet comprised of chickadee	unitless
Fraction excretion to soil	unitless

Input Parameter	Units
Fraction excretion to water	unitless
Terrestrial Omnivore - White-footed Mouse	
Body weight (BW)	kg
Population per area	# / m^2
Soil ingestion rate	kg[soil] / kg BW-day
Water_a	unitless
Water_b	unitless
Inhalation_a	unitless
Inhalation_b	unitless
Food ingestion rate	kg[food] / kg BW-day
Fraction of food diet comprised of worm	unitless
Fraction of food diet comprised of plant	unitless
Fraction excretion to soil	unitless
Fraction excretion to water	unitless
Terrestrial Herbivore - Mule Deer/Black-tailed Deer	
Body weight (BW)	kg
Population per area	# / m^2
Soil ingestion rate	kg[soil] / kg BW-day
Water_a	L[water] / kg BW-day
Water_b	L[water] / kg BW-day
Inhalation_a	unitless
Inhalation_b	unitless
Food ingestion rate	kg[food] / kg BW-day
Fraction of food diet comprised of plant	unitless
Fraction excretion to soil	unitless
Fraction excretion to water	unitless
Terrestrial Herbivore - White-tailed Deer	
Body weight (BW)	kg
Population per area	# / m^2
Soil ingestion rate	kg[soil] / kg BW-day
Water_a	L[water] / kg BW-day
Water_b	L[water] / kg BW-day
Inhalation_a	unitless
Inhalation_b	unitless
Food ingestion rate	kg[food] / kg BW-day
Fraction of food diet comprised of plant	unitless
Fraction excretion to soil	unitless
Fraction excretion to water	unitless
Semiaquatic Omnivore - Raccoon	
Body weight (BW)	kg
Population per area	# / m^2
Soil ingestion rate	kg[soil] / kg BW-day
Water_a	L[water] / kg BW-day
Water_b	L[water] / kg BW-day
Inhalation_a	unitless
Inhalation_b	unitless
Food ingestion rate	kg[food] / kg BW-day

Input Parameter	Units
Fraction of food diet comprised of benthic invertebrate	unitless
Fraction of diet comprised of water column herbivore	unitless
Fraction of diet comprised of water column omnivore	unitless
Fraction of diet comprised of benthic omnivore	unitless
Fraction of food diet comprised of worm	unitless
Fraction excretion to soil	unitless
Fraction excretion to water	unitless
Terrestrial Ground-Invertebrate Feeder - Short-tailed Shrew	
Body weight (BW)	kg
Population per area	# / m^2
Soil ingestion rate	kg[soil] / kg BW-day
Water_a	L[water] / kg BW-day
Water_b	L[water] / kg BW-day
Inhalation_a	unitless
Inhalation_b	unitless
Food ingestion rate	kg[food] / kg BW-day
Fraction of food diet comprised of worm	unitless
Fraction of food diet comprised of soil arthropod	unitless
Fraction excretion to soil	unitless
Fraction excretion to water	unitless
Terrestrial Ground-Invertebrate Feeder - Trowbridge Shrew	
Body weight (BW)	kg
Population per area	# / m^2
Soil ingestion rate	kg[soil] / kg BW-day
Water_a	L[water] / kg BW-day
Water_b	L[water] / kg BW-day
Inhalation_a	unitless
Inhalation_b	unitless
Food ingestion rate	kg[food] / kg BW-day
Fraction of food diet comprised of soil arthropod	unitless
Fraction excretion to soil	unitless
Fraction excretion to water	unitless
PLANTS - TERRESTRIAL	
Agricultural Leaf	
Water content	unitless
Lipid content	kg / kg wet weight
Correction exponent, octanol to lipid	unitless
Volume of wet leaf weight per unit area	m^3 / m^2
Density of wet leaf	kg / m^3
Mass of leaf per unit area	kg[fresh leaf] / m^2[area]
Dry mass of leaf per unit area	kg[dry leaf] / m^2[area]
Leaf wetting factor	m
1-sided leaf area index	m^2[leaf] / m^2[area]
Vegetation attenuation factor	unitless
Particle washoff rate constant	1 / day
Diffusion coefficient of water in air	m^2 / d
Date litterfall begins	MM / DD

Input Parameter	Units
Date litterfall ends	MM / DD
Date of harvest	MM / DD
Fraction of foliage harvested	unitless
Plant-air boundary layer thickness	m
Length of leaf	m
Deciduous Forest Leaf	
Water content	unitless
Lipid content	kg / kg wet weight
Correction exponent, octanol to lipid	unitless
Volume of wet leaf weight per unit area	m^3 / m^2
Density of wet leaf	kg / m^3
Mass of leaf per unit area	kg[fresh leaf] / m^2[area]
Dry mass of leaf per unit area	kg[dry leaf] / m^2[area]
Leaf wetting factor	m
1-sided leaf area index	m^2[leaf] / m^2[area]
Vegetation attenuation factor (to calc interception fraction)	unitless
Particle washoff rate constant	1 / day
Diffusion coefficient of water in air	m^2 / d
Plant-air boundary layer thickness	m
Length of leaf	m
Coniferous Forest Leaf	
Water content	unitless
Lipid content	kg / kg wet weight
Correction exponent, octanol to lipid	unitless
Volume of wet leaf weight per unit area	m^3 / m^2
Density of wet leaf	kg / m^3
Mass of leaf per unit area	kg[fresh leaf] / m^2[area]
Dry mass of leaf per unit area	kg[dry leaf] / m^2[area]
Leaf wetting factor (to calc interception fraction)	m
1-sided leaf area index	m^2[leaf] / m^2[area]
Vegetation attenuation factor	unitless
Particle washoff rate constant	1 / day
Diffusion coefficient of water in air	m^2 / d
Plant-air boundary layer thickness	m
Length of leaf	m
Herb/Grassland Leaf	
Water content	unitless
Lipid content	kg / kg wet weight
Correction exponent, octanol to lipid	unitless
Volume of wet leaf weight per unit area	m^3 / m^2
Density of wet leaf	kg / m^3
Mass of leaf per unit area	kg[fresh leaf] / m^2[area]
Dry mass of leaf per unit area	kg[dry leaf] / m^2[area]
Leaf wetting factor	m
1-sided leaf area index	m^2[leaf] / m^2[area]
Vegetation attenuation factor (to calc interception fraction)	unitless
Particle washoff rate constant	1 / day

Input Parameter	Units
Diffusion coefficient of water in air	m^2 / d
Plant-air boundary layer thickness	m
Length of leaf	m
Root - Nonwoody Only	
Wet density of root	kg / m^3
Water content of root	unitless
Lipid content of root	kg / kg wet weight
Correction exponent for octanol and lipids	unitless
Correction exponent for the differences between octanol and lipids	unitless
Total volume of dry roots in domain per unit area	m^3 / m^2
Areal density agriculture	kg / m^2
Areal density grass/herb	kg / m^2
Stem - Nonwoody Only	
Density	g / cm^3
Water content of stem	unitless
Lipid content	kg/kg wet weight
Volume of wet stem per unit area	m^3 / m^2
Density of phloem fluid	kg / m^3
Density of xylem fluid	kg / cm^3
Volume of wet weight in domain per unit area	m^3 / m^2
Flow rate of transpired water per leaf area	m^3[water] / m^2 [leaf]
Fraction of transpiration flow rate that is phloem rate	unitless
Correction exponent between foliage lipids and octanol	unitless
TEMPORAL ENVIRONMENTAL SETTING DATA	
Site-specific	
Day of first frost	unitless
Day of last frost	unitless
Deciduous Forest and Grassland	
Litterfall begin date	unitless
Litterfall end date	unitless
Uptake by leaf, end date	unitless
Uptake by root (herb/grass), end date	unitless
LAI = 0, date	unitless
Uptake by leaf, begin date	unitless
LAI = default value, date	unitless
Litterfall rate constant	1 / day
Coniferous Forest	
Uptake by leaf, end date	unitless
Uptake by leaf, end date	unitless
Litterfall rate constant	1 / day
BIOTIC CHEMICAL-SPECIFIC DATA	
ANIMALS - AQUATIC	
Water-column Carnivore - Bass	
Carnivore-omnivore partition coefficient	kg / kg
Alpha for carnivore	unitless
t_{alpha}	day

Input Parameter	Units
Assimilation efficiency	percent
Gamma	
Water-column Herbivore - Bluegill	
Herbivore-algae partition coefficient	kg / kg
Alpha for herbivore	unitless
t_{alpha}	day
Assimilation efficiency	percent
Gamma	
Water-column Omnivore - Channel Catfish	
Omnivore-herbivore partition coefficient	kg / kg
Alpha for omnivore	unitless
t_{alpha}	days
Assimilation efficiency	percent
Gamma	
Benthic Invertebrate (represented by Mayfly)	
Benthic invertebrate-sediment partition coefficient	kg / kg
Alpha for omnivore	unitless
t_{alpha}	days
Benthic Carnivore (represented by Largemouth Bass)	
Carnivore-omnivore partition coefficient	kg / kg
Alpha for omnivore	unitless
t_{alpha}	day
Assimilation efficiency	percent
Benthic Omnivore (represented by Channel Catfish)	
Omnivore-invertebrate partition coefficient	kg / kg
Alpha for omnivore	unitless
t_{alpha}	day
Assimilation efficiency	percent
PLANTS - AQUATIC	
Macrophyte	
Macrophyte-water partition coefficient	L / g
Alpha for macrophyte	unitless
t_{alpha}	days
Phytoplankton - Algae	
D_{ow}	unitless
Uptake rate	mm^2-d^{-1}-L
ANIMALS - TERRESTRIAL	
Soil Detritivore - Earthworm	
Earthworm-soil partitition coefficient, dry	mg/kg per mg/kg
t_{alpha} for worm ↔ soil	day
Alpha for worm ↔ soil	unitless
Soil Detritivore - Soil Arthropod	
Arthropod-soil partition coefficient	kg / kg wet wt
t_{alpha} for arthropod ↔ soil	day
Alpha for arthropod ↔ soil	unitless
Terrestrial Ground-Invertebrate Feeder - Black-capped Chickadee	
First-order transformation rate constant for Hg(0)→Hg(2)	1 / day

Input Parameter	Units
First-order transformation rate constant for MHg→Hg(2)	1 / day
First-order transformation rate constant for Hg(0)→MHg	1 / day
First-order transformation rate constant for Hg(2)→MHg	1 / day
First-order transformation rate constant for Hg(2)→Hg(0)	1 / day
First-order transformation rate constant for MHg→Hg(0)	1 / day
Assimilation efficiency for inhalation for Hg(0)	unitless
Assimilation efficiency for inhalation for Hg(2)	unitless
Assimilation efficiency for inhalation for MHg	unitless
Semiaquatic Piscivore - Kingfisher	
First-order transformation rate constant for Hg(0)→Hg(2)	1 / day
First-order transformation rate constant for MHg→Hg(2)	1 / day
First-order transformation rate constant for Hg(0)→MHg	1 / day
First-order transformation rate constant for Hg(2)→MHg	1 / day
First-order transformation rate constant for Hg(2)→Hg(0)	1 / day
First-order transformation rate constant for MHg→Hg(0)	1 / day
Assimilation efficiency for inhalation for Hg(0)	unitless
Assimilation efficiency for inhalation for Hg(2)	unitless
Assimilation efficiency for inhalation for MHg	unitless
Semiaquatic Predator/Scavenger - Bald Eagle	
First-order transformation rate constant for Hg(0)→Hg(2)	1 / day
First-order transformation rate constant for MHg→Hg(2)	1 / day
First-order transformation rate constant for Hg(0)→MHg	1 / day
First-order transformation rate constant for Hg(2)→MHg	1 / day
First-order transformation rate constant for Hg(2)→Hg(0)	1 / day
First-order transformation rate constant for MHg→Hg(0)	1 / day
Assimilation efficiency for inhalation for Hg(0)	unitless
Assimilation efficiency for inhalation for Hg(2)	unitless
Assimilation efficiency for inhalation for MHg	unitless
Semiaquatic Piscivore - Common Loon	
First-order transformation rate constant for Hg(0)→Hg(2)	1 / day
First-order transformation rate constant for MHg→Hg(2)	1 / day
First-order transformation rate constant for Hg(0)→MHg	1 / day
First-order transformation rate constant for Hg(2)→MHg	1 / day
First-order transformation rate constant for Hg(2)→Hg(0)	1 / day
First-order transformation rate constant for MHg→Hg(0)	1 / day
Assimilation efficiency for inhalation for Hg(0)	unitless
Assimilation efficiency for inhalation for Hg(2)	unitless
Assimilation efficiency for inhalation for MHg	unitless
Semiaquatic Omnivore - Mallard	
First-order transformation rate constant for Hg(0)→Hg(2)	1 / day
First-order transformation rate constant for MHg→Hg(2)	1 / day
First-order transformation rate constant for Hg(0)→MHg	1 / day
First-order transformation rate constant for Hg(2)→MHg	1 / day
First-order transformation rate constant for Hg(2)→Hg(0)	1 / day
First-order transformation rate constant for MHg→Hg(0)	1 / day
Assimilation efficiency for inhalation for Hg(0)	unitless
Assimilation efficiency for inhalation for Hg(2)	unitless

Input Parameter	Units
Assimilation efficiency for inhalation for MHg	unitless
Terrestrial Predator/Scavenger - Red-tailed Hawk	
First-order transformation rate constant for Hg(0)→Hg(2)	1 / day
First-order transformation rate constant for MHg→Hg(2)	1 / day
First-order transformation rate constant for Hg(0)→MHg	1 / day
First-order transformation rate constant for Hg(2)→MHg	1 / day
First-order transformation rate constant for Hg(2)→Hg(0)	1 / day
First-order transformation rate constant for MHg→Hg(0)	1 / day
Assimilation efficiency for inhalation for Hg(0)	unitless
Assimilation efficiency for inhalation for Hg(2)	unitless
Assimilation efficiency for inhalation for MHg	unitless
Terrestrial Insectivore - Tree Swallow	
First-order transformation rate constant for Hg(0)→Hg(2)	1 / day
First-order transformation rate constant for MHg→Hg(2)	1 / day
First-order transformation rate constant for Hg(0)→MHg	1 / day
First-order transformation rate constant for Hg(2)→MHg	1 / day
First-order transformation rate constant for Hg(2)→Hg(0)	1 / day
First-order transformation rate constant for MHg→Hg(0)	1 / day
Assimilation efficiency for inhalation for Hg(0)	unitless
Assimilation efficiency for inhalation for Hg(2)	unitless
Assimilation efficiency for inhalation for MHg	unitless
Terrestrial Herbivore - Meadow Vole	
First-order transformation rate constant for Hg(0)→Hg(2)	1 / day
First-order transformation rate constant for MHg→Hg(2)	1 / day
First-order transformation rate constant for Hg(0)→MHg	1 / day
First-order transformation rate constant for Hg(2)→MHg	1 / day
First-order transformation rate constant for Hg(2)→Hg(0)	1 / day
First-order transformation rate constant for MHg→Hg(0)	1 / day
Assimilation efficiency for inhalation for Hg(0)	unitless
Assimilation efficiency for inhalation for Hg(2)	unitless
Assimilation efficiency for inhalation for MHg	unitless
Terrestrial Herbivore - Long-tailed Vole	
First-order transformation rate constant for Hg(0)→Hg(2)	1 / day
First-order transformation rate constant for MHg→Hg(2)	1 / day
First-order transformation rate constant for Hg(0)→MHg	1 / day
First-order transformation rate constant for Hg(2)→MHg	1 / day
First-order transformation rate constant for Hg(2)→Hg(0)	1 / day
First-order transformation rate constant for MHg→Hg(0)	1 / day
Assimilation efficiency for inhalation for Hg(0)	unitless
Assimilation efficiency for inhalation for Hg(2)	unitless
Assimilation efficiency for inhalation for MHg	unitless
Terrestrial Predator/Scavenger - Long-tailed Weasel	
First-order transformation rate constant for Hg(0)→Hg(2)	1 / day
First-order transformation rate constant for MHg→Hg(2)	1 / day
First-order transformation rate constant for Hg(0)→MHg	1 / day
First-order transformation rate constant for Hg(2)→MHg	1 / day
First-order transformation rate constant for Hg(2)→Hg(0)	1 / day

Input Parameter	Units
First-order transformation rate constant for MHg→Hg(0)	1 / day
Assimilation efficiency for inhalation for Hg(0)	unitless
Assimilation efficiency for inhalation for Hg(2)	unitless
Assimilation efficiency for inhalation for MHg	unitless
Semiaquatic Omnivore - Mink	
First-order transformation rate constant for Hg(0)→Hg(2)	1 / day
First-order transformation rate constant for MHg→Hg(2)	1 / day
First-order transformation rate constant for Hg(0)→MHg	1 / day
First-order transformation rate constant for Hg(2)→MHg	1 / day
First-order transformation rate constant for Hg(2)→Hg(0)	1 / day
First-order transformation rate constant for MHg→Hg(0)	1 / day
Assimilation efficiency for inhalation of Hg(0)	unitless
Assimilation efficiency for inhalation of Hg(2)	unitless
Assimilation efficiency for inhalation of MHg	unitless
Terrestrial Omnivore - White-footed Mouse	
First-order transformation rate constant for Hg(0)→Hg(2)	1 / day
First-order transformation rate constant for MHg→Hg(2)	1 / day
First-order transformation rate constant for Hg(0)→MHg	1 / day
First-order transformation rate constant for Hg(2)→MHg	1 / day
First-order transformation rate constant for Hg(2)→Hg(0)	1 / day
First-order transformation rate constant for MHg→Hg(0)	1 / day
Assimilation efficiency for inhalation for Hg(0)	unitless
Assimilation efficiency for inhalation for Hg(2)	unitless
Assimilation efficiency for inhalation for MHg	unitless
Terrestrial Herbivore - Mule Deer/Black-tailed Deer	
First-order transformation rate constant for Hg(0)→Hg(2)	1 / day
First-order transformation rate constant for MHg→Hg(2)	1 / day
First-order transformation rate constant for Hg(0)→MHg	1 / day
First-order transformation rate constant for Hg(2)→MHg	1 / day
First-order transformation rate constant for Hg(2)→Hg(0)	1 / day
First-order transformation rate constant for MHg→Hg(0)	1 / day
Assimilation efficiency for inhalation for Hg(0)	unitless
Assimilation efficiency for inhalation for Hg(2)	unitless
Assimilation efficiency for inhalation for MHg	unitless
Terrestrial Herbivore - White-tailed Deer	
First-order transformation rate constant for Hg(0)→Hg(2)	1 / day
First-order transformation rate constant for MHg→Hg(2)	1 / day
First-order transformation rate constant for Hg(0)→MHg	1 / day
First-order transformation rate constant for Hg(2)→MHg	1 / day
First-order transformation rate constant for Hg(2)→Hg(0)	1 / day
First-order transformation rate constant for MHg→Hg(0)	1 / day
Assimilation efficiency for inhalation for Hg(0)	unitless
Assimilation efficiency for inhalation for Hg(2)	unitless
Assimilation efficiency for inhalation for MHg	unitless
Semiaquatic Omnivore - Raccoon	
First-order transformation rate constant for Hg(0)→Hg(2)	1 / day
First-order transformation rate constant for MHg→Hg(2)	1 / day

Input Parameter	Units
First-order transformation rate constant for Hg(0)→MHg	1 / day
First-order transformation rate constant for Hg(2)→MHg	1 / day
First-order transformation rate constant for Hg(2)→Hg(0)	1 / day
First-order transformation rate constant for MHg→Hg(0)	1 / day
Assimilation efficiency for inhalation for Hg(0)	unitless
Assimilation efficiency for inhalation for Hg(2)	unitless
Assimilation efficiency for inhalation for MHg	unitless
Terrestrial Ground-Invertebrate Feeder - Short-tailed Shrew	
First-order transformation rate constant for Hg(0)→Hg(2)	1 / day
First-order transformation rate constant for MHg→Hg(2)	1 / day
First-order transformation rate constant for Hg(0)→MHg	1 / day
First-order transformation rate constant for Hg(2)→MHg	1 / day
First-order transformation rate constant for Hg(2)→Hg(0)	1 / day
First-order transformation rate constant for MHg→Hg(0)	1 / day
Assimilation efficiency for inhalation for Hg(0)	unitless
Assimilation efficiency for inhalation for Hg(2)	unitless
Assimilation efficiency for inhalation for MHg	unitless
Terrestrial Ground-Invertebrate Feeder - Trowbridge Shrew	
First-order transformation rate constant for Hg(0)→Hg(2)	1 / day
First-order transformation rate constant for MHg→Hg(2)	1 / day
First-order transformation rate constant for Hg(0)→MHg	1 / day
First-order transformation rate constant for Hg(2)→MHg	1 / day
First-order transformation rate constant for Hg(2)→Hg(0)	1 / day
First-order transformation rate constant for MHg→Hg(0)	1 / day
Assimilation efficiency for inhalation for Hg(0)	unitless
Assimilation efficiency for inhalation for Hg(2)	unitless
Assimilation efficiency for inhalation for MHg	unitless
PLANTS - TERRESTRIAL	
Leaf	
First-order transformation rate constant for Hg(0)→Hg(2)	1 / day
First-order transformation rate constant for Hg(2)→MHg	1 / day
First-order transformation rate constant for MHg →Hg(2)	1 / day
Washout ratio Hg(2) vapor	unitless
Washout ratio Hg(0) vapor	unitless
Washout ratio Hg particulate	unitless
Root	
Alpha for root ↔ root-zone soil	unitless
t_{alpha}	day
Dry root/root-zone-soil partition coefficient	mg / kg per mg / kg
Stem	
Transpiration stream concentration factor	kg / m^3 per kg / m^3
Leaf Surface	
Transfer factor from leaf to leaf surface (Hg)	1 / day
Transfer factor from leaf surface to leaf (Hg particle)	1 / day

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APPENDIX E
Prototypes I - IV

This appendix provides a description of the process of applying the TRIM.FaTE methodology (Chapter 4) to cases of increasing complexity (referred to as "prototypes"). Section 1 discusses the computer implementation of the prototypes; Section 2 describes the development process for each prototype; Section 3 addresses the features of the prototypes, including the types of compartments and links simulated; and Section 4 discusses the chemical-specific parameters and values used in prototype 4. The goals of this appendix are to: (1) illustrate the flexibility of TRIM.FaTE for application at different levels of spatial and temporal resolution; (2) illustrate how different multimedia configurations with TRIM.FaTE are set up; and (3) document the historical development of TRIM.FaTE leading up to Prototype V.

E.1 COMPUTER IMPLEMENTATION OF PROTOTYPES

The concepts discussed in Chapter 4 have been implemented in all the prototypes using a combination of Microsoft Visual Basic™, Fortran, and Microsoft Excel™ software. An object-oriented architecture was implemented using Visual Basic 5 application environment imbedded within Excel 97 to model the hierarchy of components of TRIM.FaTE. This hierarchy includes volume elements, compartment types, compartments, links, and sources. The coding architecture is not tied to any specific ecosystem configuration. A preliminary algorithm library that utilized this coding architecture was also implemented.

If all transport processes are simulated as a first-order process, the result is a system of linear ordinary differential equations, as explained in Section 4.2. This system must be solved to determine the redistribution of chemical mass as a function of time. For TRIM.FaTE, this system is solved using the Livermore Solver for Ordinary Differential Equations (LSODE) (Radhakrishnan and Hindmarsh 1993), a Fortran program freely available via several online numerical algorithm repositories.

The LSODE subroutine solves systems of first-order ordinary differential equations of the form (Hindmarsh 1983):

$$d\mathbf{y}/dt = F(t,\mathbf{y}),\ \mathbf{y}(t_0) = \mathbf{y}_0$$

where y is an n-dimensional time-dependent vector, *i.e.*,

$$\mathbf{y}(t) = [y_1(t), y_2(t), ..., y_n(t)].$$

The system of differential equations can be stiff or non-stiff. In the stiff case, it treats the Jacobian matrix (Schneider and Barker 1989) as either a full or banded matrix. It uses Adams (Schneider and Barker 1989) methods (predictor-corrector) in the non-stiff case, and backward differentiation formula methods in the stiff case. The linear systems that arise are solved by direct methods. LSODE supersedes the older GEAR and GEARB packages.

The only restriction on the size of the system of differential equations is that imposed by computer memory. This code was modified so that it could be accessed by Visual Basic 5 in Excel 97. Another Fortran code was used, in a similar manner, to determine the steady-state solution to the system of linear differential equations (Barrodole and Stuart 1981).

Microsoft Excel spreadsheets were used for general preprocessing, postprocessing, and data storage (additional databases for spatial data were also created using Visual Basic and accessed by Excel). Excel spreadsheets also served as a convenient interface to the Visual Basic and Fortran subroutines.

The approach taken for testing the methodology made it possible to investigate the implications of draft algorithms and to work on the development of a flexible system for addressing conceptual site models with many compartments. The pre- and postprocessing for the ultimate implementation of TRIM.FaTE may require a more sophisticated platform. However, with some modification, much of the Visual Basic code, and all of the Fortran code, can be used in other computer programming languages.

E.2 PROTOTYPE DEVELOPMENT

Multiple prototypes were developed with increasing complexity to model the movement of a chemical through an ecosystem. This section describes features of the prototypes in increasing order of complexity.

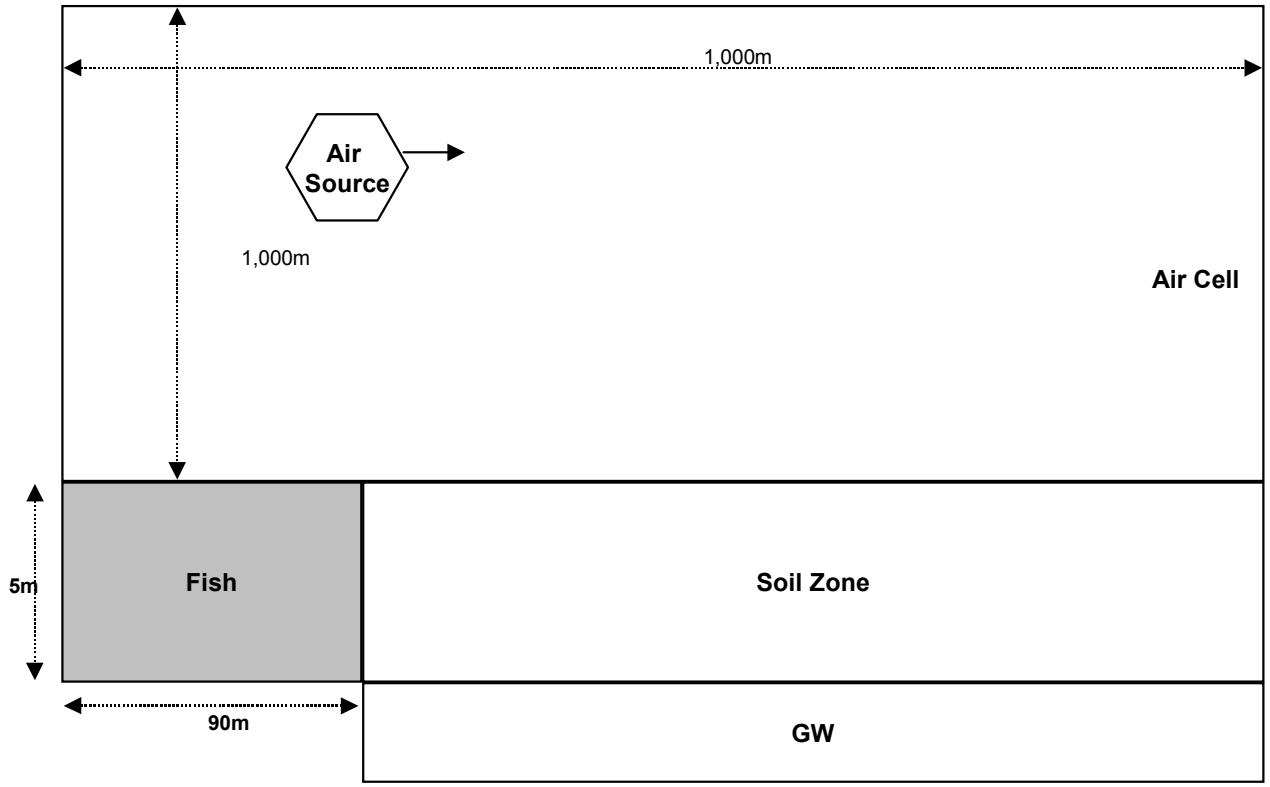
E.2.1 PROTOTYPE I

Prototype I (P1) was designed to test the mass transfer methodology (Section 4.2) and the LSODE utility. Air, surface, soil, ground water, surface water, and fish compartment types were simulated in P1 as illustrated in the conceptual site model shown in Figure E-1. P1 includes a uniform volume source emission of benzene into the air compartment volume. Benzene was selected because most of its transfer factors were readily available from CalTOX (Maddalena et al. 1995).

Some transfer factors were derived independently of CalTOX for the air to air sink, soil to ground water, fish to water, and water to fish transfers. The remaining factors were taken directly from CalTOX. The dimensions of the terrain were adapted from CalTOX to facilitate comparison of results. Chemical reaction was not simulated in this prototype.

The runs produced estimates of benzene mass throughout the system, and no problems were experienced in running the LSODE subroutine. The resulting mass distribution of benzene in various compartments was examined qualitatively to ensure that the numerical routines were producing stable and realistic solutions. A quantitative analysis of the results was not performed because the input parameters were selected only to test the implementation infrastructure. The results were approximately commensurate with theoretical expectations with no unstable or anomalous values. These results prompted further testing of the modeling approach on a more complex ecosystem.

Figure E-1
Conceptual Site Model for Prototype I



E.2.2 PROTOTYPE II

Prototype II (P2) includes more spatial detail sophistication than P1 in both the types and number of compartments used. Unlike P1, P2 included multiple volume elements for both the soil and air compartment types and included the use of plant and sediment compartments. In addition, the links between compartments had multiple-phase (*i.e.*, gas, liquid, and solid) mass transfers. P2 included a volume source emission of benzo(a)pyrene (B[a]P) into only one of the air compartment volumes. This made possible a very simple representation of spatial transport. B(a)P was selected as a test chemical for this and subsequent prototypes because of its persistence in the environment and because it is a HAP (a chemical of concern in the CAA). The derivation of the transfer factors is described in detail in the second volume of this document. The conceptual site model for P2 is shown in Figure E-2.

Multiple-phase (liquid, gas, and solid) transport within a compartment was introduced in P2. The phases are assumed to be at chemical equilibrium, with the ratios of the concentrations in the individual phases constant.

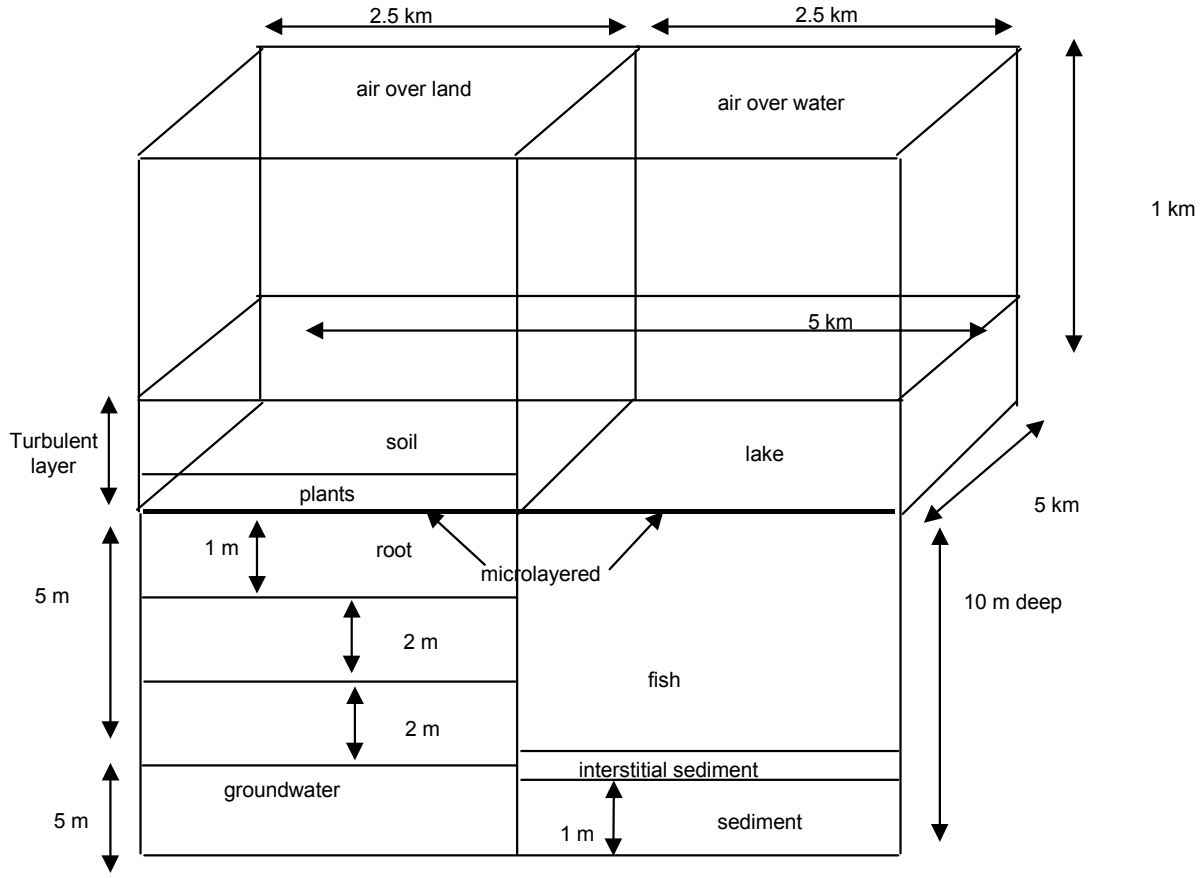
P2 was run for four different conditions that included constant source terms under pristine conditions, an artificially lower organic carbon partioning coefficient (K_{oc}) value for B(a)P, a constant source term with non-pristine conditions in surface water, and a time-varying source-term condition. In all cases, under steady-state conditions, most of the B(a)P accumulated in the plants, with minimal penetration into the subsurface. In the water column, most of the B(a)P was found in the sediment sink, with minimal accumulation seen in the fish compartment. Decrease of the K_{oc} value resulted in corresponding increase in mass in subsurface soil. Only the air compartment type seemed to be responsive to the varying source-term condition.

The transfer factors and steady-state outputs of P2 were compared to runs performed on CalTOX (Maddalena et al. 1995). Most of the transfer factors used in P2 were very similar to those in CalTOX; the mass distributions of B(a)P were similar in air, soil, and surface water compartments and differed by three orders of magnitude in plant, sediment, and ground water (aquifer) compartments. This led to refinement of the TRIM.FaTE algorithms for plant and sediment compartment types. The difference in the ground water masses was due to the fact that both TRIM and CalTOX have a simple approximations to model transport in ground water.

E.2.3 PROTOTYPE III

Prototype III (P3) focuses on code and input data structure refinements because the code and input data are significantly more complex than either P1 or P2. P3 was developed both to incorporate lessons learned from P2, which has a refined set of abiotic algorithms, and to set up the TRIM.FaTE model for the case study model run Prototype IV (P4). P3 includes a conceptual site that approaches the spatial scale (approximately 10-kilometer [km] radius) of the ecosystem used for the testing the full prototype (P4). The conceptual site model for P3 is shown in Figure E-3. The vertical dimensions of individual air compartments are not indicated because these dimensions were allowed to vary with time according to a set of specified meteorological conditions. The soil and surface water compartments were split into finer grid structures relative to P2, and several new biotic algorithms were added. The source term simulated in P3 was a

Figure E-2
Conceptual Site Model for Prototype II



volume-source emission of B(a)P into only one of the four air compartments. This was used to make an approximation to a continuous point-source release.

The differences of P3 relative to P2 include:

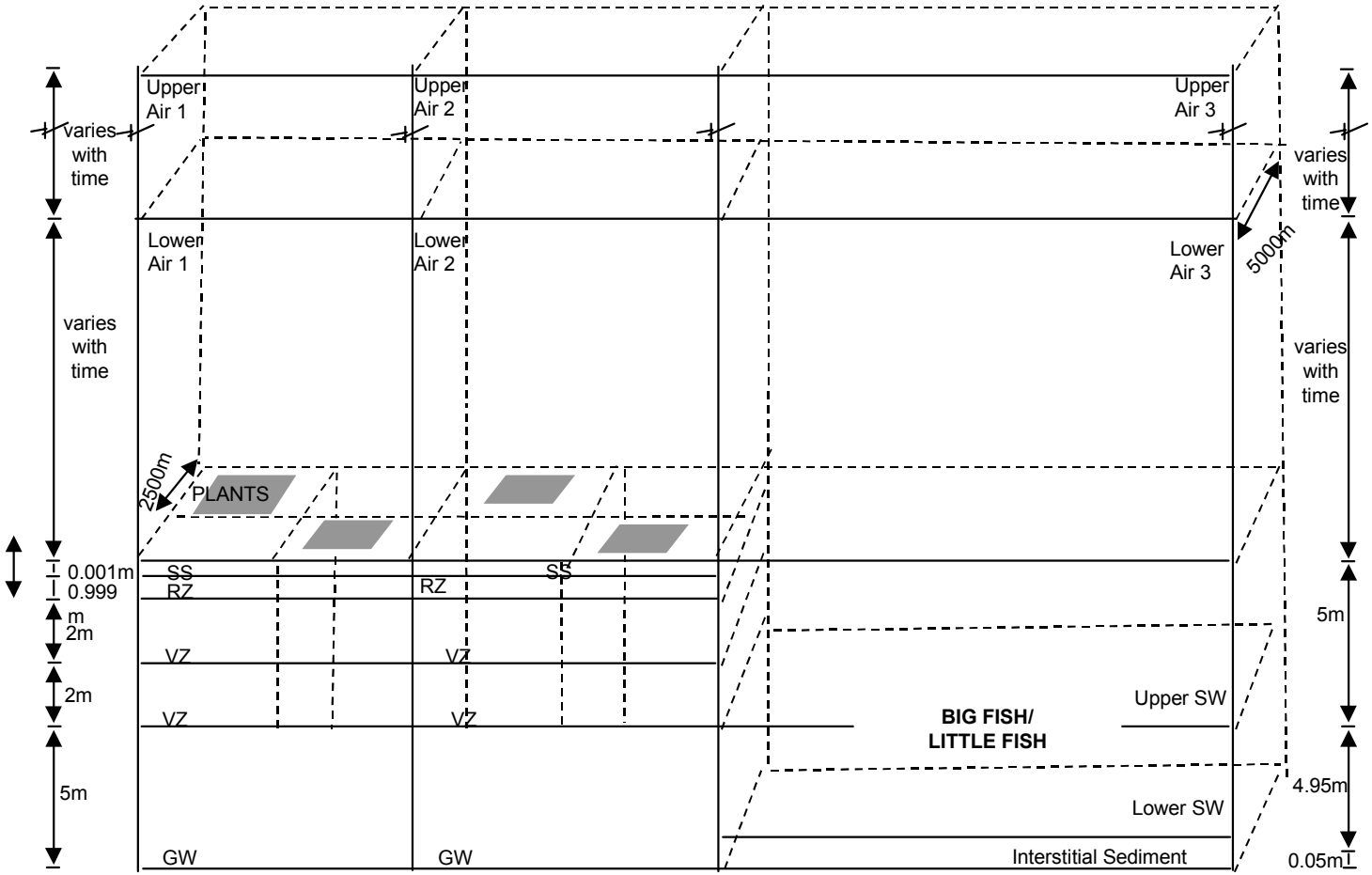
- Addition of terrestrial earthworm, kingfisher, and mouse compartment types;
- Addition of aquatic food-web system;
- Addition of macrophyte compartment type;
- Addition of compartments with varying heights for air;
- Division of soil compartments horizontally;
- Introduction of "thermoclines" and refinement of mixing for surface water;
- Refinement of plant algorithms;
- Refinement of soil diffusion algorithms;
- Addition of erosion in the soil compartment types;
- Refinement of ground water algorithm;
- Introduction of flexible code design; and
- Introduction of temporal variation for a few key input parameters.

As in the case of P2, several runs were performed for P3. The results showed that the plant, macrophyte, and sediment compartments are major sinks of B(a)P in the environment. The model showed that B(a)P mass distribution in the environment is sensitive to total macrophyte volume in the water column. The model results were extremely responsive in most compartments to varying source-term conditions. Comparisons of P3 outputs with CalTOX outputs showed that B(a)P mass distributions in the ecosystem being simulated were in closer agreement than was seen in the case of P2. This was believed to be a result of refining the algorithms as previously stated and implied that the prototype was appropriate for application to a more complicated test case.

E.2.4 PROTOTYPE IV

Whereas P1 through P3 used generic inputs and were intended for evaluation simulations, P4 was designed to be applied to an actual site. P1 through P3 were used to develop and test the TRIM.FaTE algorithms. P4 was developed and used to illustrate and evaluate the likely limits of TRIM.FaTE with respect to the number of land parcels and length of time steps used. This prototype had the shortest plausible time step (1 hours), a large number of land units in the planar view (20 parcels), and 21 different biotic compartment types. This level of detail resulted in several hundred compartments, including abiotic and biotic compartments, and the sinks necessary to account for transformation and transport losses outside of the system boundary. To test the model using a realistic ecosystem, P4 was applied to an area in the northwestern region of the United States.

Figure E-3
Conceptual Site Model for Prototype III



E.3 PROTOTYPE FEATURES

The specific features modeled in the prototypes are discussed in this section. Section 3.1 presents the abiotic compartment types modeled; Section 3.2 includes the biotic compartment types modeled; and Section 3.3 discusses the abiotic and biotic links associated with the prototypes.

E.3.1 ABIOTIC COMPARTMENTS

In P1 (Figure E-1), the air, soil, and surface water each consist of a single volume element and compartment. Ground water was simulated simply as a sink to the soil compartment. P2, as shown in Figure E-2, divides the air into four volume elements (two upper air and two lower air layers); divides the soil into four volume elements (surface soil, root zone, and vadose zones one and 2); and simulated ground water, surface water, and sediment as single volume elements. In P3, (Figure E-3) the air consists of six volume elements (two lower air and two upper air over soil, and a lower air and upper air over surface water); the soil was divided into 32 volume elements (eight surface soil, eight root zone, eight vadose zone 1, and eight vadose zone 2); ground water and surface water were both simulated with two volume elements; and sediment was simulated as a single volume element. P4 simulates 129 abiotic volume elements. Parcels were defined in P4 and divided vertically based on compartment type. The 129 abiotic compartments associated with the parcels in P4 are summarized in Table E-1.

E.3.2 BIOTIC COMPARTMENTS

In P1 and P2, a single fish species is modeled and only uptake and loss of chemical through the gills is simulated. In the transition to P3 and P4, the number of biotic water column compartments was expanded from a single fish species to an aquatic food web represented by several feeding trophic levels (compartment types). Bioaccumulation by herbivores, as well as omnivores and carnivores, is accommodated within the P3 and P4 simulations. It is important to note, however, that the trophic level representations were simplified to reflect primary uptake and loss from a single representative species from each trophic level.

Both P3 and P4 include terrestrial wildlife as compartments. Wildlife may be exposed to chemicals through food, soil, and water ingestion, and through inhalation of chemicals in air. Elimination of chemicals from body tissues may occur through metabolic breakdown of the chemical and excretion through urine, feces, milk (mammals only), and eggs (birds only). Terrestrial and semiaquatic biota were not considered in P1 and P2. Two species were introduced in P3: a white-footed mouse (*Peromyscus leucopus*) and the belted kingfisher (*Ceryle alcyon*). These species were selected because they are taxonomically dissimilar (mammal versus bird) and represent differing compartment types (terrestrial omnivore and semiaquatic piscivore, respectively). P4 simulated a more complex terrestrial, aquatic, and semiaquatic system, as summarized in Table E-2.

Table E-1
Types of Abiotic Compartments and Number of Volume Elements Modeled

Compartment Type	Number of Volume Elements[a]			
	P1	P2	P3	P4
Air	1 - Air	2 - Upper Air Layer 2 - Lower Air Layer	3 -Upper Air Layer 3 - Lower Air Layer	20 -Upper Air Layer 20 - Lower Air Layer
Soil	1 - Soil (general) 1 - Ground water	1 - Surface Soil 1 - Root Zone 1 - Vadose Zone 1 1 - Vadose Zone 2 1 - Ground water	8 - Surface Soil 8 - Root Zone 8 - Vadose Zone 1 8 - Vadose Zone 2 2 - Ground water	14 - Surface Soil 14 - Root Zone 14 - Vadose Zone 1 14 - Vadose Zone 2 14 - Ground water
Surface Water	1 - Surface Water	1 - Surface Water	1 - Upper Surface Water Layer 1 - Lower Surface Water Layer	1 - Upper Lake Layer 1 - Lower Lake Layer 5 - River Segments
Sediment	NA	1 - Interstitial Water 1 - Sediment	1 - Interstitial Water 1 - Sediment	6 - Interstitial Water 6 - Sediment
TOTAL NUMBER	**4 Volume Elements**	**12 Volume Elements**	**44 Volume Elements**	**129 Volume Elements**

[a] Reaction and advection sinks are not listed in this table.

Table E-2
Biotic Compartments Modeled

Compartment	P1	P2	P3	P4
Aquatic Ecosystem	Single Fish Species	Single Fish Species	• Macrophytes (Benthic Herbivores) • Aquatic Herbivores • Aquatic Omnivores • Aquatic Carnivores	• Macrophytes (Benthic Herbivores) • Mayfly (Benthic Herbivores) • Bluegill (Modeled as Herbivore) • Channel Catfish (Omnivore) • Bass (Carnivore) • Mallard (Herbivore) • Raccoon (Omnivore) • Tree Swallow (Insectivore)
Terrestrial Ecosystem	NA	NA	• White-footed Mouse (Omnivore) • Earthworm (Soil Detritovore) • Plant Leaves, Roots, Xylem and Stem	• White-footed Mouse (Omnivore) • Earthworm (Soil Detritovore) • Black-capped Chickadee (Insectivore) • Red-tailed Hawk (Predator) • Long-tailed Weasel (Predator) • Black-tailed Deer (Herbivore) • Long-tailed Vole (Herbivore) • Mink (Piscivore) • Trowbridge Shrew (Ground Invertebrate Feeder) • Insects • Plant Leaves, Roots, Xylem and Stem
Semi-Aquatic Ecosystem	NA	NA	• Belted Kingfisher (Piscivore)	• Belted Kingfisher (Piscivore) • Wetland Plant Leaves, Roots, Xylem and Stem

P3 and P4 also simulated pollutant transfer to earthworms. The concentration in earthworms was assumed to be in equilibrium with the solid, liquid, and vapor-phase concentrations of the chemical in the root zone compartments.

Plants were introduced to the TRIM.FaTE framework in P2. The plant component of the ecological model implemented for P2, P3, and P4 is comprised of leaves, roots, xylem, and stem. Plants are divided into these compartment types because: (1) the literature suggests that concentrations of non-ionic organic chemicals in foliage are primarily related to those in air and that concentrations in roots are generally related to those in soil (with stems serving as the conduit between the two), and (2) herbivores may eat part but not all of a plant. Each compartment type was assumed to be homogeneously-mixed. The plant algorithms implemented in P2 through P4 are applicable for mature plants only, and did not address plant growth.

E.3.3 LINKS

If mass can move from one compartment to another compartment without first moving through intervening compartments, then the two compartments are considered "linked." Each link is associated with an algorithm that determines the direction and rate of mass flow between the two compartments. Links may be between compartments in adjacent volume elements or compartments within a volume element. At a given spatial location, and within a single volume element, more than one compartment may exist and linkages may exist between these compartments.

Table E-3 shows examples of generalized links applied in P1 through P4. This table is generic and can be used in conjunction with Tables E-1 and E-2 to define a specific link. For example, in P2 through P4, transfer of a pollutant can occur from an upper air compartment to adjacent upper air compartments and to a lower air compartment. This is represented in Table E-3 by the air (sending compartment) to air (receiving compartment) link. A more complex example is the links associated with the kingfisher from the semi-aquatic ecosystem. As a receiving compartment, pollutant(s) can transfer to the kingfisher from air (*i.e.*, lower air), soil (*i.e.*, surface soil), surface water (*i.e.*, upper lake layer), and aquatic (*i.e.*, bluegill) ecosystems.

The links from sending compartments to sinks are not shown in Table E-3. Sinks refer to the compartments of pollutant mass leaving the modeled ecosystem through a reaction or physical process(es).

Table E-3
Examples of Links Associated with Compartments Types

Sending Compartment Types	Receiving Compartment Types
Air	Air Soil Surface Water Terrestrial Ecosystem Semi-aquatic Ecosystem
Soil	Air Soil Ground water Surface Water Terrestrial Ecosystem Semi-aquatic Ecosystem
Ground water	Ground water Surface Water
Surface Water	Surface Water Sediment Aquatic Ecosystem Semi-aquatic Ecosystem Terrestrial Ecosystem
Sediment	Surface Water Aquatic Ecosystem
Terrestrial Ecosystem	Terrestrial Ecosystem Air Soil
Aquatic Ecosystem	Aquatic Ecosystem Semi-aquatic Ecosystem Terrestrial Ecosystem Surface Water
Semi-aquatic Ecosystem	Terrestrial Ecosystem Air Soil Surface Water

E.4 PAH-SPECIFIC VALUES USED IN TESTING OF PROTOTYPE IV

This section discusses the testing approach for chemical specific parameters and values. More detailed descriptions of algorithms associated with many of the parameters discussed in this section can be found in TRIM.FaTE TSD Volume II.

E.4.1 TRANSFORMATION OF PAHs BY PLANTS

Metabolism in Plants

Few studies of metabolism of organic chemicals in plants exist. Exceptions include metabolism of: atrazine by poplar trees (Burken and Schnoor 1997); pentachlorophenol in soybean and spinach (Casterline et al. 1985); trichloroethylene in carrots, spinach, and tomatoes (Schnabel et al. 1997); PCBs in plants (reviewed in Puri et al. 1997); and bromacil, diclobenil, nitrobenzene, and 1,3-dinitrobenzene in soybean plants and barley roots. Metabolic rate constants were only calculated in the first paper. Investigations of the metabolism of polycyclic aromatic hydrocarbons in plants include: metabolism of phenanthrene and anthracene by tomato and wheat (Harms 1996), metabolism of anthracene and benz[a]anthracene in bush bean (Edwards 1988), metabolism of anthracene by soybean (Edwards et al. 1982), metabolism of anthracene in bush bean (Edwards 1986), and metabolism of various PAHs by bush bean (in progress, T. McKone, personal communication, August 1997). The first two papers are somewhat useful for the calculation of a metabolic rate constant, and the ongoing study by McKone may prove most useful when completed. Unfortunately, the two papers are dynamic studies with PAH taken up through the soil and air and degraded gradually, perhaps at a first-order rate, and with metabolites present in the nutrient solution that could also be taken up.

Thus, it is difficult to calculate the metabolic rate constant. Harms (1996) provides radioactivity (percentage of applied) of parent compound (phenanthrene or anthracene) and metabolites in culture medium; parent compound, metabolites, and nonextractable residue in shoots; and parent compound, metabolites, and nonextractable residue in roots after five days of exposure. If it is assumed that a) non-extractable residues reflect the measured proportion of parent compound to metabolite, b) metabolites produced in aseptic culture medium were produced by roots rather than by shoots, c) metabolites did not move between plant organs, and d) that most of the measured parent compound was in the plant for the majority of the five days (the rate of uptake may have been rapid because of the application of phenanthrene in liposomes), a simple calculation of a first-order metabolic rate constant can be made. (Although these are poor assumptions, it is notable that the order of magnitude variability in rate constants for metabolism of phenanthrene in shoots of two plant species (below) is probably greater than errors associated with the above assumptions.)

Thus, a calculation of a lower bound on the first-order metabolic rate constant can be made. The equation used is $\ln (N/N_0) = -kt$, where N is the radioactivity of the metabolite pool after five days and N_0 is the sum of the radioactivity of the parent compound pool and metabolite pool after five days (assumed to be the total radioactivity of the parent compound in the plant close to the beginning of the experiment). If the calculation is made, the rate constants are: 0.008/d for phenanthrene in tomato leaf and stem, 0.08/d for phenanthrene in wheat leaf and stem, 0.24/d for phenanthrene in tomato root, and 0.28 for phenanthrene in wheat root. The half-lives range from 2.5 to 90 days.

Similarly, a calculation of a lower bound on the first-order metabolic rate constant for benzo(a)pyrene can be made using results from uptake and metabolism of benz(a)anthracene by bush beans in nutrient solution (Edwards 1988). The PAH was added continually to solution to

maintain a constant concentration. In a previous experiment it was determined that most of the benz(a)anthracene absorbed by roots was taken up within one day. After 30 days 25 percent of the radioactivity was parent compound and 14 percent was in the form of metabolites; the distribution of the parent compound and metabolites in the plant is presented in the paper. Using the same assumptions as above, low estimates of the rate constants are: 0.015/d for benzo(a)pyrene in root, 0.19/d for the PAH in stem and 0.12/d for the chemical in foliage.

Randy Maddalena and Tom McKone of Lawrence Berkeley Laboratory investigated the uptake of anthracene, fluoranthene, phenanthrene, and pyrene from air by leaves of bushy beans. The following calculation is based on a personal communication from Tom McKone in September 1997. These compounds appear to have reaction rates on the order of 0.1 to 0.3 /day (half-life of three to 10 days) and thus are somewhat higher than the low estimate of the rate constant for phenanthrene metabolism in leaves described above.

It is expected that metabolism in plants is estimated within an order of magnitude in TRIM.FaTE. The parameters in Table E-4 should be used for phenanthrene and benzo(a)pyrene or as defaults for other PAHs. Different numbers may be chosen in the future as additional information is obtained. As the root and leaf compartment types are connected, the rate constant for the stem is likely to change.

Table E-4
First-order Metabolic Rate Constants (d^{-1})

Chemical	root	stem	leaf
Phenanthrene	0.3	0.08	0.2
Benzo(a)pyrene	0.02	0.2	0.2

Photolysis on the Plant Surface

The process of photolysis on the plant surface was not implemented in the PAH test case of TRIM.FaTE because the leaf and leaf surface were not separate compartment types. In future runs of the model for PAHs, photolysis on the leaf surface may be included. Few investigations of the photolysis of contaminants on plant foliage have been undertaken. An exception is the photodegradation of 2,3,7,8-tetrachlorodibenzodioxin sorbed to grass foliage (k = 0.0156 hr-1). It is assumed that photolysis of organic contaminants on the leaf surface occurs at a rate that is somewhat less than that of PAHs sorbed to particulate matter in air; PAHs on leaves are probably exposed to a lower light intensity than those in air. Thus, the rate constant on leaf surfaces is assumed to be one-half of the rate constant of photolysis of PAHs on particulates in air. Kamens et al. (1987) provides measurements of the rate constant for benzo(a)pyrene when the chemical is present at a loading of 30 to 350 ng/mg particulates (0.0211 min^{-1}) and when the PAH is present at a loading of 1000 to 2000 ng/mg particulates (0.009 min^{-1}). Their more general equation for determining the rate constant (in min^{-1}) for the 30 to 350 ng/mg loading case is:

$$\ln k = -1.355 - 1.279(1/T) + 0.831(\ln(I)) + 0.816(\ln[H2O]),$$

where:

I = the average solar intensity (cal/cm^2/min)
[H2O] = water vapor concentration in g/m^3

Kamens et al. (1987) have not investigated photolysis of 3-ringed PAHs such as phenanthrene. Behymer and Hites (1988) suggest that photolysis is independent of PAH structure for substrates with a carbon content greater than five percent. In an experiment in which fifteen fly-ash substrates were irradiated using a mercury vapor lamp (17.6 W/m^2), they investigators measured photolytic rate constants for phenanthrene ranging from <0.00069 hr^{-1} to 0.0050 hr^{-1}, with a mean of 0.0019 hr^{-1}. The mean rate constant for benzo(a)pyrene was measured at 0.0035 hr^{-1}. Thus, this measurement is more than an order of magnitude lower than the numbers in the Kamens study (note that they are presented in min^{-1}).

Without knowledge of solar intensity (and with lots of uncertainty), the following rates are suggested for photolysis of contaminants on a leaf surface during the daytime hours: 0.03 hr-^{1} for benzo(a)pyrene and 0.001 hr^{-1} for phenanthrene.

E.4.2 DISTRIBUTION, ELIMINATION, AND TRANSFORMATION OF PAHs IN WILDLIFE

The toxicological literature was reviewed to identify models or parameters to describe the absorption, metabolism, and excretion of phenanthrene in both avian and mammalian species. No data were found to describe the toxicokinetics of phenanthrene in birds. Although models to describe the toxicokinetics of phenanthrene in mammals were not found, data suitable for estimating absorption, metabolism, and excretion rates following oral exposure were available. These data, and rate estimates developed from them, are outlined below. Phenanthrene appears to be readily absorbed, metabolized, and eliminated by mammals. Rahman et al. (1986) orally dosed rats with single one mg dose radiolabeled phenanthrene. Eight hours post dose, 72.74 percent of the initial radio label dose had been recovered in bile or urine, suggesting an assimilation efficiency of approximately 73 percent.

Chang (1943) orally exposed rats to an experimental diet containing one percent phenanthrene and by oral gavage of 11 or 13 mg phenanthrene. Amount of parent compound excreted in feces was measured. Because excretion rates were comparable regardless of the mode of exposure, results from both dietary and gavage exposure were pooled. Rats excreted four to seven percent (mean equals 5.75 percent) of the original dose. Conclusions from this study are limited by the small sample size used in limited description of the methods employed.

Chu et al. (1992) exposed both rats and guinea pigs to doses of radiolabeled phenanthrene of 10 mg/kg/d via gavage. After 48 hours, rats and guinea pigs had excreted 52 percent and 47 percent of the initial radiolabel. In rats, 90 percent of the excreted radiolabel was in urine and 10 percent in feces; among guinea pigs, 95 percent of the excreted radiolabel was in urine and five percent in feces . Of the radiolabel in the urine both species, 95.8 percent and 95.7 percent consisted of metabolites of phenanthrene and 4.2 percent and 4.3 percent of unmetabolized phenanthrene in rats and guinea pigs, respectively.

Female rats were orally or dermally exposed to phenanthrene, either as phenanthrene alone or as phenanthrene adsorbed to sandy or clay soil (Kadry et al. 1995). Absorption was greatest for pure phenanthrene as compared to phenanthrene adsorbed to soil. Percent absorption of the initial dose ranged from 55.7 percent to 65.3 percent and 0.7 percent to one percent for oral and dermal pathways, respectively. After 72 hours, 47.6 percent to 52.4 percent of the initial oral dose was recovered in urine; 27.8 percent to 22.1 percent was recovered in feces. After 96 hours, 36.2 percent to 48.4 percent of the initial dermal dose was recovered in urine; 8.6 percent to 14 percent was recovered in feces.

The results of these studies are listed and summarized in Table E-5. From these data, the mean excretion (E_u), metabolic (E_m), and absorption efficiencies for phenanthrene are 3.2 percent, 63.4 percent, and 33.8.0 percent, respectively. The first-order rate constants for metabolism range from 0.1 day^{-1} to one day^{-1}. Because no data were found for assimilation for water, soil, or food, assimilation via all pathways is assumed to be equal, *e.g.*, $A_a=A_w=A_s=A_s$. Because no data were found concerning uptake and elimination of phenanthrene by birds, parameters developed for mammals should be used. Due to physiological differences between birds and mammals, use of mammalian values for birds will contribute significant uncertainty to the final tissue residue estimate.

No studies data were found to enumerate elimination of phenanthrene via lactation (E_l) or elimination via egg production (E_e). However, transfer of contaminants from the diet to milk or eggs may be estimated using models reported in Travis and Arms (1988) and McKone (1993a, 1993b, 1993c).

E.4.3 UPTAKE OF PAHs BY BENTHIC INFAUNA

Uptake of PAHs is based on the water to benthic infauna transfers presented in Section 7.3.2.1 of TSD Volume II. Uptake of contaminants from water is primarily based on respiratory processes. (Stehly et al. 1990) have found that the clearance rate of B(a)P and phenanthrene from water by the mayfly is analogous to the clearance rate of oxygen during respiration. The uptake of these two PAHs can, therefore, be estimated similarly to the ratio of oxygen clearance to the volume of water passing over respiratory surfaces. With a known or assumed volume of water passing over respiratory membranes with known concentrations of B(a)P and phenanthrene, the extraction efficiency of these PAHs can be calculated. Generic algorithms in Section 7.4.2.1 of TSD Volume II were adapted from Stehly et al. (1990) for estimating PAH uptake and loss within the benthic invertebrate, based on the clearance rate driven by the volume of water cleared and the bioaccumulation factor (BCF). Uptake rates, as measured by a clearance rate constant, as well as the bioconcentration factor for 30, 60, and 120-day-old mayflies for B(a)P and phenanthrene, were provided by Stehly et al. (1990).

Table E-5
Summary of Assimilation, Metabolism, and Elimination Data for Phenanthrene

Percent of Total Dose Excreted as Phenanthrene or Metabolites (percent)	Days	First-order Excretion Rate (day^{-1})	Percent of Total Dose Metabolized[f] (percent)	First-order Metabolic Rate Constant (day^{-1})	Reference
72.74	0.33	3.9	69.68	3.6	Rahman et al. 1986
52[a]	2	0.37	49.82	0.34	Chu et al. 1992
47[b]	2	0.32	44.99	0.30	Chu et al. 1992
75.4[c]	3	0.47	72.23	0.43	Kadry et al. 1995
76.2[d]	3	0.48	73	0.44	Kadry et al. 1995
74[e]	3	0.45	70.9	0.41	Kadry et al. 1995

[a] rats
[b] guinea pigs
[c] pure phenanthrene
[d] phenanthrene adsorbed to sandy soil
[e] phenanthrene adsorbed to clay soil
[f] assumes that 95.8 percent of total excreted dose is not phenanthrene, based on Chu et al. (1992)

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APPENDIX F
TRIM.FaTE Computer Framework

The TRIM.FaTE computer framework provides the infrastructure required to conduct and analyze TRIM.FaTE simulations. The framework allow users to:

- Define the issue to be studied, including time period, geographic region, pollutants, media, and populations of interest;
- Specify and choose algorithms that will be used for simulations;
- Select modeling parameters, including emissions sources, characteristics of the environment (*e.g.*, air temperature and soil permeability), and simulation time step;
- Identify data sets to be used and created;
- Execute the simulation;
- Perform sensitivity studies; and
- Export results.

There are two versions of the framework: prototype and Version 1.0. The framework prototype has served as a testbed for evaluating approaches. It has been designed to allow changes to be quickly implemented and to allow ideas to be quickly tried. The prototype was used to conduct the simulations described in this document. Version 1.0 was completed September, 1999 and will be used for future studies. Version 1.0 incorporates lessons learned from Prototypes I through V with the addition of features that increase the usefulness of the system, such as management of multiple modeling scenarios, portability between Windows and UNIX, and improved ease of use and robustness.

This description of the TRIM.FaTE computer framework generally covers both the prototype and Version 1.0 with indications where necessary that descriptions apply to only one of the implementations. Additional information about the architecture and design of TRIM.FaTE Version 1.0 can be found in Fine et al. (1998a,1998b).

F.1 SOFTWARE ARCHITECTURE

Bass et al. (1998) provide the following definition:

> The software architecture of a program or computing system is the structure or structures of the system, which comprise software components, the externally visible properties of those components, and the relationships among them.

The prototypes and Version 1.0 have different architectures, so they are described separately.

F.1.1 ARCHITECTURE OF THE PROTOTYPES

The prototypes are implemented in an object-oriented manner, with almost all important quantities implemented as objects/classes. These include:

- parcels;
- volume elements;
- compartments;
- chemicals;
- links;
- algorithms;
- parameters (input parameters and calculated parameters);
- runs; and
- projects.

In the prototypes, a project is constructed in a hierarchical fashion: first a parcel is created, then volume elements can be added "to" the parcel, and then compartments can be added to the volume elements. Links can be created manually or can be automatically determined based on the spatial adjacency information of the project.

When a run is initiated, the needed transition matrices, source term vectors, and initial condition vector are constructed from the modeled system. This process utilizes the link topology and algorithms associated with each link, in addition to the source specified for particular compartments and the implied source terms calculated based on any boundary air concentrations specified. The transition matrices and associated source term and initial condition vectors are used in successive calls to the differential equation solver (*i.e.,* LSODE), after which the predicted chemical mass in each compartment is available.

An expression evaluator is also included within the design of the prototypes. This is used to evaluate almost all algorithms and other needed calculated quantities (*e.g.*, distribution coefficients in soil for organics, which are calculated from properties of the chemical and the soil compartment). The expressions themselves are stored as strings, using an object-oriented syntax consistent with the overall object model used. These expressions are "compiled" when a run is performed, with the objects needed to calculate each expression obtained for subsequent calculation. This allows flexible naming of variables and the creation of numerous intermediate terms that can help provide insight into the finer details of a particular run. Further, it significantly improves the quality of output reports that can be produced. For example, detailed reports can be generated that show the exact equations used to calculate a given quantity, as well as the values of the terms used in its calculation. The successful implementation of such a system in the prototype made it possible to seriously consider, and ultimately decide upon, implementing a similar capability in the TRIM.FaTE Version 1.0.

F.1.2 VERSION 1.0 ARCHITECTURE

As shown in Figure F-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) those that primarily provide data (ovals). However, each of the components except for external data sources provide both functionality and data. The architectural components that are 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 F-1 are described below.

F.1.2.1 TRIM Core

The TRIM Core primarily provides services required by multiple TRIM components or to integrate those components. The following functions are provided by the Core:

- A mapping tool that shows TRIM spatial objects, such as volume elements, and arbitrary supplemental information supplied by the user, such as soil types. The map display will also allow users to specify the X-Y extent of TRIM.FaTE volume elements.

- Coordination of TRIM graphical user interface components. This includes allowing the user to invoke TRIM modules, such as TRIM.FaTE, and maintaining lists of open windows.

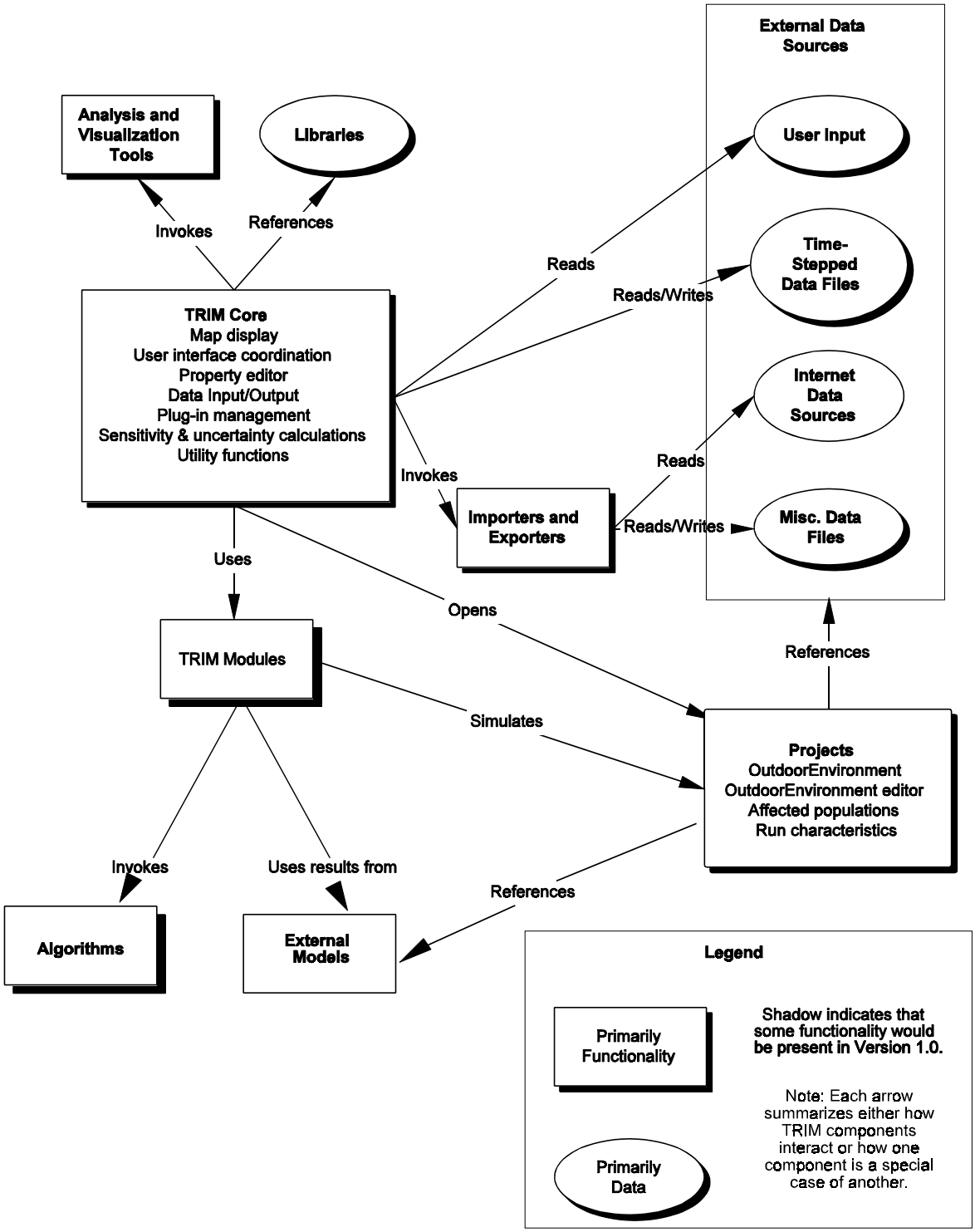
- Allowing users to edit and view property values, where a property is an attribute (*e.g.*, molecular weight) that describes an entity simulated by a model, such as a compartment or volume element. Properties include air temperature, scavenging coefficients, and chemical reaction rates.

- Management of plug-in data importers and exporters.

- Calculation of sensitivity and uncertainty using TRIM models (not supported in Version 1.0).

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

Figure F-1
TRIM Computer System Architecture



F.1.2.2 Project

All information pertinent to an environmental study is stored in a "project." Each project is also responsible for displaying the information it contains and allowing the user to change the information, in some cases relying on a TRIM Core functionality such as the property editor. A project can contain one or more "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.

F.1.2.3 TRIM Modules

Each TRIM module, such as TRIM.FaTE, provides simulation or analysis functionality. Where required, they also provide specialized graphical user interfaces to support their functionality. Version 1.0 includes the TRIM.FaTE module. Future TRIM versions will have support for additional TRIM modules.

TRIM.FaTE uses a number of algorithms that compute chemical transfer coefficients between and transformation coefficients within conceptual compartments. As new chemicals and ecosystems are studied, new algorithms will be required. To address this need, users will be able to add algorithms, which are stored in libraries and projects. The algorithms that are stored in libraries can be applied to various projects.

F.1.2.4 Libraries

A substantial amount of relatively static information is required to conduct studies of multimedia fate and transport and effects on selected populations. For instance, the measured properties of chemicals change infrequently. Also, the boundaries of a study region might stay constant for years. Users can store such information in TRIM object libraries. They can then easily reuse selected information from a library in future projects. When information from a library is used in a project, a copy is made of the information, which protects the project from future changes to the library.

F.1.2.5 External Data Sources, Importers, and Exporters

It will be common for TRIM users to access or create data sets beyond TRIM projects. Some data sets may be too large to be conveniently stored in projects, while other data sets already exist in non-TRIM formats. TRIM provides several methods for accessing external information. The TRIM Core accepts user inputs and will read and write data in native TRIM files. The format of these files is 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.

TRIM also allows users to plug in data importers and exporters. Data importers read non-TRIM data sets and set appropriate TRIM properties. For example, an importer could read files

containing measurements of surface air temperature and set properties in ground-level TRIM air domains. Data exporters provide TRIM results in a form that is suitable for use by another program or for interactive review. This could include comma-delimited files that could be imported into a spreadsheet and tabular results for people to review.

F.1.2.6 Analysis and Visualization Tools

Version 1.0 includes no analysis and visualization tools. Instead, simulation results can be easily exported to Excel or other analysis packages. In the future, TRIM will include some analysis and visualization capabilities and might allow additional capabilities to be developed and plugged-in by users.

F.2 IMPLEMENTATION APPROACHES

The computer framework has been developed using an object-oriented approach. There has been much discussion in the software engineering literature (*e.g.,* Booch 1993) on the benefits of this approach, including increased software extensibility, reuse, 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 that data (*e.g.*, compute 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. TRIM's view 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.

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 be worked out as implementation proceeds. Graphical user interface mock-ups and significant new capabilities are shown to potential users before implementation begins. 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 will not have adequate performance or will significantly limit the potential for future changes, more complex approaches will be used. As time permits, operations that cause noticeable speed or resource problems will be optimized.

F.3 IMPLEMENTATION LANGUAGE

Due to the different objectives of the framework prototypes and Version 1.0, different development languages were chosen. The rationale for each choice is described below.

F.3.1 PROTOTYPES

Microsoft's Visual Basic was used as the primary tool with which to implement the prototypes. This was due to a number of factors:

- Ease of use with Microsoft Excel, which all members on the team had (for early prototypes);
- Object-oriented features of language, while limited[1], simplify a dynamic, iterative architecture development cycle; and
- Straightforward to call needed Fortran codes (*e.g.*, differential equation solver, linear equation solver, triangulation).

F.3.2 VERSION 1.0

The Version 1.0 computer framework was developed primarily, but not entirely, in the Java programming language. Some parts of TRIM.FaTE, such as the differential equation solver, and other TRIM models, such as the exposure model, are implemented in FORTRAN, and other parts, such as the polygon overlay algorithm, are implemented in C.

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 good combination of speed of development, robustness, and support for object-oriented designs.
- Java is supported by multiple vendors. This often leads to competitive pressures to improve development tools, and it reduces the likelihood that one vendor's product strategy or financial problems will cripple TRIM development.
- Java provides built-in support for multithreading, which allows multiple operations to proceed simultaneously, and networking.

The disadvantages of using Java include the following:

- Java programs typically execute more slowly than programs written in C++ or BASIC. As the technologies for compiling and executing Java programs advance, the speed penalty for using Java should decrease.

[1] The primary limitation is that Visual Basic does not support inheritance. However, it does support polymorphism (an object/class can implement any number of interfaces), which is utilized to a large degree to simplify the logic of the programming.

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

- Java development tools are not as mature as tools for other languages, but that situation is improving.

F.4 EMBEDDED TRANSFER ALGORITHMS

As described elsewhere, TRIM.FaTE allows users to specify and choose algorithms that compute chemical transformation and transfer factors. This provides significant flexibility to describe different pollutants and environmental systems. However, some transfer algorithms are too complex to be represented as user-entered formulas. These algorithms are described below.

F.4.1 WIND SPEED BETWEEN AIR COMPARTMENTS

The wind speed from one air compartment to another is calculated as the sum of the transport and dispersive/lateral wind speed. The methods used to calculate these quantities are implemented in subroutines within the source code, rather than through the use of expressions for the expression evaluator. Details on these methods can be found in Section 3.1 of the TRIM.FaTE TSD Volume II.

F.4.2 INTERFACIAL AREA BETWEEN VOLUME ELEMENTS

The interfacial area shared by volume elements is used frequently (*e.g.*, for advective and diffusive transfers). This is calculated by subroutines in the source code itself. In the prototype, each side of a volume element that might intersect another volume element is triangulated (in conjunction with a dynamic link library for triangulation). Next, intersection of the triangulations is computed. Version 1.0 uses a more specialized but faster approach that takes advantage of current restrictions on the structure of volume elements (sides must be vertical and tops and bottoms horizontal). The X-Y projections of side-by-side volume elements are examined for line segment overlap. The length of the overlap multiplies the extent of vertical overlap. The interfacial area for volume elements that are stacked vertically is computed by intersecting the polygons that represent the X-Y projections of the volume elements and then computing the area of the resulting polygon. When more general shapes are permitted for volume elements, a more general calculation, such as the triangulation approach, will be incorporated into Version 1.0.

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