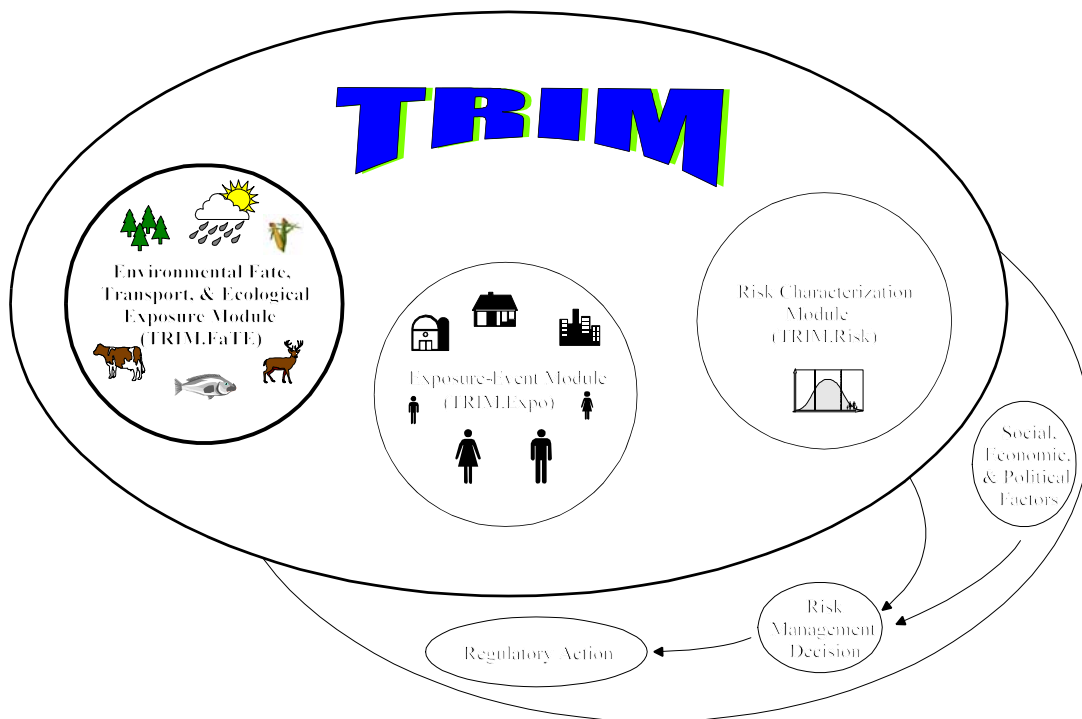




Total Risk Integrated Methodology

TRIM.FaTE Technical Support Document

Volume I: Description of Module



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TRIM
Total Risk Integrated Methodology

TRIM.FaTE
Technical Support Document
Volume I: Description of Module

U.S. Environmental Protection Agency
Office of Air Quality Planning and Standards
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PREFACE

This 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) and/or user's guidance for each of the TRIM modules. This report, which supersedes earlier versions (U.S. EPA 1998a, U.S. EPA 1999g,h), 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.

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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
MIMS	Multimedia Integrated Modeling System
MMSP	Multimedia, multipathway, and multireceptor simulation process
MPE	Multiple Pathways of Exposure
NAAQS	National ambient air quality standard
NAS	National Academy of Sciences
NATA	National Air Toxics Assessments
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
USGS	United States Geological Survey
WASP	Water Quality Analysis Simulation Program

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1. INTRODUCTION

The Office of Air Quality Planning and Standards (OAQPS) of the U.S. Environmental Protection Agency (EPA) 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:

- C Have multimedia assessment capabilities;
- C Have human health and ecological exposure and risk assessment capabilities;
- C Can perform multiple pollutant assessments (*e.g.*, ability to assess mixtures of pollutants and track chemical transformations);
- C Can explicitly address uncertainty and variability;
- C Have the ability to easily perform analyses iteratively, moving from the use of simpler assumptions and scenarios to more detailed assessments; and
- C 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 first developmental phase of TRIM, 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 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 was 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 draft Status Report and draft Technical Support Documents (TSDs) documenting this phase (U.S. EPA 1999a-f) were subjected to review by representatives from

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.

the major program offices at EPA and an EPA Models 2000² review team prior to this SAB advisory. Since review of the draft documents, TRIM.FaTE activities have focused on model evaluation, implementation of the uncertainty analysis feature, and documentation of associated libraries.

This Technical Support Document (TSD) provides technical documentation and support for TRIM.FaTE, the environmental fate, transport, and ecological exposure module of the TRIM modeling system. The TSD is divided into two volumes. Volume I 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. A glossary of key terms related to TRIM.FaTE is presented in Appendix A. Volume II of the TSD presents detailed descriptions of the equations 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 has been 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 has been 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.

C **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

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 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.

core substance (*e.g.*, mercury for methylmercury and divalent mercury) within the modeling simulation will be preserved.

- C **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.
- C **Capability for multiple pollutant, multiple media, and 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 has the following characteristics.
- **Easily accessible.** The TRIM modeling system is accessible for use with a personal computer (PC). The system will be available for download from the Internet and accessible through an Agency model system framework (*e.g.*, Multimedia Integrated Modeling System (MIMS)).
 - **Well-documented.** In addition to Technical Support Documents, Users Guidance is available to assist with setting up and running the model, and interpreting results.
 - **Clear and transparent.** The graphical user interface of the TRIM computer framework provides transparency and clarity in the functioning of the TRIM modules, and output from the modules will include information on modeling assumptions, limitations, and uncertainties.

1.2 TRIM DESIGN

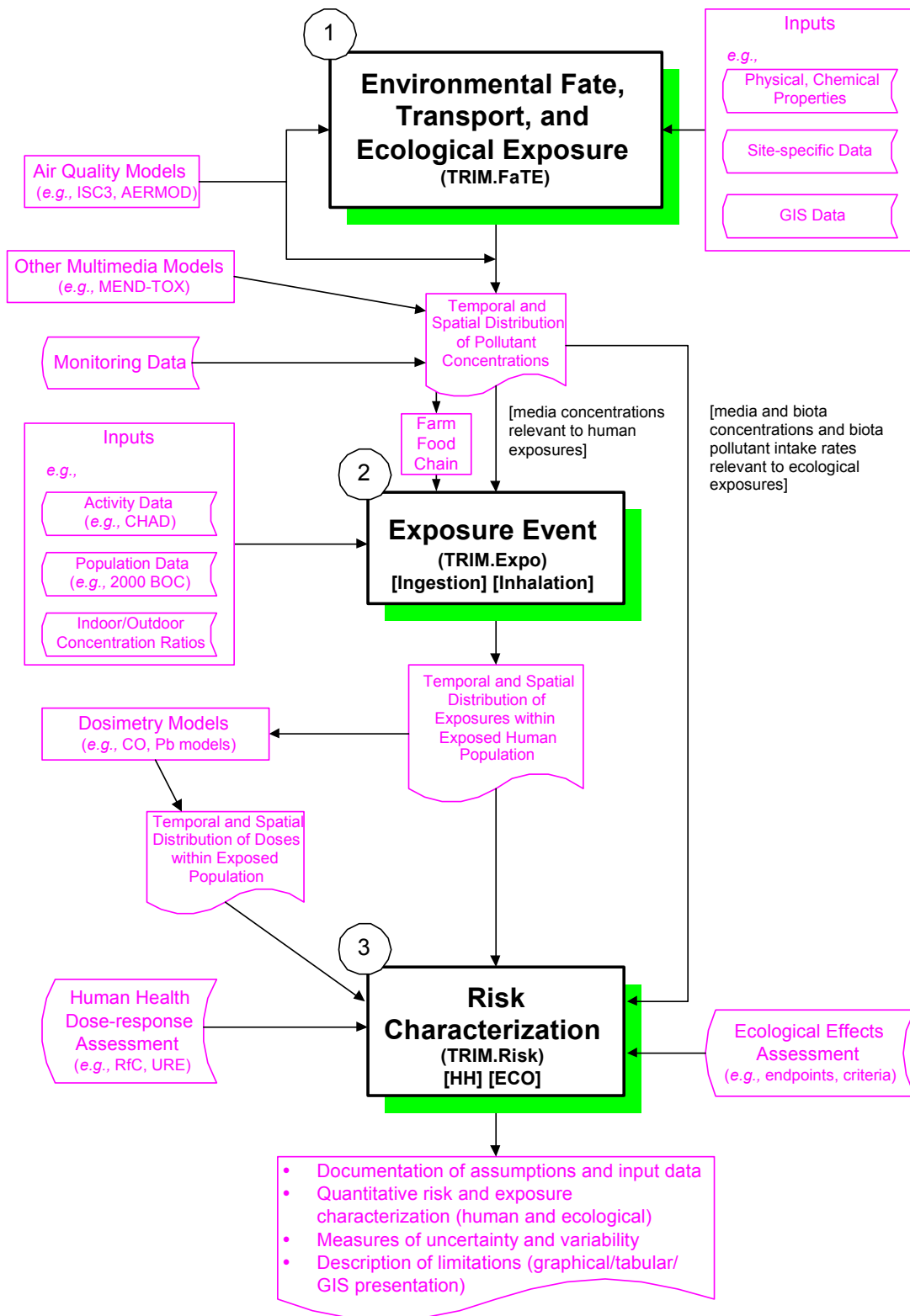
The TRIM design (Figure 1-1) includes three individual modules. The *Environmental Fate, Transport, and Ecological Exposure* module, **TRIM.FaTE**, accounts for movement of a chemical through a comprehensive system of discrete compartments (*e.g.*, media and biota) that represent possible locations of 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**.³ In TRIM.Expo, human exposures are evaluated by tracking either randomly selected individuals that represent an area's population or 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 designed to characterize ecological risks from multimedia exposures. The output from TRIM.Risk is intended to 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 to assess the overall precision of the model. The uncertainty and variability feature augments 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 have been developed in a phased approach, and refinements can be 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 without the need to run TRIM.FaTE, 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.

³ A farm food chain (FFC) model is also available as a method for deriving livestock and produce contaminant concentrations from soil and air concentrations and air deposition outputs from TRIM.FaTE.

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



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. Additional details regarding TRIM.FaTE are covered in the chapters that follow.

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 may be added in the future.

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, drinking water, foods, household dusts, and soils).

TRIM.Expo is currently comprised of two components, one for inhalation exposure and one for ingestion exposure. The inhalation component of TRIM.Expo predicts inhalation exposures of many individuals randomly selected to represent an area's population by tracking the movement of each individual through locations where chemical exposure can occur according to specific activity patterns. In a typical application, the inhalation component can combine either processed air monitoring data or air dispersion modeling results with the activity

patterns of the individuals and micro-environment concentration relationships to estimate exposures. The movements of an individual are defined as an exposure-event sequence that can be related to time periods for which exposure concentrations are estimated. Each exposure event places the individual 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 also can provide information relating to the potential for pollutant uptake (*e.g.*, respiration rate). Exposures associated with these events are aggregated to predict an exposure concentration for the time period of interest.

The primary purpose of the ingestion component of TRIM.Expo is for the assessment of ingestion exposure to air pollutants that are persistent and/or bioaccumulative. The ingestion component calculates the ingestion exposure (in units of mg of constituent per kg of body weight per day) to human receptor groups from media and food concentrations. In a typical application, the ingestion component can accept TRIM.FaTE output data or other pollutant concentration data for media and biota to estimate human exposure. TRIM.FaTE can be used to provide an inventory of chemical concentrations in environmental media and in biota across the ecosystem at selected time intervals (*e.g.*, days, hours). A farm food chain module is also available to provide livestock and produce contaminant estimates from air and soil concentrations and air deposition estimates provided by TRIM.FaTE or from an external file.

In addition to directly providing human population exposure estimates, the TRIM.Expo module is intended to contribute to a number of health-related assessments, including risk assessments and status and trends analyses.

1.2.3 DESCRIPTION OF TRIM.Risk

Risk characterization is the final step in risk assessment and is primarily used to integrate the information from the other three key steps (*i.e.*, hazard identification, dose-response assessment, exposure assessment). Within the TRIM framework, TRIM.Risk, the risk characterization module, will be used to integrate the information on exposure (human or ecological receptor) with that on dose-response or hazard assessment and to provide quantitative

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.

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 and associated tools will provide the capability to summarize or highlight the major points from each of the analyses conducted in the TRIM modules. In general, this will include: (1) documentation of assumptions and input data, (2) risk calculations and data analysis, and (3) presentation of results and supporting information.

Current and proposed EPA guidance on risk characterization will guide the development of TRIM.Risk and associated tools. 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 types 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,⁴ 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.*, similar to the 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. Consequently, review of existing models and consideration of other current modeling efforts has been an important part of TRIM development activities. Reviews of relevant models existing at the initiation of development activities for TRIM.FaTE are described in Chapter 2 of this document. Additionally, EPA has incorporated TRIM into EPA's MIMS, which is essentially a modeling framework that accommodates linkages among multiple models and the sharing of common tools and data.

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 review has been an integral part of the TRIM development plan. Following the first phase of TRIM development, OAQPS submitted TRIM (U.S. EPA 1998a, U.S. EPA 1998b) to SAB under their advisory method of review. In May 1998 in Washington, DC, the Environmental

⁴ 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.

Models Subcommittee (Subcommittee) of the Executive Committee of SAB reviewed the TRIM project, assessing the overall conceptual approach of TRIM and the specific approach of TRIM.FaTE. The Subcommittee reported that the development of TRIM and the TRIM.FaTE module was conceptually sound and scientifically based (U.S. EPA 1998c) and provided specific recommendations related to six specific charge questions. These recommendations are detailed in Chapter 2 of the 1999 TRIM Status Report (U.S. EPA 1999b), along with brief responses. Changes to TRIM.FaTE based in part on the SAB recommendations are highlighted in Chapter 4 of the 1999 TRIM Status Report.

TRIM was again submitted to SAB advisory review in December 1999, when the Subcommittee met to review progress on TRIM (U.S. EPA 1999a,b, U.S. EPA 1999g,h). In providing comments and recommendations the Subcommittee found “ongoing efforts to develop TRIM as a flexible, state-of-the-art system for evaluation multimedia chemical fate, transport, exposure and risk, to be effective and innovative” (U.S. EPA 2000). In consideration of SAB’s comments and recommendations, TRIM.FaTE was refined, including the development of new and updated capabilities and the development and limited testing of methodologies for model set-up, uncertainty and variability analysis, and evaluation. This TRIM.FaTE documentation has also gone through internal Agency peer review, involving reviewers across the Agency from major program offices, the Office of Research and Development, and staff involved in the Agency’s Models 2000 efforts, as well as the SAB reviews described above.

In addition to consulting with Agency scientists during future TRIM development (*i.e.*, peer involvement), OAQPS will, as appropriate, seek peer review of new aspects in 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.

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 (HAP) (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 such as National Air

Toxics Assessments (NATA) are described as one of the program's key components.⁵ NATA include both national- and local-scale activities. The TRIM system is intended to provide tools in support of local-scale assessment activities, including multimedia analyses.

One of the Agency's most immediate needs for TRIM comes in the Residual Risk Program, in which there are many upcoming statutory deadlines 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 National Ambient Air Quality Standards (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. The 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 methodology⁶ 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

EXAMPLES OF TRIM APPLICATIONS

- C 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.
- C An assessment of human health risks associated with air emissions of a criteria air pollutant (e.g., ozone) or one or several volatile HAPs in a metropolitan area could be developed using an external air model or ambient concentration data from fixed-site monitors coupled with TRIM.Expo and TRIM.Risk.

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

⁶ In support of the *Mercury Report to Congress* (U.S. EPA 1997) 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 titled 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).

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.

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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 initial development of TRIM.FaTE, EPA 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 the existing models addressed the following characteristics desired for TRIM.FaTE:

- C Ability to address varying time steps (of one hour or greater) and provide sufficient spatial detail at varying scales (site-specific to urban scale);
- C Conservation of pollutant mass within the system being assessed;
- C Transparency, as needed for use in a regulatory context; and
- C 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 was necessary to develop a new, truly coupled, multimedia modeling framework. In developing TRIM.FaTE, the Agency has incorporated several features that improve upon the capabilities of the existing models considered during the review. These key features are summarized in Section 2.3. A complete description of the TRIM.FaTE computer framework is presented in Appendix D.

2.1 REVIEW OF EXISTING FATE AND TRANSPORT MODELS

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,b,c) 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.

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 and Johnson 1996), examined several multimedia models. Two additional EPA studies conducted in 1997 (IT 1997a,b) 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).

A brief summary of the key multimedia models that were evaluated for applicability to the TRIM.FaTE effort follows. Other models that were reviewed are documented in the previously mentioned background reports (Mosier *et al.* 1996, IT 1997a, IT 1997b).

- **Indirect Exposure Methodology (IEM).** The version of IEM reviewed by OAQPS during initial TRIM development efforts consisted of a set of multimedia fate and exposure algorithms developed by EPA's Office of Research and Development. This methodology was, and remains today, a significant 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), a major addendum was issued in 1993 (U.S. EPA 1993), and an updated guidance

document was published in 1999 (U.S. EPA 1999d).¹ The IEM assessed by OAQPS had undergone extensive scientific review, including review by SAB, which was useful in focusing efforts in the development of TRIM. The SAB identified several limitations of IEM that were pertinent to its application to the design qualifications for TRIM (U.S. EPA 1994b). Concurrently with IEM development, EPA also developed and applied a closely related set of multimedia models in a variety of dioxin assessments (U.S. EPA 1994c).

Descriptions of fate and transport algorithms, exposure pathways, receptor scenarios, and dose algorithms are presented in the existing IEM documentation. The IEM includes procedures for estimating the indirect human exposures and health risks that could 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.

During its review of the IEM methodology, OAQPS identified several limitations in the IEM approach relative to the TRIM.FaTE design criteria and OAQPS' needs. For example, the version of IEM evaluated could be applied only to chemicals that were emitted to the air. This limited 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 has moved 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 was crucial in the initial development of TRIM, and remains true today, that a sense of continuity be maintained between IEM and 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 could not provide detailed time-series estimation (*e.g.*, for time steps less than one year) of media concentrations and concomitant exposure, could not maintain full mass balance, and, because it was not a truly coupled multimedia model, did not have the ability to model "feedback" loops between media or secondary emissions (*e.g.*, re-emission of deposited pollutants). Furthermore, IEM did not provide for the flexibility OAQPS considered as necessary in site-specific applications or in estimating population exposures. Significant site-specific adjustment would be necessary to allow for spatially

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 was 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.

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

Therefore, while IEM met its own design criteria quite well (*e.g.*, could adequately estimate long-term average exposure media concentrations in the vicinity of an air source for contaminants for which indirect impacts were important), it did not fully meet the needs of OAQPS at the time of initial TRIM development for the reasons noted above.

- **California Department of Toxic Substance Control's Multimedia Risk Computerized Model (CalTOX).** First issued in 1993 (McKone 1993a,b,c) and updated in 1995, 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 version of CalTOX reviewed by OAQPS was a dynamic multimedia transport and transformation model that could 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 was a seven-compartment regional and dynamic multimedia fugacity model. The seven compartments were: (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 were 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 were treated as time-varying state variables. Contaminant concentrations in ground water were based on the leachate from the vadose-zone soil.

The multipathway exposure model reviewed at the time of initial TRIM development encompassed 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 consisted 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 distinguished CalTOX from many other exposure models. In addition, all parameter values used as inputs to CalTOX were 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 employed. This stochastic approach allowed both sensitivity and uncertainty to be directly incorporated into the model operation.

As indicated in the literature review reports, the CalTOX model appeared 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 could have been directly applied to meet the TRIM goals. However, OAQPS identified several limitations to CalTOX that prevented it from being entirely imported into the TRIM approach. These limitations resulted 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, or for a limited range of chemicals (*e.g.*, non-ionic organic chemicals in a liquid or gaseous state). As a result, the model did 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, was the fact that the CalTOX model, as it existed at the time of initial TRIM efforts, did not allow spatial tracking of a pollutant as was required in the TRIM approach.

- **SimpleBOX.** Based on OAQPS' review, SimpleBOX was identified as a steady-state, non-equilibrium partitioning, mass balance model (van de Meent 1993, Brandes *et al.* 1997). It consisted of eight compartments, three of which were soils of differing use and properties. It also produced 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 represented the Netherlands. SimpleBOX used the classical concentration concept to compute the mass balance (van de Meent 1993). While its goals were comparable to TRIM to the extent that it simulated regional systems, its coarse spatial and temporal complexity and lack of exposure media concentration estimates caused it to fall short of TRIM's goals.
- **Integrated Spatial Multimedia Compartmental Model (ISMCM).** At the time of initial TRIM efforts, ISMCM had 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, was under evaluation by the EPA Office of Research and Development's National Exposure Research Laboratory.

OAQPS review found that the version of ISMCM available during early TRIM efforts considered all media, biological and non-biological, in one integrated system and included both spatial and compartmental modules to account for complex transport of pollutants through an ecosystem. Assuming mass conservation, ISMCM was 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, was that it was 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 was the fact that the links and compartments (spatial

configuration) of this model were predetermined (van de Water 1995). 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. OAQPS review during initial TRIM efforts showed that this model consisted of single-media transport models linked together under appropriate boundary conditions and considered four primary types of pollutant pathways (ground water, overland, surface water, and atmospheric) in evaluating human exposure. MEPAS also contained an exposure and risk module. The model was unique in its ability to estimate multipathway risks for chemicals and radionuclides. The nature of its algorithms made it a screening tool, rather than a detailed assessment tool. The model was updated periodically and the latest version of MEPAS (Version 3.1) evaluated by OAQPS during its review contained an uncertainty and variability analysis module (Buck *et al.* 1995).

Based on OAQPS review during initial TRIM efforts, the mathematical design of this model did not include mass balance and could not be integrated into TRIM. As with IEM, MEPAS represented a "linked" model system that utilized 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 did not allow for the temporal tracking of the pollutants and concomitant exposure necessary to meet the needs of TRIM.

Based on the results of these review efforts, OAQPS concluded that while certain features of existing models were desirable for TRIM, none of the models reviewed at that time would fully address the needs for the TRIM modeling system. Therefore, OAQPS determined that it would be necessary to develop an improved fate and transport modeling tool. Reasons for this conclusion are discussed in the next section.

2.2 APPROACH TO DEVELOPING TRIM.FaTE

During initial TRIM development, OAQPS determined that the currently existing OAQPS fate and transport models for hazardous and criteria air pollutants did not address multimedia exposures, and currently existing OAQPS HAP models did not adequately estimate temporal and spatial patterns of exposures. Adopting or incorporating existing models into a tool that meets OAQPS' needs represented 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 was no single fate and transport model that met the needs of OAQPS (outlined in Chapter 1) and that could be adopted as part of TRIM. Most models were limited in the types of media and environmental processes addressed. Simply, no single model at that time could 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 was unlikely that one individual model could be developed to address this wide range of concerns. Therefore, the TRIM framework was constructed to

emphasize 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.

Multimedia models existing at the time of initial TRIM development could be divided into two basic categories: “linked” single medium model systems and mass-conserving models. Mass-conserving models could 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). OAQPS concluded that the linked single medium and mass-conserving models each had their own strengths and limitations.

“Linked” single medium modeling systems were identified as those composed of several independent single medium models. The linked system typically calculated 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 were several highly sophisticated single medium models to choose from when constructing a linked system. However, the linked design did not assure conservation of mass because the dynamic feedback loops and secondary pollutant transfers were not treated in a fully coupled manner. In addition, the level of detail provided by the linked model system could not be 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. Although the fugacity concept provides a convenient method for quantifying the multimedia fate of chemicals (Cowen *et al.* 1995),² 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 could technically handle inorganic chemicals, but temporal and spatial resolution would be limited by the rigid compartmentalized structure or boxes used to represent the environmental media. Spatial compartmental models (*e.g.*, ISMCM) represented the closest current models to an integrated multimedia system. However, as previously described, ISMCM did not meet the TRIM design criterion for a flexible architecture.

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

² Fugacity is a method of expressing the escape tendency of a substance using units of pressure. If this concept is considered as a measure of chemical intensity, the chemical potential of a substance in any phase can be expressed as a fugacity, using the gas phase of that substance as a reference phase. When two or more phases are at equilibrium, the fugacities of the substance’s phases are equal; therefore, the fugacity concept can be used to determine the fractional distribution of mass within different phases in a compartment.

Another model, the multimedia, multipathway and multireceptor risk assessment (3MRA, formerly FRAMES-HWIR), was also under development during the initial TRIM development phase. Development on this model has continued through the present time as a methodology for EPA to support risk assessment decisions made regarding waste concentration limits for chemicals in industrial waste management units. 3MRA 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 18 individual modules (*e.g.*, air, watershed, human exposure). Similar to IEM, the 3MRA methodology includes procedures for estimating the indirect human exposures and health risks that could result from the transfer of emitted air pollutants to soil, vegetation, and water bodies. This model is designed to predict long-term impacts from continuous sources, using a one-way process through a series of linked models and algorithms incorporating IEM concepts. The methodology addresses exposures via inhalation, food, water, and soil ingestion, and dermal contact. However, like IEM, 3MRA is not a truly coupled, mass-balanced multimedia model.

2.3 KEY CAPABILITIES OF TRIM.FaTE

As mentioned above, several key characteristics were identified as essential to the design of TRIM.FaTE:

- C Ability to address varying time steps (of one hour or greater) and provide sufficient spatial detail at varying scales (site-specific to urban scale);
- C Conservation of pollutant mass within the system being assessed;
- C Transparency, as needed for use in a regulatory context; and
- C 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 ChemCan³ 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 at the time of initial TRIM development. These key features included:

- C Implementation as a truly coupled multimedia model framework;

³ 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.

- C The adaptability to match a simulation to the spatial and temporal scales needed for a broad range of pollutants and geographical areas;
- C 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;
- C An accounting of the pollutant mass distributed within, as well as entering and leaving, the environmental system;
- C An embedded procedure to characterize uncertainty and variability; and
- C The capability to be used as an exposure model for ecological receptors.

This section summarizes these features along with some of the potential limitations of the TRIM.FaTE framework.

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 assists the user in not 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.

General recommendations for designing the spatial extent and subdivision of a modeling region based on existing TRIM.FaTE test cases will be incorporated into TRIM.FaTE User Guidance (EPA 2002a). However, the flexibility inherent to TRIM.FaTE allows the user a nearly limitless number of unique layout options for a single modeling application, including untested approaches and potentially problematic configurations. Consequently, the user must be careful to maintain a balance between the advantages and the uncertainties of spatial complexity.

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 three 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.

TRIM.FaTE does not currently estimate the concentrations of chemicals in vertebrate organs; therefore, models that relate toxicity to organ concentration are not easily implemented. However, given the inherent flexibility of TRIM.FaTE, the user, if armed with prerequisite information to describe pollutant movement among the internal compartments of a particular animal, could implement a scenario in TRIM.FaTE to make use of such models.

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. Note that the Glossary presented in Appendix A also provide brief definitions for key terms related to TRIM.Fate. 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 different meanings in different disciplines. Three 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 (<i>e.g.</i> , spatial, temporal, environmental, source, chemical) used to define a TRIM.FaTE model set-up for a particular simulation or set of simulations.
Simulation:	A single application of TRIM.FaTE to estimate chemical transport and fate, based on a given scenario and any initial input values needed.
Project:	A TRIM.FaTE computer framework for saving one or more scenarios and all of the data properties for the scenarios that pertain to a single model application.

The primary objective of the TRIM.FaTE module is to estimate the fate and transport of a chemical pollutant or pollutants over time 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 a 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 polycyclic aromatic hydrocarbons (PAHs), methylmercury, elemental mercury, and benzene.

3.1 BASIC TRIM.FaTE TERMINOLOGY

In the TRIM.FaTE module, chemicals are contained within compartments. The term “compartment” is in some ways similar to what is referred to as a “medium” in environmental fate and transport modeling literature. However, 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. Simply, a **compartment** is defined as the TRIM.FaTE modeling unit that contains chemical mass. Within TRIM.FaTE, chemical mass is transported between and transformed within compartments. A specific compartment is characterized by its physical and spatial composition and its relationship to other compartments. It is assumed, for modeling purposes, that all chemical mass within a compartment 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 generally assumed to be in equilibrium with respect to chemical partitioning (see TRIM.FaTE TSD Volume II for exceptions). Compartments can be either biotic, such as a deer compartment, or abiotic, such as a surface water 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 (or in some cases community, or other subgroup) within a specified spatial volume or area.

The term **compartment type** is used to denote a particular kind of compartment, such as an air compartment type or a soil detritivore compartment type. Compartment types are typically distinguished from each other by their basic characteristics and the way they exchange chemical mass with other compartment types. A compartment type can be thought of as a “template” for a specific, spatially defined and located compartment. A specific compartment is defined for a modeling scenario by first adding a copy of that “template” to the scenario and then defining its location and establishing its site-specific properties. Compartments of the same type are distinguished from each other in a given scenario by their location and sometimes also by the values that define their composition at a particular location. For example, two different surface soil compartments may have organic carbon fractions of 0.015 and 0.01, respectively, but they are both described by the compartment type called “surface soil.”

SINKS

A sink is a special kind of compartment type that accounts for chemical mass no longer available for transport or uptake within a TRIM.FaTE simulation. Like other compartment types, sinks are linked to compartments, but sinks do not have a volume and, by definition, they do not have any loss processes associated with them (*i.e.*, they “receive” mass but do not “send” mass). There are three types of sinks: advection sinks, flush rate sinks, and degradation/reaction sinks. Advection sinks are linked to the outside edges of certain compartments (*e.g.*, air compartments) to account for chemical mass removed from the entire modeling region via advection from these compartments. Flush rate sinks are needed for each water body that “flushes” or releases water out of the modeled domain (*e.g.*, a river that flows across the boundary of the modeled region, or a lake that flushes its contents outside of the region). Degradation/reaction sinks are needed when modeling chemicals that degrade or are transformed into products whose fate after degradation/transformation is not tracked by the model.

In general, compartment types are classified as either abiotic or biotic (see also the text above describing sinks). An abiotic compartment type consists primarily of a non-living environmental medium¹ (e.g., air, soil) for which TRIM.FaTE calculates chemical masses and concentrations. A biotic compartment type consists 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. Abiotic and biotic compartment types are discussed in more detail in Section 3.2.

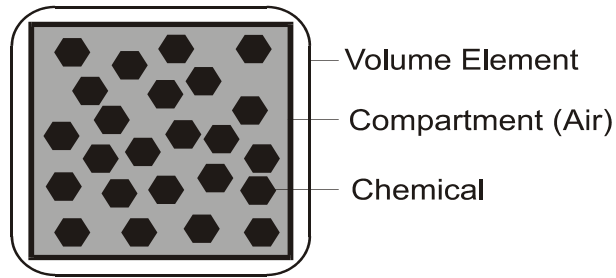
Each compartment is associated with (contained within) a volume element. A **volume element** is a bounded three-dimensional space that defines the location of one or more compartments. This term is introduced to provide a consistent method for locating and organizing objects that have a natural spatial relationship. In applications of TRIM.FaTE thus far, one (and only one) abiotic compartment is contained within any one volume element, and each volume element is identified by the abiotic compartment type it contains (e.g., surface soil volume element, ground water volume element). In addition to the abiotic compartment, numerous biotic compartments may be contained within a single volume element (e.g., multiple terrestrial biota compartment types along with a surface soil compartment may be contained within a surface soil volume element). Animals are typically associated with surface soil or surface water compartment types depending on where they usually reside and/or feed. For example, mallards generally feed in the water, so the mallard compartment type, when included in modeling, is placed along with the surface water compartment in one or more surface water volume elements. Terrestrial biota included in modeling are placed with the surface soil compartment in one or more surface soil volume elements. It should be noted, however, that animals are not restricted to feeding only in the volume element where they are located. The user may designate that a particular biotic compartment (e.g., bald eagle) obtains its diet from compartments (e.g., mouse) in more than one volume element.

The size and shape of volume elements for a given TRIM.FaTE application depend 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 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 associated with 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 an air volume element. Likewise, the volume element in Figure 3-2 is referred to as a surface 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 defining the compartments to be modeled within this framework.

¹ When chemical transformation or degradation is modeled, an abiotic compartment may implicitly contain biota in the form of the microorganisms responsible for chemical transformation.

Figure 3-1
Simple TRIM.FaTE System^a



^aChemicals 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

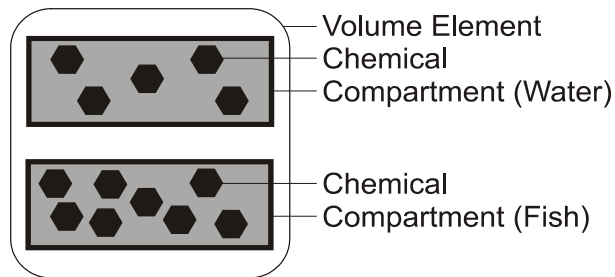
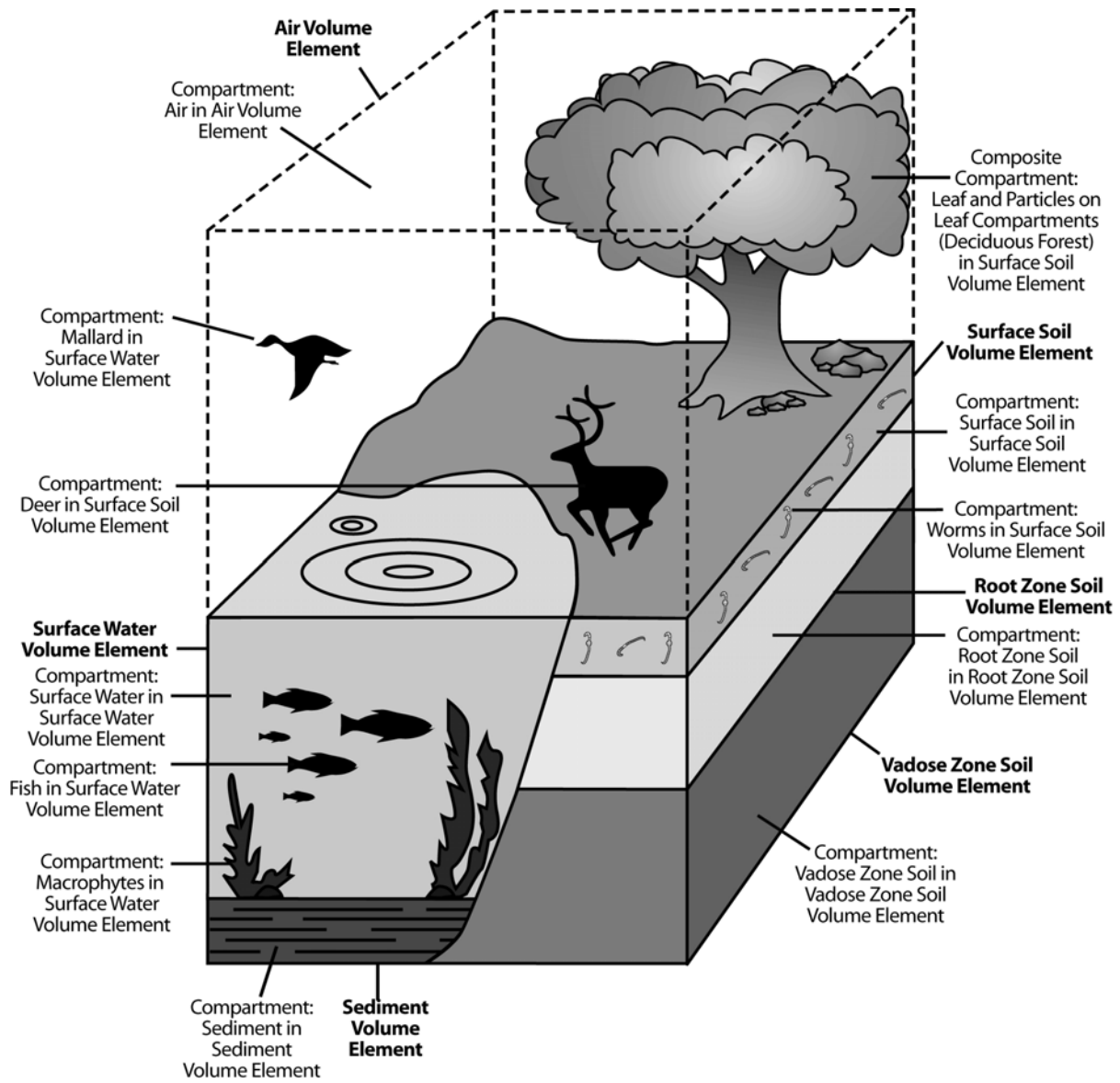


Figure 3-3
Example of a Hypothetical Environment (Multiple Volume Elements, Multiple Compartments)



Abiotic compartments (*e.g.*, surface soil, air) generally possess the same dimensions (*i.e.*, height, length, and width), and hence the same volume, as the containing volume element. Note that a sediment compartment may include both the sediment particles and the interstitial pore water, with the chemical in phase equilibrium between them. The total volume of this sediment compartment would consist of water (with a volume fraction equal to x) and sediment particles (with a volume fraction equal to $(1 - x)$). Similarly, surface water compartments include both particulate and dissolved phases, and air compartments contain particulate and vapor phases (see Section 4.3).

Although biotic compartments are associated with volume elements as a part of the TRIM.FaTE modeling structure, they do not “take up space” within a volume element. Concentrations in biotic compartments are calculated on the basis of biomass (refer to TRIM.FaTE TSD Volume II for more detailed information). For the purposes of estimating chemical mass and concentration in the abiotic compartment, the volumes associated with biotic compartments are considered insignificant compared with the volumes of the associated abiotic compartment (*e.g.*, air, soil, water). See the text box

above for two examples of the conceptual relationship between biotic compartments and volume elements for the hypothetical environment shown in Figure 3-3.

**Biotic Compartments and Volume Elements:
Examples from Figure 3-3**

The **fish compartment** is associated with the Surface Water Volume Element and is assumed to exist as a population evenly spread throughout the surface water compartment within that volume element. Characteristics for the fish population are defined by the user (*e.g.*, average body weight, number of fish per square meter of water body). However, the volume occupied by the biomass of the fish is not calculated, and the volume fraction of the surface water compartment that consists of fish is not estimated or subtracted from the volume of water in the compartment for any of the calculations in TRIM.FaTE.

The **mallard compartment** is also associated with the Surface Water Volume Element, and some of the same population characteristics (*e.g.*, average body weight, number of individuals per area) are defined by the user. The mallard population is assumed to feed on both aquatic invertebrates (associated with the same volume element) and terrestrial plants (associated with one or more neighboring volume elements). Thus, in terms of feeding habits, the mallard population is not physically restricted to the volume element with which it is associated.

3.2 COMPARTMENT TYPES

The openness and flexibility of TRIM.FaTE give the user wide latitude in defining the compartment types for any particular modeling scenario. The discussion in the two sections that follow describes compartment type implementations that have been used and evaluated thus far. TRIM.FaTE provides the user the capability to define scenarios using these or alternate compartment type strategies. With this flexibility, however, comes the responsibility to consider the ramifications of the selected strategy. Observations of complexity evaluations described in the TRIM.FaTE Evaluation Report (USEPA 2002b) and discussion in TRIM.FaTE User Guidance (USEPA 2002a) may be of assistance, particularly in considering the strategy for including biota in a TRIM.FaTE scenario.

3.2.1 ABIOTIC COMPARTMENT TYPES

Abiotic compartment types consist primarily of a non-living environmental medium. The adjacent text box lists the abiotic compartment types currently included in TRIM.FaTE. Within the TRIM.FaTE system, chemical mass is initially transported to biotic compartments based on their relationships with abiotic compartment types. In addition to the abiotic compartment types listed here, compartment types defined within the TRIM.FaTE system that are not associated with biota also include advection and flush rate sinks (to account for mass transported outside of the modeled region) and reaction/degradation sinks (to account for the results of chemical transformation reactions when the fate of the reaction product is no longer tracked by TRIM.FaTE). Sinks are described in more detail in the text box in Section 3.1 and in the discussion of the TRIM.FaTE mass balance framework (Chapter 4).

ABIOTIC COMPARTMENT TYPES IN TRIM.FaTE	
Air Surface Soil Root Zone Soil Vadose Zone Soil	Ground Water Surface Water Sediment

The properties of abiotic compartment types are set by the user who can give them differing or identical values throughout the modeling region. For example, parameter values for all surface soil compartments in a modeling scenario can be assumed to be the same. However, if site-specific data are available for different compartments in a scenario, these data can be entered as compartment-specific properties. For example, where multiple water bodies are represented in a scenario, the user may need to specify differing values for the surface water and sediment compartment properties (*e.g.*, current velocity, water pH, sediment particle density).

3.2.2 BIOTIC COMPARTMENT TYPES

Biotic compartment types generally are differentiated from one another based on their links with other compartment types. Thus, each biotic compartment type represents a different trophic/taxonomic group or has a different route of uptake. The compartment types are further distinguished by the ecosystem (*i.e.*, terrestrial or aquatic) in which the biotic compartment feeds or is located. Mammalian and avian wildlife, soil detritivores, fish, aquatic (benthic) invertebrates, and aquatic plants are considered different compartment types because they belong to unique trophic groups and/or occupy different ecosystems. Those groups can be further subdivided based on their habitat (*e.g.*, terrestrial, semi-aquatic) and/or general feeding patterns (*e.g.*, herbivore, omnivore). For example, some wildlife species are considered to be entirely terrestrial (*e.g.*, deer), while others are considered to be semi-aquatic (*e.g.*, mink), feeding on prey from both aquatic and terrestrial habitats. The different biotic compartment types that have been used to date in TRIM.FaTE are listed in Table 3-1.

For terrestrial and semi-aquatic wildlife (*i.e.*, birds and mammals), one or more species can represent each trophic/functional group. For example, a single species, the short-tailed shrew, might represent terrestrial ground invertebrate feeders for the terrestrial portions of the modeling region. For a terrestrial predator trophic group, both the red-tailed hawk and the

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

Biotic Compartment Type	Representative Subgroup or Species
Aquatic Plants	
Macrophyte	[User input] ^a
Benthic Fauna	
Benthic invertebrate	[User input] ^a
Benthic omnivore	[User input] ^a
Benthic carnivore	[User input] ^a
Water-Column Fauna	
Water-column herbivore	[User input] ^a
Water-column omnivore	[User input] ^a
Water-column carnivore	[User input] ^a
Semi-Aquatic Fauna	
Semi-aquatic piscivore	Belted kingfisher Common loon Mink
Semi-aquatic predator/scavenger	Bald eagle
Semi-aquatic aerial insectivore (<i>i.e.</i> , feeding on adults of emergent insects such as mayflies, mosquitos, damselflies)	Tree swallow
Semi-aquatic omnivore	Mallard Raccoon
Terrestrial Plants^b	
Plant leaf	Defined as appropriate for coniferous or deciduous forest, grass/herb fields, or agricultural systems.
Particle on leaf	
Plant stem	
Plant root	
Terrestrial Fauna	
Terrestrial omnivore	American robin White-footed mouse
Terrestrial insectivore	Black-capped chickadee
Terrestrial predator/scavenger	Long-tailed weasel Red-tailed hawk

Biotic Compartment Type	Representative Subgroup or Species
Terrestrial vertebrate herbivore	Black-tailed deer Bobwhite quail Long-tailed vole Meadow vole Mule deer White-tailed deer
Terrestrial ground-invertebrate feeder	Short-tailed shrew Trowbridge shrew American woodcock
Flying insect ^c	Mayfly
Soil detritivore	Earthworm Soil arthropod

^a In applications to date, the fish compartments have been employed to represent trophic niches arising either from a benthic (*i.e.*, sediment-based) or water-column contaminant source. In addition, the term omnivore has been a misnomer in the applications to date, because the water-column “omnivore” has fed only on the water-column herbivore, and the benthic “omnivore” only on benthic invertebrates. Thus, these compartment types have not been parameterized using the concept of a single representative species that might feed on organisms from more than one trophic level or from both the benthic and water-column environments. Rather, the total biomass for a single representative fish species that feeds from both benthic and water-column sources has been divided into two compartments for that species: one that feeds from benthic sources and one that feeds from water-column sources, respectively. The water-column “herbivore” also is a misnomer in that zooplankton are implicitly included in the diet and represent an intermediate trophic level between the phytoplankton and the fish herbivore. Further discussion of this is provided in the TRIM.FaTE Evaluation Report and the TRIM.FaTE TSD, Volume II, Chapter 6. As mentioned previously, however, alternate strategies may be evaluated and employed, as appropriate.

^b Terrestrial plant parts constitute different compartment types even though they are not different trophic groups.

^c For applications thus far, flying insects have been represented by the benthic invertebrate compartment type, thus essentially assuming that the concentration of chemical in the adult flying insect is the same as the concentration of chemical in the aquatic nymph from which it emerged.

long-tailed weasel might be included in one or more surface soil volume elements of the modeling region. In that case, the diet of each of those species would be specified and compartments representing the prey species would also need to be included in the model. The diet of fish and wildlife can range from a single diet item (*e.g.*, 100 percent algae for an herbivorous fish) to multiple diet items (*e.g.*, 5 percent shrews, 20 percent mice, 25 percent ducks, 25 percent benthic invertebrates, and 25 percent water-column herbivorous fish for mink). The selection of wildlife compartments and assignment of corresponding diet, biomass, and other parameter values will depend on the location of the site, the habitat types found at the site, the area covered by the modeling region, and other factors as described in the TRIM.FaTE User Guidance.

There are similarities between constructing an aquatic food web and constructing a food web for terrestrial wildlife. The user can specify fish compartments appropriate to the site and can specify the diet for each fish compartment. A given fish compartment might be parameterized to represent an entire trophic group, or one or more species considered representative of that group can be used to assign values to the parameters for one or more compartments. Biomass relevant to the distribution of the pollutant being modeled should be

accounted for. For example, the entire biomass of aquatic organisms in the surface water body being modeled should be accounted for in the set of aquatic compartments implemented to ensure appropriate chemical partitioning in the aquatic ecosystem.

In some cases, composite compartment types may be implemented within the TRIM.FaTE framework. A **composite compartment type** is a group of different compartment types that are consistently interconnected. Each individual compartment within a composite compartment requires the presence of other compartments. Conceptually, a composite compartment type may be considered as a term of convenience for the user rather than a structural component of the TRIM.FaTE system; that is, TRIM.FaTE distributes mass between the individual compartments, not into the compartment type as a single unit. Currently, plant composite compartment types have been defined within TRIM.FaTE, with root, stem, leaf, and particle on leaf² compartments comprising the plant composite compartment type (given the difficulty in modeling woody stems and roots, only the leaf and particle on leaf compartments are currently included in the coniferous and deciduous forest composite compartments). Note that different types of plant communities (*e.g.*, deciduous forest, grass and herb community) may be represented by separate composite compartments.

Given the flexibility of the TRIM.FaTE framework, the user can design and implement their own approach to modeling pollutant movement through biotic compartments. This can include custom definitions of compartment types, feeding habits, biomass densities, and other parameters. As mentioned previously, with this flexibility comes an inherent responsibility to consider the ramifications of a given design and consequently its appropriateness for the objectives of the assessment. For example, although the animals in an ecosystem are not considered to play a large role in the distribution of pollutant mass within that ecosystem (*i.e.*, the balance will occur in abiotic media), distribution of pollutant mass among the various animals in TRIM.FaTE is influenced by the relationships among them (*e.g.*, predator-prey, relative abundance, dietary preferences).

3.3 LINKS

There are two general processes that can affect the presence of chemical mass within a given compartment:

- (1) the transfer of chemical mass from and/or to another compartment; and
- (2) the transformation of one chemical to another chemical within a compartment.

In order to evaluate the occurrence and magnitude of these processes, the relationships, or links, between and within the compartments must be determined. A **link** is defined as a “connection” between compartments (for transfer processes) or within a compartment (for

² The “particle on leaf” compartment type represents those particles deposited from air onto a leaf surface via wet and dry deposition. The chemical mass that is associated with the “particle on leaf” compartment can be transferred into the leaf or blown off the leaf surface, or can remain associated with the particles on the surface of the leaf.

transformation processes³) that allows one of these processes to occur. Each link contains an algorithm or multiple algorithms that mathematically represent the mass transfer or transformation. Figure 3-4 expands on the concepts presented in Figure 3-2 by showing links representing transfers 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.

The algorithms that mathematically represent mass transfer or transformation are assigned to links which specify the compartments involved in the transfer and the direction of transfer. This concept is demonstrated in Figure 3-5 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. For a transformation process, the link exists within a compartment to allow transformation between two chemicals (parent chemical and reaction product) within the same compartment (see Figure 3-6).

In the TRIM.FaTE framework, links provide for the organization and application of algorithms that describe chemical mass transfer among, and transformation within, compartments. Links “contain” the algorithms describing the one or more processes governing mass transfer across that link, as well as any properties specific to the link itself (but *not* those properties of the compartments or chemicals involved). For example, a link between two particular surface soil compartments may contain algorithms for advection of mass via erosion and runoff processes as well as information on the fraction of overland advective flow from one soil compartment to another. A soil-to-shrew link may contain an algorithm for intake of chemical mass via soil ingestion by the shrew. The algorithms contained on both of these links would also use properties of the sending and receiving compartments and the chemicals being modeled (*e.g.*, erosion rate, liquid volume of soil, ingestion rate of soil by the shrew, chemical partition factors) to calculate transfer factors.

3.4 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 and boundary contributions. A **source** is an external component that introduces chemical mass directly into an abiotic compartment. A common example of a source would be the factory emissions of a chemical into an air compartment. TRIM.FaTE is designed to accommodate single or multiple source scenarios. Currently, sources in TRIM.FaTE can introduce chemical mass into air compartments only.

³ Note that in TRIM.FaTE, chemical transformations that result in degradation products or metabolites of a parent chemical whose fate will not be tracked in the modeling scenario are considered “degradation” processes (see Chapter 4). Thus, chemical mass can be lost from the system of modeled compartments in two ways: (1) mass transferred into advection or flush rate sinks, and (2) mass transferred into degradation/reaction sinks due to degradation processes.

Figure 3-4
Two Linked Compartments in Separate Volume Elements

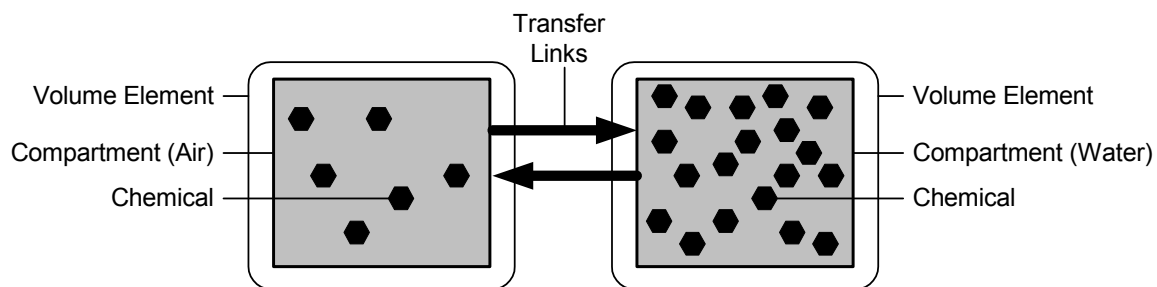


Figure 3-5
Three Linked Compartments in Two Volume Elements

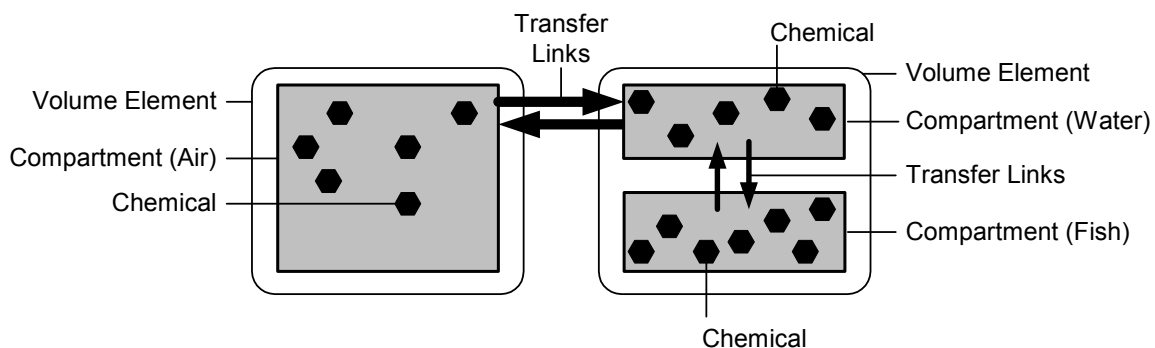
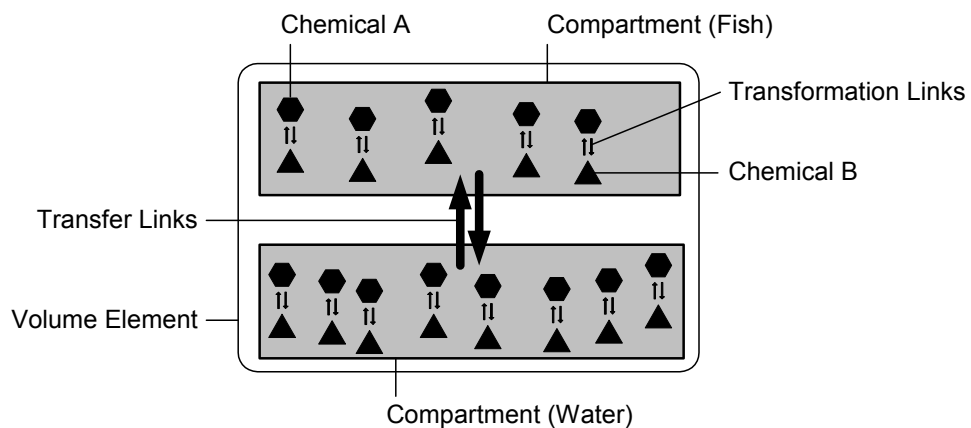


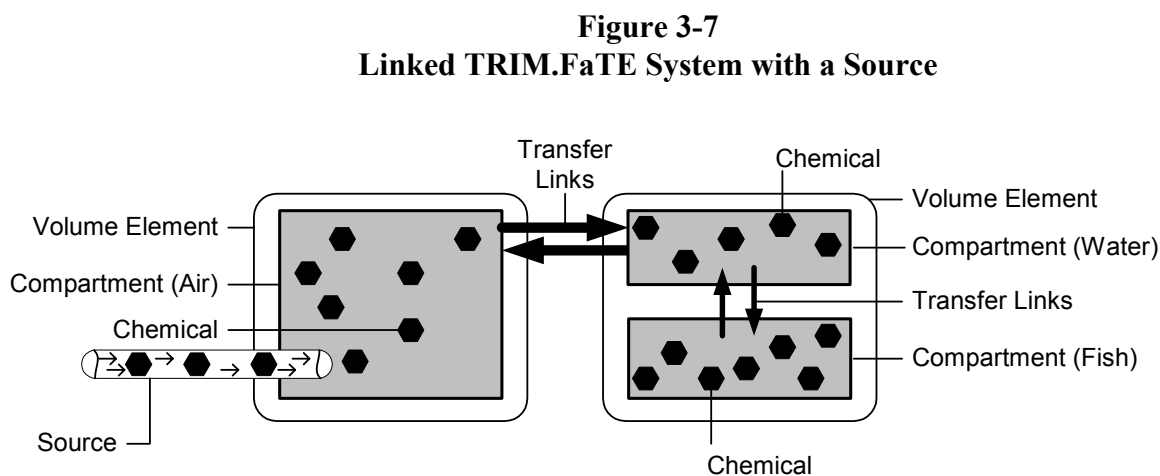
Figure 3-6
Transformation Links Between Chemicals within a Compartment



TRIM.FaTE differentiates between sources emitting within the modeling region (*e.g.*, air emissions from a facility stack) and sources of chemicals derived from outside the scenario modeling boundaries; the latter are referred to as boundary contributions (or boundary conditions) within the TRIM.FaTE framework. Sources emit chemicals directly to the primary abiotic compartment within which the source emission point(s) is located, as specified by coordinates (including height) assigned to the source. The emission rate of chemical entering this compartment (either a constant or time-varying rate) is specified by the user. A **boundary contribution** may be set for any outside interface of a compartment located on the outer sides of the modeled region. For air, a boundary concentration (which may be set by the user for the outer volume elements) establishes the concentration of a chemical in the air on the external (*i.e.*, non-modeled) side of the modeled region. Chemical mass enters the outside compartments via air advection algorithms that depend on wind speed, wind direction, and boundary concentration. Although currently implemented in TRIM.FaTE only for air compartments, boundary contributions could be set for other compartments as well (*e.g.*, flowing surface water compartments).

In addition, chemical mass can be included in the starting conditions for a scenario based on initial concentrations set by the user for abiotic or biotic compartments included in the TRIM.FaTE modeling scenario. The addition of mass to a scenario as an **initial concentration** in one or more compartments is a one-time event and represents concentrations in environmental media just before the simulation period begins. Outside of the TRIM.FaTE framework and terminology, this concept is often referred to as “background” concentrations. However, within the TRIM.FaTE framework, the word background is not used; the term “initial concentration” is used. A related TRIM.FaTE feature that can be useful for evaluation and diagnostic purposes is the ability to fix the concentration in any compartment to a user-specified value for the duration of the simulation.

Figure 3-7 adds to Figure 3-5 by showing a source emitting into the air compartment.



3.5 TIME-RELATED TERMS AND CONCEPTS

3.5.1 BASIC TIME TERMINOLOGY

TRIM.FaTE is a dynamic model (*i.e.*, the model accepts time-varying inputs and produces time-varying outputs), which makes it important that the time-related terminology is clearly defined and consistently used. There are three main time-related terms that are central to understanding how TRIM.FaTE relates input data, fate and transport calculations, and model outputs: **simulation period**, **input data time step**, and **output time step**. Definitions of these terms for the purposes of TRIM.FaTE are given below.

For a given TRIM.FaTE model run, the **simulation period** (or modeled time period) is the entire length of time over which the simulation occurs and compartment masses and concentrations are calculated – in other words, the time period from the beginning date and time of the simulation until the ending date and time. The simulation period is set by the user through specification of the simulation begin and end date and time. For most anticipated applications of TRIM.FaTE, the simulation period is expected to be one year or longer. Source emissions can occur for either all or part of the simulation period (*i.e.*, source modeling periods can be shorter than the simulation period), or even none of the simulation period if the analysis objective is to assess boundary conditions only (see Section 3.4).

Simulation period is the length of time over which the simulation occurs.

Input data time step dictates the points in time at which TRIM.FaTE calculates a new matrix of transfer factors.

Output time step is the frequency at which results are provided by the model.

The **input data time step** dictates the points in time at which TRIM.FaTE calculates new transfer factors (*i.e.*, a new transition matrix as described in Section 4.2). The input data time step refers to the interval between changes in value of any time-varying input (*e.g.*, wind speed data may be provided at hourly intervals). The input data time step (or time increments by which time-varying input data change) is recognized by the model during the run and can vary both across and within data types. That is, values for a particular data input can even be provided for erratically-spaced times during the simulation period (*e.g.*, Day 1, Day 2, Day 5, Day 7, Day 8, Day 9). In moving through the simulation time period, the model recalculates the relevant parts of the matrix of transfer factors with each occurrence of a change in input data. This up-to-date matrix is then relied on by TRIM.FaTE for its calculation of the distribution of chemical among the compartments.

The model can output results for any hourly time interval greater than or equal to one hour. The user specifies the frequency at which results are output (sometimes referred to as “**output time step**”) through the use of two model parameters: simulation time step and number

of simulation steps per output. Setting the simulation time step to 12 hours and the number of simulation steps per output step at 2, the model will write out results at 24-hour intervals throughout the simulation period. Setting the number of simulation steps per output step to 1 would produce results at 12-hour intervals (*i.e.*, that specified by the simulation time step). That is, the product of the two parameters is the time interval between model outputs (*i.e.*, the output time step). The results at each output time are those derived for that time point (*i.e.*, a “snapshot”), and are **not** an average over any time period. The time series results output from TRIM.FaTE can also be averaged over various time periods of interest (*e.g.*, each day, month, year) using an averaging feature of TRIM.FaTE.

For a modeling scenario with 100 compartments, a 30-year (262,800 hour) simulation period, a simulation time step of 1 hour, and the number of simulation time steps per output equal to 2, there would be 13,140,000 ($100 \times 262,800 \div 2$) reported values **each** for moles, mass, and concentration results for **each** chemical modeled.

TRIM.FaTE also can be run in a steady-state mode. In this mode, there are no time-varying inputs, no simulation period, and no output time step; the model’s run time is negligible compared to the dynamic modeling mode. In the steady-state mode, TRIM.FaTE calculates single values for chemical moles, mass, and concentration for each compartment. These values approximate the levels that the chemical would reach if the dynamic form of the model was run for a long enough period of time to allow all mass “inputs” and “outputs” to balance for each compartment (*i.e.*, to reach a steady-state).

3.5.2 OTHER TIME-RELATED CONCEPTS

Much of TRIM.FaTE’s data are, in reality, time-varying and can be treated as such by the model, although it is expected that typically most would be treated as being constant over time. However, inputs such as meteorological data (*e.g.*, wind speed and direction), stream flow, and source emissions rate typically would be treated as time-varying in TRIM.FaTE model runs where sufficient data are available. Values for time-varying parameters can be provided to TRIM.FaTE in any time increment selected by the user, generally based on data availability and run time considerations. For example, meteorological data (*e.g.*, wind speed, precipitation measurements) may be available at hourly increments, and source emission rate data may be available at monthly increments; TRIM.FaTE can readily accommodate these different input data time increments. However, using smaller time increments for time-varying input data can increase the model’s run time.

TRIM.FaTE can model certain processes that vary by season and time of day. Including seasonal changes in chemical fate and transport modeling can be advantageous for at least two reasons: (1) a seasonally dependent model can be applied to regions where below-freezing temperatures occur, and (2) model runs can be implemented for durations greater than a single growing system. However, model realism gained by accounting for seasonality must be balanced with the burden on the user to collect site-specific data on seasonal processes.

Two seasonal processes are currently implemented for plants in TRIM.FaTE: litterfall, which allows chemical mass to be transferred from the leaves to the surface soil, and growing

season, which allows uptake of chemicals by plants only between the day of last and first frost.⁴ These processes are implemented by enabling or disabling certain links and the associated transfer algorithms depending on the date. Additional seasonal processes may be considered in future refinements to TRIM.FaTE (*e.g.*, dynamics of snow accumulation and snowmelt, timing and rate of growth of algae during and following a bloom, dietary and habitat changes by wildlife). In addition, day-night is simulated in TRIM.FaTE to allow for different exchanges between the plants and air or soil during the day and night. These processes are implemented by enabling or disabling certain links depending on the time of day.

⁴ In addition, seasonality in weather patterns is accounted for by the use of time-varying meteorological and streamflow data.

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 and mathematical framework 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 specific algorithms used to implement the approach are documented in Volume II of the TRIM.FaTE TSD.

4.1 CONCEPTUAL DESIGN

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

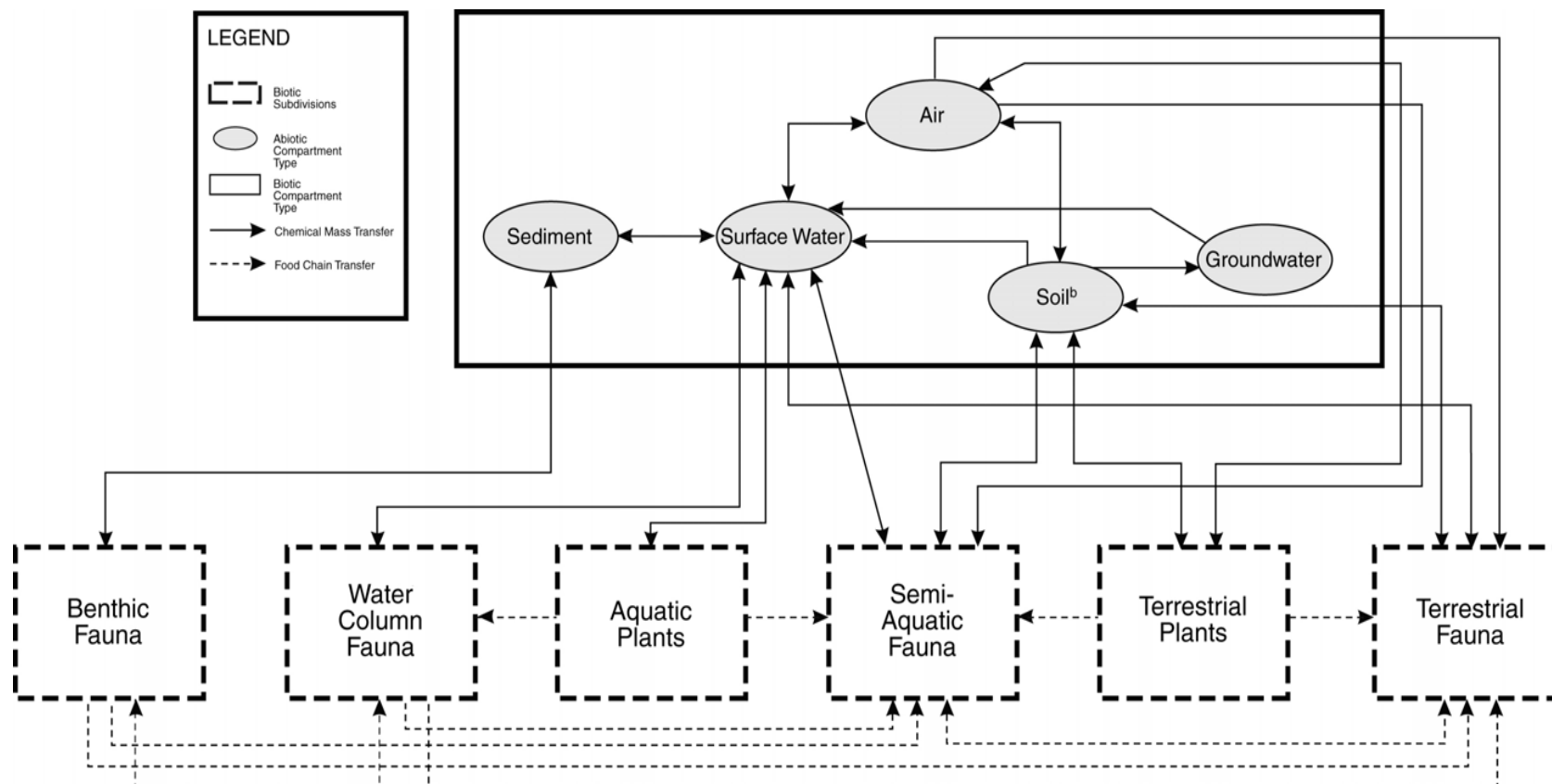
The development of TRIM.FaTE began with a conceptual diagram of the relationships and processes that affect chemical transport within the environment. The current version of this diagram is shown in Figure 4-1. In this figure, biotic compartments are represented by rectangles and abiotic compartments are represented by ovals. The arrows illustrate the potential chemical transfers between each of the components of the ecosystem. Chemical transformations, which may occur within compartments in TRIM.FaTE, are not included in Figure 4-1.

4.2 MASS BALANCE CONCEPTS AND EQUATIONS

TRIM.FaTE has been developed with an emphasis on maintaining a mass balance within the modeling system. That is, all inputs and outputs of the chemical of interest are tracked to ensure that the results are not unrealistic with regard to the relationship between the amount of that chemical being introduced to the system and the amounts predicted to be retained in and lost from the system. More specifically, it means that the amounts of the chemical of interest predicted to be retained in and lost from the system always sum to the amount of chemical introduced into the system. When applied to a specific compartment (*e.g.*, soil, or a mouse population), the mass balance approach implies that, over a given time period, the amount of the chemical of interest in the compartment at the end of the period is equal to the sum of the amount of that 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.

It should be noted that in order to accommodate transformation of a chemical and modeling of the fate of the transformation product chemicals, the mass balance aspect of TRIM.FaTE is achieved for the chemical entity of interest (*i.e.*, the “core chemical”). Inherent to the application of this approach is that the core chemical, which may be a part of the chemical

Figure 4-1
Simplified Conceptual Diagram for TRIM.FaTE^a



^a Sinks are not shown. Chemical transformation processes are not depicted but may occur in all compartment types. Transformation products may be tracked within compartments in TRIM.FaTE or transferred out of compartments to reaction/degradation sinks.

^b Includes surface soil, root zone soil, and vadose zone soil compartment types.

introduced into the system rather than the whole chemical (*e.g.*, the X molecule of a hypothetical chemical of formula XY_2), is an entity that maintains its chemical integrity throughout the modeling system. To date, certain mercury compounds are the only chemicals for which TRIM.FaTE applications have incorporated transformation among chemicals that are explicitly modeled. In this case, the mercury atom (in elemental or ionic form) is the core chemical for which mass balance is maintained within the system, and the model predicts distribution of that core chemical occurring as elemental, divalent, and methyl mercury within the system. That is, the mass of mercury atoms (regardless of its speciation or the compound of which it may be a part) that is introduced to the system is in balance with the sum of the mass and number of conserved units predicted to remain in and predicted to exit from the system.

To date, TRIM.FaTE has been implemented primarily for first-order linear transfer and transformation processes. Therefore, the following discussion is limited to algorithms of that type. It is important to note that higher order nonlinear methods can also be implemented within the TRIM.FaTE modeling structure.

First-order transfers between compartments are described by transfer factors, referred to as T-factors. T-factors are in units of inverse time and are not dependent on the sending and receiving chemicals or the amount of chemical in the sending compartment. The T-factor is the *instantaneous* flux of chemical normalized to the amount of that chemical in the sending compartment. The actual *instantaneous* flux (*i.e.*, the amount of chemical passing across an interface per unit time) can be calculated using the T-factor and the amount of chemical in the sending compartment.¹

First-order transformation of chemicals is described by a reaction rate, referred to as R. Conceptually similar to (and mathematically identical to) the T-factor, R is measured in units of inverse time. Due to the structure of TRIM.FaTE, a chemical molecule cannot be transferred to a different compartment and transformed simultaneously. Thus, when both a transformation and a transfer occur, two separate processes are modeled in TRIM.FaTE.² Transformations occur for chemicals *within* a compartment, and the reaction products (and remaining parent compound) may subsequently be transferred to another compartment or out of the system. A transformation in which a chemical of interest is converted to a chemical species for which transport and fate are *not* modeled is handled by transferring the chemical moles out of the system of compartments to a degradation/reaction sink. This kind of transformation is treated as an irreversible loss from the system.

¹ T-factors are actually applied to the moles of the chemical in the compartment, rather than mass, to facilitate the modeling of transformation. Although some of the transfer (*e.g.*, advection, diffusion) and degradation algorithms used in TRIM.Fate may be based on mass relationships, there is no mathematical impact of applying the T-factors to moles instead of mass when the sending and receiving chemical are the same. The algorithms involving inter-transformation processes between chemicals are based on mole relationships.

² When there are multiple processes being modeled for a chemical in a given compartment (*e.g.*, multiple transfer processes, simultaneous transfer and transformation), the processes are modeled separately but calculated concurrently based on the same starting number of moles (*i.e.*, the number of moles present in a compartment at the start of the series of calculations for a particular point in time).

A chemical also can be transferred to a sink via advective transport that moves the chemical beyond the physical boundaries of the modeled system (*e.g.*, moles of chemical that are blown out of the modeled area with the air or flushed out with surface water). This kind of sink is referred to as either an advection sink or a flush rate sink depending on the physical processes involved in transferring the chemical. The transfer of chemical to a sink by either advective transport or degradation/reaction is irreversible because after the chemical is transferred to a sink, it can no longer move to any other compartments.

Although TRIM.FaTE models chemical transfers among compartments and chemicals (where transformation is involved) on the basis of moles, it also provides the results in units of mass or concentration by multiplying the resultant moles in each compartment by the molecular weight of each complete chemical being modeled, or the weight of the entity of interest (*e.g.*, methyl mercury mass and concentration results can be provided either in units of methyl mercury or units of methylmercury, as mercury). Figure 4-2 illustrates the mass to moles to mass conversions in TRIM.FaTE.

A simplification of a first-order transfer process involving a single chemical (*i.e.*, no transformation between chemicals) is shown in the top part of Figure 4-3 for a system of one chemical, two compartments, and two degradation/reaction sinks, where degradation is treated as an irreversible loss. For this system, it can be seen that:

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

$$\text{Chemical losses for compartment A} = T_{ab} N_a + R_a N_a \quad (2)$$

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

$$\text{Chemical losses for compartment B} = T_{ba} N_b + R_b N_b \quad (4)$$

where:

- N_a = amount of chemical in compartment A, units of *moles*
- N_b = amount of chemical in compartment B, units of *moles*
- S_a = chemical source outputting to compartment A, units of *moles/time*
- T_{ab} = transfer factor for movement of chemical from compartment A to compartment B, units of */time*
- T_{ba} = transfer factor for movement of chemical from compartment B to compartment A, 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
Chemical Mass/Mole Conversions in TRIM.FaTE
(Example for a single chemical)

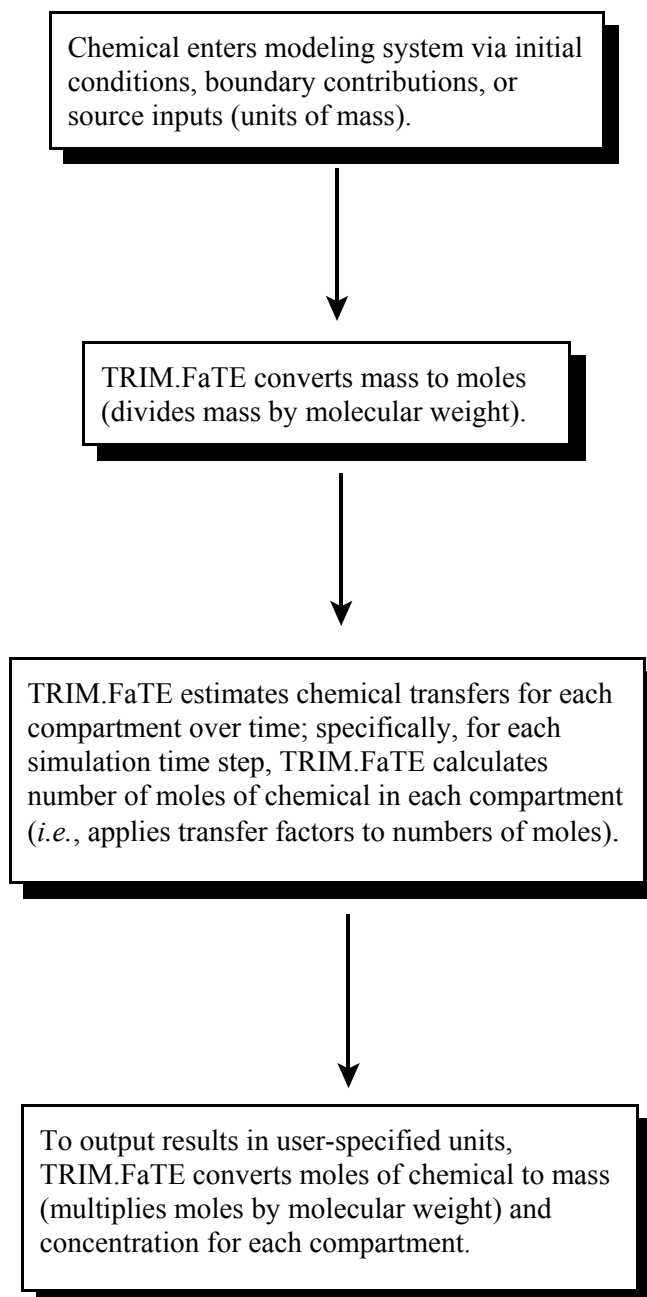
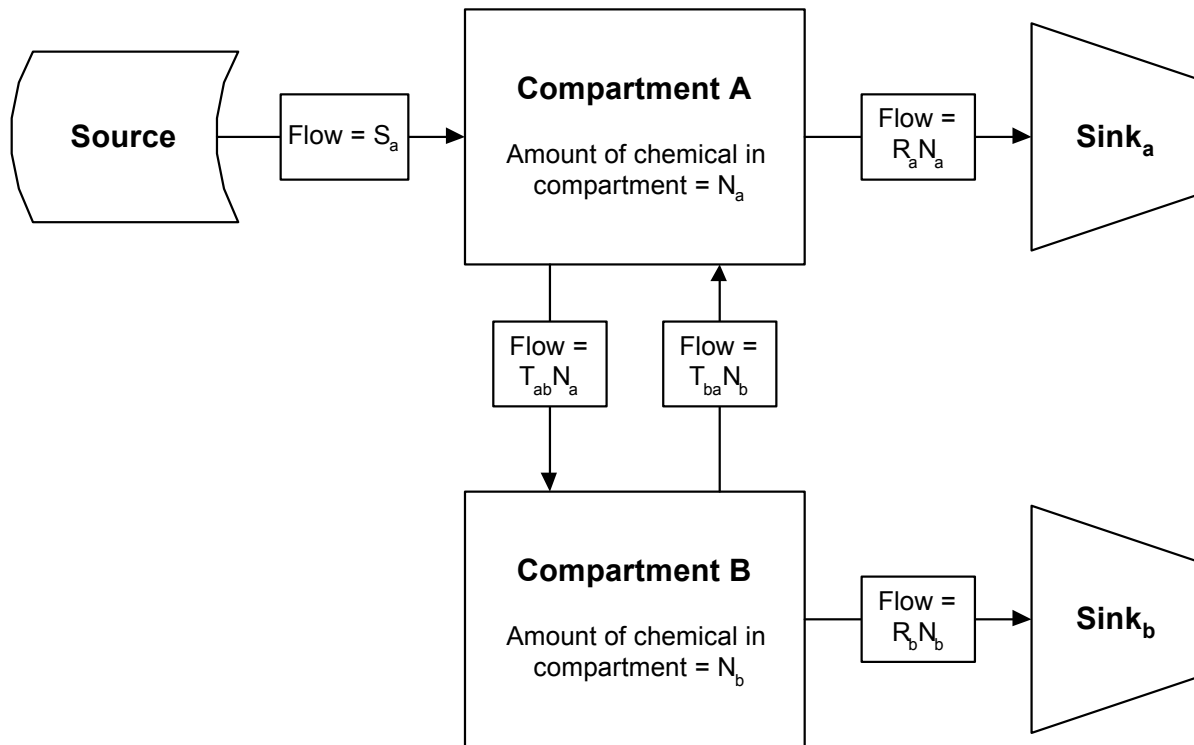


Figure 4-3
Example of First-order Transfer Processes for Two Compartments, One Chemical^a



$$\begin{bmatrix} dN_a/dt \\ dN_b/dt \\ d\text{Sink}_a/dt \\ d\text{Sink}_b/dt \end{bmatrix} = \begin{bmatrix} -(T_{ab} + R_a) & T_{ba} & 0 & 0 \\ T_{ab} & -(T_{ba} + R_b) & 0 & 0 \\ R_a & 0 & 0 & 0 \\ 0 & R_b & 0 & 0 \end{bmatrix} \begin{bmatrix} N_a \\ N_b \\ \text{Sink}_a \\ \text{Sink}_b \end{bmatrix} + \begin{bmatrix} S_a^0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (5)$$

^a In this one-chemical example, transformation is treated as an irreversible sink (*i.e.*, a degradation/reaction process). Note that the boxes in this figure labeled *flow* (and similar boxes designating either flow or reaction in subsequent figures) represent the transfer of chemical between compartments A and B as either $(T_{ab} \times N_a)$ or $(T_{ba} \times N_b)$, depending on the direction of the transfer. This “flow” represents the instantaneous change in chemical moles (*i.e.*, mole transfer) with respect to time and is not a constant value. The value for the mole transfer depends on the number of moles (*i.e.*, N_a or N_b) in the sending compartment. Because the number of moles changes continually as transfer process occur, the value for the mole transfer can change continually over time as moles are removed from and added to the sending compartment.

As discussed earlier, the constraint that mass balance must be preserved means that, over any time interval, the change in amount of chemical in a compartment is equal to the gains minus the losses over the time interval. For compartments A and B, this change in amount is the difference in equations (1) and (2), and (3) and (4), respectively. The instantaneous change in amount 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 of the two compartments A and B 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 mass that is accumulated in the degradation/reaction sinks. Thus, two additional compartments are added to the system as sinks and serve as the repository of the chemicals after a reaction creates a form of the chemical that is no longer modeled in the system. After the chemical is transferred to a sink, it cannot move to any other compartments within the system. $Sink_a$ and $Sink_b$ denote the mass in the degradation/reaction sinks for compartments A and B, respectively. Now the complete system can be described using equations (6) and (7) above along with (8) and (9) presented below:

$$\frac{d Sink_a}{dt} = R_a N_a \quad (8)$$

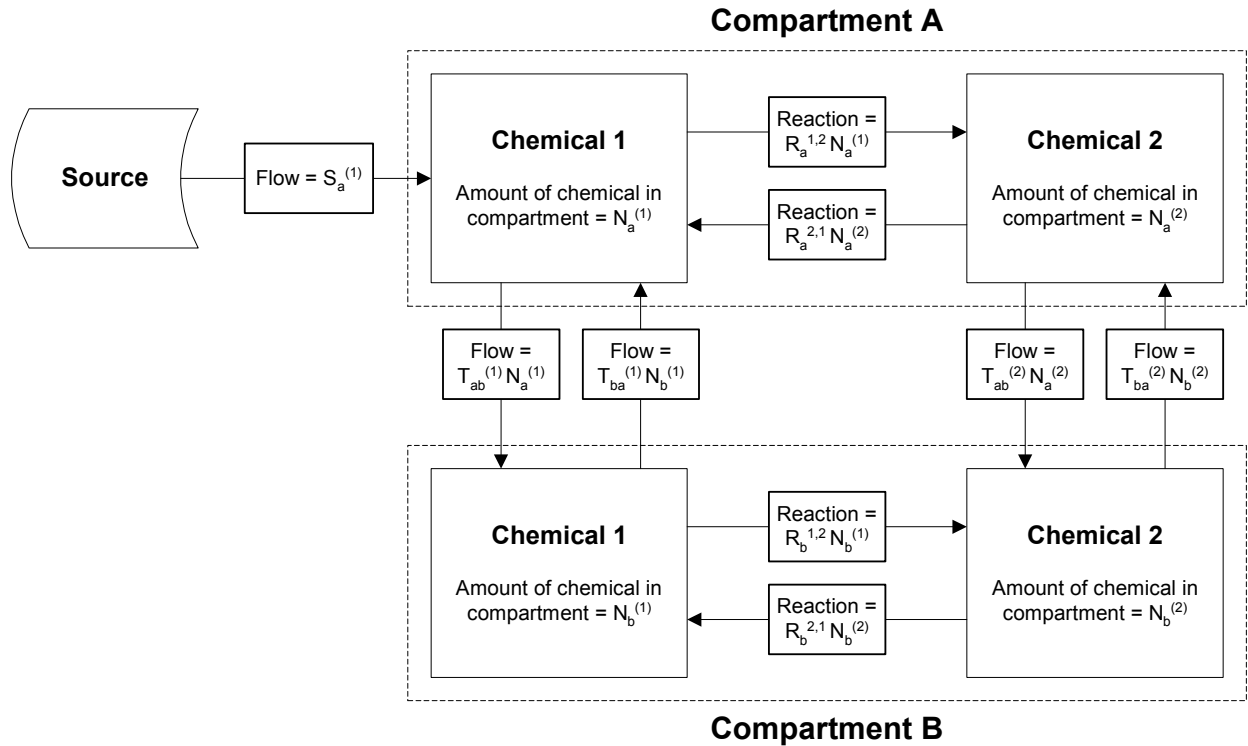
$$\frac{d Sink_b}{dt} = R_b N_b \quad (9)$$

This system of equations (equations (6) through (9)) is shown in matrix form in Equation (5) at the bottom of Figure 4-3.

For TRIM.FaTE, systems of linear ordinary differential equations are 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 use of LSODE in TRIM.FaTE is described in more detail in Appendix C of this document.

If the fate of the chemical created by a transformation reaction is to be modeled explicitly, and the necessary algorithms and input data are available for this transformation product, then the mass balance approach described above can be modified accordingly to include this transformation product. Figure 4-4 shows a generalization of the previous example to the case where the transformed chemical is modeled in addition to the parent chemical. In this case, in addition to the reaction rate, T-factors are added for the transformed chemical to account for additional possible transfers between compartments.

Figure 4-4
Example of First-order Transfer Processes for Two Compartments, Two Chemicals^a



^a This example illustrates the transformation and independent physical movement of two chemicals that can transform into each other.

Using the same approach used for the system in Figure 4-3, the more complex system in Figure 4-4 can be expressed as a set of four differential equations, as follows:

$$\frac{dN_a^{(1)}}{dt} = -T_{ab}^{(1)} N_a^{(1)} - R_a^{1,2} N_a^{(1)} + T_{ba}^{(1)} N_b^{(1)} + R_a^{2,1} N_a^{(2)} + S_a^{(1)} \quad (10)$$

$$\frac{dN_b^{(1)}}{dt} = T_{ab}^{(1)} N_a^{(1)} - T_{ba}^{(1)} N_b^{(1)} - R_b^{1,2} N_b^{(1)} + R_b^{2,1} N_b^{(2)} \quad (11)$$

$$\frac{dN_a^{(2)}}{dt} = R_a^{1,2} N_a^{(1)} - T_{ab}^{(2)} N_a^{(2)} - R_a^{2,1} N_a^{(2)} + T_{ba}^{(2)} N_b^{(2)} \quad (12)$$

$$\frac{dN_b^{(2)}}{dt} = R_b^{1,2} N_b^{(1)} + T_{ab}^{(2)} N_a^{(2)} - T_{ba}^{(2)} N_b^{(2)} - R_b^{2,1} N_b^{(2)} \quad (13)$$

where:

- $N_a^{(1)}$ = amount of core chemical 1 in compartment A, units of *moles*
- $N_a^{(2)}$ = amount of core chemical 2 in compartment A, units of *moles*
- $N_b^{(1)}$ = amount of core chemical 1 in compartment B, units of *moles*
- $N_b^{(2)}$ = amount of core chemical 2 in compartment B, units of *moles*
- $T_{ab}^{(1)}$ = transfer factor for movement of chemical 1 in compartment A to compartment B, units of */time*
- $T_{ab}^{(2)}$ = transfer factor for movement of chemical 2 in compartment A to compartment B, units of */time*
- $T_{ba}^{(1)}$ = transfer factor for movement of chemical 1 in compartment B to compartment A, units of */time*
- $T_{ba}^{(2)}$ = transfer factor for movement of chemical 2 in compartment B to compartment A, units of */time*
- $R_a^{(1,2)}$ = reaction/transformation of chemical 1 to chemical 2 in compartment A, units of */time*
- $R_a^{(2,1)}$ = reaction/transformation of chemical 2 to chemical 1 in compartment A, units of */time*
- $R_b^{(1,2)}$ = reaction/transformation of chemical 1 to chemical 2 in compartment B, units of */time*
- $R_b^{(2,1)}$ = reaction/transformation of chemical 2 to chemical 1 in compartment B, units of */time*
- $S_a^{(1)}$ = source for chemical 1 outputting to compartment A, units of *moles/time*

This system of equations can be summarized in matrix form as follows:

$$\begin{bmatrix} dN_a^{(1)}/dt \\ dN_b^{(1)}/dt \\ dN_a^{(2)}/dt \\ dN_b^{(2)}/dt \end{bmatrix} = \begin{bmatrix} -(\Gamma_{ab}^{(1)} + R_a^{1,2}) & \Gamma_{ba}^{(1)} & R_a^{2,1} & 0 \\ \Gamma_{ab}^{(1)} & -(\Gamma_{ba}^{(1)} + R_b^{1,2}) & 0 & R_b^{2,1} \\ R_a^{1,2} & 0 & -(\Gamma_{ab}^{(2)} + R_a^{2,1}) & \Gamma_{ba}^{(2)} \\ 0 & R_b^{1,2} & \Gamma_{ab}^{(2)} & -(\Gamma_{ba}^{(2)} + R_b^{2,1}) \end{bmatrix} \begin{bmatrix} N_a^{(1)} \\ N_b^{(1)} \\ N_a^{(2)} \\ N_b^{(2)} \end{bmatrix} + \begin{bmatrix} S_a^{(1)} \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (14)$$

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:

$$\frac{d\vec{N}}{dt} = A(t)\vec{N}(t) + \vec{s}(t), \quad \vec{N}(t_0) = \vec{N}_0 \quad (15)$$

where:

- $\vec{N}(t)$ = an M -dimensional time-dependent vector whose i th entry is the moles of chemical in the i th compartment
- $A(t)$ = an $M \times M$ -dimensional time-dependent matrix
- $\vec{s}(t)$ = an M -dimensional time-dependent vector accounting for the source terms contributing to each compartment.

The vector \vec{N}_0 is the initial distribution of chemical moles among the compartments. The vector $\vec{N}(t)$ is the distribution of chemical moles among the compartments over time. 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 transition matrix is used in TRIM.FaTE to solve for the T-factors at each time step. The vector $\vec{s}(t)$ accounts for pollutant sources emitting the chemical to specific compartments over time.

4.3 PHASES

Chemicals in the environment can exist in various phases (*e.g.*, liquid, gas, solid). The chemical mass in each phase is tracked in TRIM.FaTE because transfer factors are phase-dependent (*e.g.*, the transfer factor for suspended particulate deposition from air is applied only to the chemical mass in the particulate phase of air). There are multiple environmental phases modeled within the abiotic compartments in TRIM.FaTE. A chemical's phase distribution is generally assumed to be at chemical equilibrium within a compartment (see Volume II of the TSD for exceptions). For example, chemical mass sorbed to suspended particulate matter (solid phase) exists in equilibrium along with chemical mass present as vapor (gas phase) in an air compartment. The adjacent text box lists the phases currently implemented in TRIM.FaTE for each abiotic compartment type.³

PHASES CURRENTLY IMPLEMENTED IN TRIM.FaTE

Air

- vapor/gas
- suspended particulate

Soil^a

- soil pore water
- vapor/gas
- soil solids

Surface water

- water
- suspended solids-algae
- suspended solids-other

Sediment

- sediment pore water
- sediment solids

Groundwater

- soil pore water
- soil solids

^a Includes surface, root zone, and vadose zone soil compartment types.

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 generally assumed, the ratios of the concentrations in the individual phases are constant over time for a given chemical. The fraction of the chemical that is in each phase in a compartment is calculated in TRIM.FaTE using either partitioning or fugacity concepts. Both concepts are mathematical approaches to describe the same physical phenomena. Partitioning coefficients are empirical relationships that show the distribution of a specific chemical between two phases. Fugacity is a measure of a chemical's potential to remain in any particular phase based on its chemical properties. Transfer between two phases is dependent on the fugacity capacity of a chemical, or the tendency for the chemical to "escape," or transfer, to another phase. Details and calculations for the implementation of phases in TRIM.FaTE are presented in Chapter 2 of Volume II of the TRIM.FaTE TSD.

³ Algae are included as a phase within surface water rather than a separate compartment type because of the limited data available to explicitly model chemical movement between algae and surface water at the time TRIM.FaTE was being developed for mercury. Given the available uptake algorithm for algae, uptake was assumed to occur by passive diffusion and could thus be most simply represented by equilibrium partitioning.

4.4 FATE, TRANSFORMATION, AND TRANSPORT PROCESSES

In TRIM.FaTE, the following physical, chemical, and biological processes are implemented as first-order mathematical processes for modeling the transfer and transformation of chemicals:

- Advection;
- Dispersion;
- Diffusion;
- Biotic processes; and
- Reaction and transformation.

Qualitative descriptions of these five types of processes are presented in the subsections below. 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.

Fate and transport algorithms developed for early prototypes of TRIM.FaTE were specific to nonionic organic compounds (*i.e.*, phenanthrene and benzo(a)pyrene). Transfer factors used in the algorithms contained in these prototypes relied upon the concept of fugacity for modeling some types of chemical transfers; however, the concept of fugacity cannot generally be applied to metals and other inorganic compounds. In order to address the fate and transport of metals and other inorganic compounds using TRIM.FaTE, non-fugacity-based algorithms can be developed. The current version of TRIM.FaTE includes algorithms specifically developed for mercury and mercury compounds as well as several individual PAHs; it is expected that many of these algorithms can be used for other metals and organic and inorganic compounds as well. The flexibility of the TRIM.FaTE framework allows for the development of additional algorithms specific to other chemicals.

4.4.1 ADVECTION

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 (*i.e.*, mass per time traveling across an interface) is the velocity of the moving phase and the amount of the chemical that is in the moving phase. Examples of advective processes included in TRIM.FaTE for transport of a chemical include erosion from a surface soil compartment to a surface water compartment, runoff of water from a surface soil compartment to a surface water compartment, and transport from one air compartment to another due to the wind.

4.4.2 DISPERSION

Dispersion refers to the “spreading out” of a chemical during advective transport and can result in movement in any direction relative to the direction of advective flow (including

perpendicular to the flow). Dispersion can be partially explained by Brownian motion, which is the movement of small particles as they are randomly bombarded by the molecules of the surrounding medium. In the current version of TRIM.FaTE, dispersion is explicitly addressed (as a first-order process) in transfers between surface water compartments using the methods presented in the Water Quality Analysis Simulation Program (WASP) water transport model (Ambrose et al. 1995).

Horizontal dispersion between air compartments is not currently modeled in TRIM.FaTE due to the complexity of accurately modeling this process in a compartment-based model. Currently, vertical dispersion is not modeled either. For a compartment-based model like TRIM.FaTE, however, the assumption that chemicals are instantaneously distributed evenly throughout a compartment volume results in three-dimensional “numerical dispersion” in the air compartments. The effective dilution that results from this assumption is generally much larger than the effects of dispersion in air.

4.4.3 DIFFUSION

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

4.4.4 BIOTIC PROCESSES

The transport of chemicals to biota (*i.e.*, into biotic compartments) consists of advective and diffusive processes, though the former term is rarely used by biologists. For example, chemicals deposit onto plant leaves with particles in air, an advective process; chemicals also diffuse into plant leaves from air and from the plant surface. 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 macrophytes and benthic invertebrates by diffusion. The major advective process for the transport of chemicals into animals is food intake by fish, birds, and mammals. The transport of chemicals out of biota and into the surrounding abiotic compartment is also modeled within TRIM.FaTE by the same types of processes (*e.g.*, diffusion by benthic invertebrates, excretion by mammals).

The only transport process within biota (*i.e.*, within the biological system in the biotic compartments) that is included in TRIM.FaTE is advective transport within the composite leaf compartment between the leaves and the plant stem via xylem and phloem fluids. Modeling the distribution of chemicals among organs in fish and wildlife is not currently a feature of TRIM.FaTE; however, this increased complexity could be accommodated within the current TRIM.FaTE framework.

4.4.5 REACTION AND TRANSFORMATION

Reaction and transformation processes in the abiotic media include biodegradation (*i.e.*, the biotically mediated breakdown of the chemical in abiotic compartments), photolysis, hydrolysis, and oxidation/reduction. In biota, metabolic processes can transform the chemical to another chemical of concern tracked in the system or can break down (*i.e.*, degrade) the chemical into metabolites that are not followed in the system. Transformation is modeled in TRIM.FaTE as a reversible reaction using first-order rate equations, as discussed in Section 4.2. In all TRIM.FaTE applications to date, transformation is modeled as a bi-directional process between two inter-transforming chemicals that occurs via a pair of transformation algorithms, whereas degradation is modeled as an irreversible first-order reaction. The first-order transformation and degradation rates may be process-specific, or they may incorporate more than one of the processes involved. First-order rate constants are equivalently described in TRIM.FaTE as transformation half-lives (*i.e.*, a rate constant can be mathematically converted to a half-life and vice-versa). 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.

5. APPLICATION OF TRIM.FaTE

This chapter illustrates 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. Note that the text here is simply a summary based on the applications of TRIM.FaTE to date and the associated chemicals, algorithms, compartment specifications, and properties. Future applications may expand upon these or implement alternatives. However, it is expected that the basic framework for model application will remain as presented here.

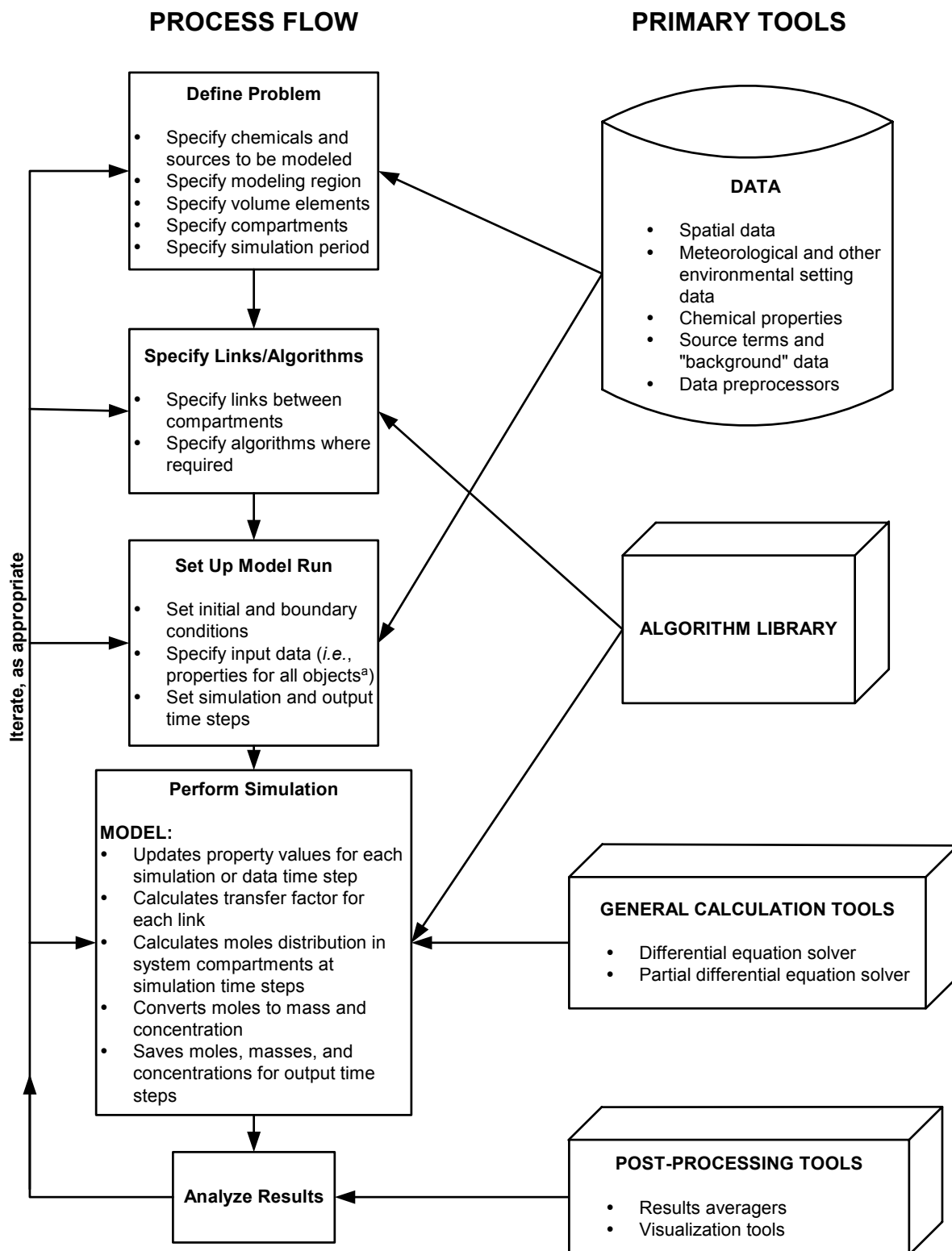
This chapter is not intended to serve as a user's guide to the model; rather, it provides a broad understanding of how TRIM.FaTE works by explaining in general terms how it is used to simulate the multimedia fate and transport of air emissions from one or more sources. For detailed information on installing and navigating TRIM.FaTE software, applying the model for a specific scenario, and other aspects of operating TRIM.FaTE, refer to the TRIM.FaTE User Guidance.

5.1 GENERAL PROCESS FOR A TRIM.FaTE SIMULATION

TRIM.FaTE is designed to be an iterative and flexible model. Although there are a number of steps that the user must include in the development and application of a TRIM.FaTE simulation, some of the order in which these steps are completed is flexible. The general process is shown in Figure 5-1. The boxes on the left side of the figure categorize the basic steps involved in the completion of TRIM.FaTE simulation: problem definition, specification of links, simulation set-up, model execution, and analysis of results. In an actual application, progression through the modeling process might not be quite as linear as that shown in the figure. However, all of the tasks identified in the basic steps must be addressed during the course of developing and executing a TRIM.FaTE simulation.

The vertical arrows linking the steps under the "Process Flow" heading represent the typical order of events in an application. The arrows to the left indicate that model application might involve multiple iterations as the modeling scenario is refined. Primary components of the analysis are illustrated under the "Primary Tools" heading and linked with arrows to the relevant steps in the "Process Flow" column. To focus on key aspects of the TRIM.FaTE approach, only selected tools are shown. There are other tools that may be relied upon that are not indicated in this figure (*e.g.*, sensitivity analysis and Monte Carlo features, steady state solver).

Figure 5-1
TRIM.FaTE Modeling Sequence



^a The term objects refers to sources, chemicals, volume elements, compartments, and the scenario.

5.2 PROBLEM DEFINITION

TRIM.FaTE is not intended for use in assessments involving air pollutant emissions where the air is the medium of interest; rather, it is intended for applications involving air pollutant emissions where the assessment focus is on non-air media. The first step in the TRIM.FaTE modeling process is articulating a clear statement of the problem and then translating that into the TRIM.FaTE structure. In defining the problem for a TRIM.FaTE application, the chemical(s), source(s), primary spatial features of the ecosystem, and simulation period are defined. Using the nomenclature presented in Chapter 3, the volume elements and compartments within the volume elements are specified.

The TRIM.FaTE problem definition is based directly on the underlying objectives of the fate and transport/exposure/risk assessment to be performed. As recommended in recent EPA and other risk guidance, a clear problem formulation should be developed for the fate and transport/exposure/risk assessment before any modeling begins. This is particularly important for highly flexible models like TRIM.FaTE.

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

The sources and chemicals to be included in the TRIM.FaTE simulation are identified in the first step of the problem definition process. Generally, this identification flows directly from the overall problem formulation for the fate and transport/exposure/risk assessment. This step must be performed first because the chemical(s) and location of the source(s) can influence how the region to be modeled is delineated and subdivided. In determining the chemicals to be modeled, the user should consider the objective of the modeling exercise, the available emissions information, and the potential effects and receptors of concern. The user must decide, given the objectives and resources available for the analysis, which sources and chemicals should be included in the modeling analysis. The process of identifying chemicals of concern and associated sources should be referenced to existing EPA guidance when possible.

5.2.2 DETERMINING SCALE AND SPATIAL RESOLUTION

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. Definitions for the important spatial terms used in this section are discussed in more detail in Chapter 3 and are summarized in the adjacent text box. After the initial scenario is constructed and a simulation has been completed, the preliminary results

A **parcel** is a planar (*i.e.*, two-dimensional), horizontal geographical area used to subdivide the modeling region. Parcels, which are polygons of 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 (soil or surface water).

A **volume element** is a bounded three-dimensional space that defines the location of one or more compartments.

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

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 the TRIM.FaTE User Guidance.

It is important to note that TRIM.FaTE is designed to model the fate and transport of air pollutant emissions into non-air media. Scenarios may be created that range from general and conceptual (*e.g.*, an environment consisting of air, soil, and a water body) to more detailed and site-specific (*e.g.*, capturing major land and water topographic variation in a 25 square mile area). The compartment-based design, with its assumptions of homogeneity within compartments, is not intended to provide fine scale resolution of predicted pollutant concentrations. When such detail is desired for particular media (*e.g.*, a water body), it may be appropriate to also consider use of a detailed model specific to that medium (*e.g.*, a water quality model). As noted previously, for assessments of air pollutant emissions where the air is the medium of interest, users should rely on an air quality model.

5.2.2.1 Specifying the Modeling Region

The first step in determining the scale and spatial resolution of a TRIM.FaTE scenario is to determine the scale of the modeling region (*i.e.*, external spatial boundaries of the analysis). In this step, the user specifies the geographical extent of the area to be modeled. A user should consider factors such as mobility of the modeled chemical(s), location of source(s), location of sensitive populations, and background concentrations of the chemical(s). A scoping step using air dispersion modeling may be appropriate to evaluate the predicted spatial pattern of deposition. When the predominant wind direction is variable, the modeling region may need to extend beyond the region of primary interest to account for the possibility of pollutant mass leaving and re-entering the system. After the scale of the modeling region has been chosen, one must consider whether that scale is appropriate when compared to other sources of model uncertainty.

5.2.2.2 Specifying Parcels

Once the scale of the analysis is determined, the next step is to specify the spatial resolution of the modeling region using two-dimensional parcels—essentially polygons—that subdivide the modeling region. **Parcels** need to be defined for the air and for the land surface (*i.e.*, soil and surface water); these two sets of parcels do not need to have the same spatial layout (*i.e.*, their individual and combined boundaries do not need to line up). A larger number of parcels in a given scenario can be used to provide higher spatial resolution and/or greater areal coverage. It is noted however, that more parcels correspond to greater resource requirements, both in terms of model set-up and data collection as well as model run time.

Beyond complexity and 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);

- The locations of natural and land use boundaries; and
- The locations of important environmental or biological receptors. These can include populations of receptors (*e.g.*, human or ecological cohorts) or landscape components (*e.g.*, lake, agricultural area) of interest.

For the chemical(s) of interest, three important factors in determining the likely pattern of transport and transformation are the atmospheric transport of chemical mass, rapidity of chemical transport in media other than air, and transformation or 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 picture of the general path of chemical transport, helping the user determine where higher spatial resolution may be beneficial.

Information about the mobility and transformation or degradation of the chemical(s) of interest in soils and water, when combined with information on land use, 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 modeling region.

Natural boundaries are also an important consideration in developing the parcel layout. For example, an airshed boundary can be defined by a combination of geographical and meteorological conditions such as large valleys where inversion layers and diurnal wind patterns may result in a confined and relatively well mixed air mass within the area for extended periods of time. Airshed boundaries can also include smaller valleys when meteorological conditions produce a long residence time for the air mass in the bounded region. Airshed boundaries are useful in providing information about the scale of the overall modeling 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 surface parcels within the system, especially if chemical concentrations in a particular lake or stream are of interest. Watershed boundaries can be identified from existing references (*e.g.*, United States Geological Survey (USGS) applications) 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 it.

Land use and land cover data should be considered in defining land parcels. That is, it may be appropriate for the parcel layout to capture the pattern of land use and cover, including forest type, rangeland, or agriculture lands,¹ as land use homogeneity can be desirable within

¹ For example, it is useful to consider variation in vegetation type which may be important for the subsequent step of assigning vegetation and other biotic compartments.

parcels. Land use or land cover can also correspond with a particular receptor of interest (*e.g.*, ecological receptor(s) in a coniferous forest, or residents on small farms). The location of the receptor(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 receptor(s) and resolution to be finer in areas that may have a greater impact.

The illustrative approach to specifying parcels described in the TRIM.FaTE User Guidance provides a starting point for any given analysis objective for which TRIM.FaTE is used. The approach is intended to impart some consistency and transparency into the spatial set-up process while maintaining an adequate level of flexibility.

5.2.2.3 Specifying Volume Elements

After the parcels have been determined for a scenario, the volume elements corresponding to those parcels are specified. This step involves specifying the appropriate vertical dimension and resolution of the modeling region. Whereas parcels only represent the modeling region in two dimensions (*i.e.*, a horizontal plane), volume elements add the component of depth, thus representing the modeling region in three dimensions (the location and horizontal two-dimensional planar shape of a volume element correspond exactly to the relevant parcel). The volume elements are determined based on various factors, including knowledge of mixing heights in air, average depth of water bodies or approximate levels of stratification, and typical demarcations in the soil horizon (or demarcations of interest to a particular assessment). The specification of volume elements represents the final step in specifying the spatial dimensions of the modeling region.

TRIM.FaTE allows the specification of multiple layers of volume elements, when the additional complexity and resource requirements of doing so are offset by the desire for greater spatial resolution. In addition, the user must ensure that algorithms to model the transfer of chemical mass between multiple layers (or multiple vertically stacked volume elements) are included in the library. Although use of a single volume element (*i.e.*, no vertical stacking of volume elements), may be sufficient for the application at hand, use of multiple vertically stacked volume elements of the same type (*e.g.*, air, surface water) may be useful in particular assessments. For example, instead of one set of volume elements for the vadose zone (*i.e.*, one layer), additional vertical resolution can be gained by dividing the vadose zone into two or more vertically stacked layers of volume elements. Without such assignment of multiple volume elements of the same type, however, TRIM.FaTE currently accommodates vertical variation in soil through the use of separate volume elements of different types for the three major soil zones (*i.e.*, surface, root zone, and vadose zone) and the availability in the TRIM.FaTE library of algorithms describing vertical transport among them.

EXAMPLES OF VOLUME ELEMENTS USED IN TRIM.FaTE	
Air	Surface Water
Surface Soil	Sediment
Root Zone Soil	Ground Water
Vadose Zone Soil	

5.2.3 DETERMINING COMPARTMENTS

5.2.3.1 Abiotic Compartments

Abiotic compartment types are assigned as appropriate to each volume element (*e.g.*, air compartments in air volume elements, surface water compartments in surface water compartments). At least one abiotic compartment must be contained within each volume element. Although not currently implemented, the model framework supports multiple abiotic compartments within a volume element. In most cases, the determination of abiotic compartments is an implied step because these compartments are simply defined by the abiotic medium designation of the volume element.

5.2.3.2 Biotic Compartments

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 the modeled scenario and those that significantly affect concentration in the compartments of interest in the assessment. In applying the model to PAHs, for example, 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 only results of interest for a particular application were concentrations in abiotic compartments. In addition to plants, the TRIM.FaTE scenario should include those biotic compartment types that significantly affect chemical concentrations in the compartments of interest to the assessment.

The flexibility of TRIM.FaTE can accommodate a variety of designs for compartmentalization of biota for a modeling scenario. For example, a user can perform a TRIM.FaTE assessment for a whole trophic group using parameter values for a single species selected to be representative of all of the species in the group. In addition, a user can choose particular animal species of concern (*e.g.*, threatened or endangered populations) and parameterize the model for those species.

5.2.4 DETERMINING SIMULATION PERIOD

After determining the sources and chemicals to be modeled, the user determines the appropriate simulation period by considering the modeling objectives (per the problem definition), the lifetime of the modeled source(s), the persistence and mobility of the modeled chemical(s), and the effects of concern. The user should also consider resource limitations when determining the simulation period because this parameter directly affects the computing time. In addition to the dynamic modeling mode, TRIM.FaTE includes a feature for obtaining a steady solution. This is desirable for some assessments or for parts of some assessments, and provides substantial savings in computing time over a multi-year dynamic simulation.

5.3 DETERMINING LINKS/ALGORITHMS

The second step shown in Figure 5-1 is to assign the links, as appropriate, between the compartments and sinks specified for a given scenario (the compartment types currently available in TRIM.FaTE are listed in Chapter 3). Generally, for abiotic compartment types, the user will want to link all adjacent compartments to each other and link compartments at the edge of the modeling region to advection sinks. Biotic compartment types need to be linked to the appropriate abiotic compartments, as well as to other biotic compartments, depending on their relationships to each other in terms of the transfer of chemical mass. For example, each biotic compartment should be linked to all compartments that comprise its diet or in any way provide it a source of chemical mass (*e.g.*, terrestrial biota need to be linked to air compartments for inhalation of chemical), as well as to all compartments to which that biotic compartment provides chemical mass (*e.g.*, via excretion or by acting as a dietary component). TRIM.FaTE has a “SmartLink” feature that facilitates setting links, particularly among abiotic compartments. However, it is still necessary, particularly for biotic compartments, to carefully identify what links should be in place and confirm their placement or assignment within the TRIM.FaTE scenario.

The system of links is one of the most critical components of TRIM.FaTE. This component is critical because the links provide for the assignment of the algorithms describing the processes that drive chemical transfer and transformation. By specifying a link between two compartments, it is assumed that one or more algorithms² exist by which to estimate the transfer of chemical through the link via the prevailing processes. 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 described in the TRIM.FaTE User Guidance. Tables 5-1 and 5-2 present examples of links between abiotic and biotic compartment types, respectively, which are supported by non-transforming mass transfer algorithms in the current TRIM.FaTE library. In addition, Table 5-3 presents links that are implemented if the user chooses to apply the equilibrium model for bioaccumulation by fish (see Volume II of the TRIM.FaTE TSD for more information regarding this model for fish). To support the modeling of chemical transformation (*i.e.*, transportation of mass between different chemicals within the same compartment), TRIM.FaTE includes a feature that automatically creates links for each compartment with itself. At this time, the TRIM.FaTE library includes transformation algorithms for mercury species.

TRIM.FaTE also has the flexibility to use model results from single-medium models (*e.g.*, ISC) in place of 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. It is noted, however, that this could have ramifications on the mass balance feature of

² Where multiple process operate to transport chemical across a link (*e.g.*, deposition and diffusion between an air compartment and a soil compartment), multiple algorithms may be active (*i.e.*, enabled) on a single link. Additionally, there may be more than one algorithm, derived by different methods, which could be used to describe chemical movement across a link via the same process. In that case, the user must identify the algorithm preferred for the process in the current scenario and disable the other(s).

Table 5-1
Abiotic Compartment Type Links and Mass Transfer Processes

(Table includes non-transformation related examples supported by the current TRIM.FaTE algorithm library.)

Links Between Compartment Types		Mass Transfer Processes Addressed
Sending	Receiving	
Air	Air	Bulk Advection
	Surface Soil	Dry Deposition (of particles) Wet Deposition (of particles and vapors) Diffusion
	Surface Water	Dry Deposition (of particles) Wet Deposition (of particles and vapors) Diffusion
	Air Advection Sink	Bulk Advection Beyond System Boundary
Surface Water	Air	Diffusion ^a
	Surface Water	Bulk Advection Dispersion
	Sediment	Suspended Sediment Deposition Pore Water Diffusion
	Surface Water Advection Sink	Bulk Advection Beyond System Boundary
Sediment	Surface Water	Resuspension Pore Water Diffusion
	Sediment Burial Sink	Solids Advection Beyond System Boundary
Surface Soil	Air	Diffusion ^a Resuspension
	Surface Soil	Erosion Runoff
	Root Zone Soil	Percolation Diffusion
	Surface Water	Erosion Runoff
	Surface Soil Advection Sink	Erosion Beyond System Boundary Runoff Beyond System Boundary
Root Zone Soil	Surface Soil	Diffusion
	Root Zone Soil	Percolation (if multiple root zone layers)
	Vadose Zone Soil	Percolation Diffusion

Links Between Compartment Types		Mass Transfer Processes Addressed
Sending	Receiving	
Vadose Zone Soil	Root Zone Soil	Diffusion
	Vadose Zone Soil	Percolation (if multiple vadose zone layers)
	Ground Water	Percolation
Groundwater	Surface Water	Bulk Advection (recharge)

^a Includes volatilization.

Table 5-2
Biotic Compartment Type Links and Mass Transfer Processes

(Table includes non-transformation related examples supported by the current TRIM.FaTE algorithm library.^a)

Links Between Compartment Types		Mass Transfer Processes Addressed
Sending	Receiving	
Air	Plant Leaf	Uptake ^b
	Terrestrial and Semi-aquatic Wildlife (birds and mammals)	Inhalation ^c
Air (Particulates)	Particle on Leaf	Wet Deposition ^c Dry Deposition ^c
Air (Rain Water)	Leaf	Wet Deposition ^c
Plant Leaf	Particle on Leaf	Diffusion
	Surface Soil	Litterfall ^c
	Air	Diffusion/Advection
	Terrestrial Vertebrate Herbivore and Omnivore	Diet ^c
	Semi-aquatic Herbivore	Diet ^c
	Plant Stem	Uptake ^b (advection only)
Particle on Leaf	Surface Soil	Particle Washoff ^c Litterfall ^c
	Plant Leaf	Uptake ^b (diffusion only)
	Terrestrial Herbivore and Omnivore	Diet ^c
	Semi-aquatic Herbivore and Omnivore	Diet ^c
Plant Stem	Plant Leaf	Uptake ^b (advection only)
Plant Root	Root Zone Soil	Equilibrium Partitioning

Links Between Compartment Types		Mass Transfer Processes Addressed
Sending	Receiving	
Surface Soil	Terrestrial Ground-invertebrate Feeder	Diet ^c
	Terrestrial Vertebrate Herbivore and Omnivore	Diet ^c
	Semi-aquatic Herbivore	Diet ^c
	Plant Stem	Uptake ^b (advection only)
Root Zone Soil	Plant Root	Uptake ^b (equilibrium partitioning)
	Soil Detritivore	Uptake ^b
	Plant Stem	Uptake ^b (advection only)
Surface Water	Macrophyte	Equilibrium Partitioning ^b
	Fish ^e	Gill Exchange ^{bd}
	Water-column Herbivore	Diet (algae as phase of surface water) ^c
Macrophyte	Surface Water	Equilibrium Partitioning ^b
Sediment	Benthic Invertebrate (Flying Insect) Herbivore ^f	Uptake ^b
Terrestrial and Semi-aquatic Predator/Scavenger	Surface Soil	Excretion ^b
Terrestrial Vertebrate Herbivore	Semiaquatic Omnivore	Diet ^c
	Terrestrial and Semi-aquatic Predator/Scavenger	Diet ^{cg}
	Surface Soil	Excretion ^b
Terrestrial Omnivore, Insectivore, and Ground-invertebrate Feeder	Terrestrial Predator/Scavenger	Diet ^c
	Semi-aquatic Piscivore	Diet ^c
	Surface Soil	Excretion ^b
Soil Detritivore	Surface Soil (soil arthropod)	Equilibrium Partitioning
	Root Zone Soil (earthworms)	Equilibrium Partitioning
	Terrestrial Ground-invertebrate Feeder (earthworms)	Diet ^c
	Terrestrial Insectivore (arthropods)	Diet ^c
	Terrestrial Omnivore, Semi-aquatic Omnivore, and Terrestrial Predator/Scavenger (worms and arthropods)	Diet ^c

Links Between Compartment Types		Mass Transfer Processes Addressed
Sending	Receiving	
Water-column Herbivore and Omnivore	Semi-aquatic Omnivore	Diet ^c
	Semi-aquatic Piscivore	Diet ^c
	Water-column Carnivore	Diet ^{cd}
	Surface Water	Elimination ^{cd}
	Semi-aquatic Predator/Scavenger	Diet ^c
Water-column Carnivore	Semi-aquatic Omnivore	Diet ^c
	Semi-aquatic Piscivore	Diet ^c
	Surface Water	Elimination ^{cd}
	Semi-aquatic Predator/Scavenger	Diet ^c
All Semi-aquatic Wildlife	Surface Soil	Excretion ^b
	Surface Water	Excretion ^b
Benthic Omnivore	Benthic Carnivore	Diet ^{cd}
	Surface Water	Elimination ^{cd}
Benthic Carnivore	Surface Water	Elimination ^{cd}
Benthic Invertebrate	Semi-aquatic Omnivore	Diet ^c
	Sediment	Equilibrium Partitioning ^b
	Benthic Omnivore	Diet ^c
Flying Insect (emerged from benthic larval insect) ^f	Semiaquatic Predator/Scavenger	Diet ^c
	Semi-aquatic Insectivore	Diet ^c

^a Examples of links among aquatic fish compartments that are supported by the time-to-equilibrium model for bioaccumulation by fish are not shown here; they are presented in Table 5-3.

^b Uptake, filtration, or partitioning which includes diffusion, advection, and/or active accumulation and elimination by organism.

^c Advection processes.

^d Bioenergetic model for bioaccumulation by fish.

^e "Fish" include the following compartment types: benthic omnivore, benthic carnivore, water-column herbivore, water-column omnivore, and water-column carnivore.

^f The flying insect compartment is modeling an insect with an aquatic benthic larval phase; assumes insect emerges and becomes a flying adult invertebrate with the same body concentration as aquatic larval phase.

^g The presence of the terrestrial herbivore to terrestrial predator/scavenger link will depend on the species or groups selected to represent these compartment types for particular site (e.g., a mouse could be prey for red-tailed hawks or mink, but a deer might not be prey for any predators).

Table 5-3
Biotic Compartment Type Links and Mass Transfer Processes:
Time-to-Equilibrium Model for Bioaccumulation by Fish ^a

(Table includes non-transformation related examples supported by the current TRIM.FaTE algorithm library.)

Links Between Compartment Types		Mass Transfer Process Addressed
Sending	Receiving	
Surface Water (algae as phase of surface water)	Water-column Herbivore	Equilibrium Partitioning
Water-column Herbivore	Surface Water (algae as phase of surface water)	(Equilibrium Partitioning)
Sediment	Benthic Invertebrate (Flying Insect) Herbivore ^b	Equilibrium Partitioning
Benthic Invertebrate (Flying Insect) Herbivore ^b	Sediment	Equilibrium Partitioning
Water-column Herbivore	Water-column Omnivore	Equilibrium Partitioning
Water-column Omnivore	(Water-column Herbivore)	(Equilibrium Partitioning)
	Water-column Carnivore	Equilibrium Partitioning
Water-column Carnivore	(Water-column Omnivore)	(Equilibrium Partitioning)
Benthic Invertebrate	Benthic Omnivore	Equilibrium Partitioning
Benthic Omnivore	(Benthic Invertebrate)	(Equilibrium Partitioning)
	Benthic Carnivore	Equilibrium Partitioning
Benthic Carnivore	(Benthic Omnivore)	(Equilibrium Partitioning)

^a In the current library, the algorithms implementing this model are limited to use with mercury species.

^b The flying insect compartment represents an insect with an aquatic benthic larval phase; assumes insect emerges and becomes a flying adult with the same body concentration as aquatic larval phase.

TRIM.FaTE. A description of how external models can be integrated with TRIM.FaTE is presented in Appendix B.

5.4 SIMULATION SET-UP

The third step shown in Figure 5-1 is providing the relevant input data for the simulation. 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, environmental data needed by the selected algorithms, and the simulation and output time steps. Note that some properties must be specified before links can be made. The role of these inputs in estimating the chemical fate and transport is briefly explained in this section. A complete list

of all the parameters for the currently implemented algorithms is presented in Appendix D of Volume II of the TRIM.FaTE TSD.

5.4.1 CHEMICAL PROPERTIES

To estimate the fate and transport of chemical mass through the system, certain 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 or degradation rate (in each environmental medium)
- Henry's Law constant
- melting point
- molecular weight

ILLUSTRATIVE EXAMPLES OF BIOTIC CHEMICAL PROPERTIES

- half-life or rate of metabolic degradation (for each modeled animal or plant species)
- chemical transformation rates (in modeled plant leaves and animal species)
- elimination rate (for modeled animal species)

5.4.2 INITIAL AND BOUNDARY CONDITIONS

For each compartment and chemical in a scenario, the user has the option of specifying an initial concentration. In addition, the user can specify boundary concentrations for volume elements that include an external interface (*e.g.*, air volume elements located around the outer edge of the modeled domain). Boundary contribution algorithms for air compartments in outer volume elements can then be applied to account for continuing contribution of chemical to the modeled region from external sources (*e.g.*, the cumulative effect of non-local sources). Default values of zero may be assumed for boundary concentrations for pollutants that have a relatively short half-life in the air or if the objective of the simulation is to assess the effects of a modeled source (or sources) in the absence of "background." If the objective is to assess "cumulative" exposures, or if results of the analysis are to be compared with measurement data, however, the initial concentration and boundary contribution features may be essential. Refer to Section 3.5 for additional discussion of initial and boundary conditions in TRIM.FaTE.

Additionally, the user can specify concentrations (in one or more compartments of any type) to be held constant (or fixed) throughout the simulation period. This feature is useful for evaluation or diagnostic simulations.

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
- chemical-specific emission rate

5.4.4 ENVIRONMENTAL SETTING DATA

Whereas initial and boundary 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 environmental data necessary for TRIM.FaTE to estimate mass transfers in abiotic media: 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 data are required for many of the transport-related algorithms. For example, the air advection algorithms rely on wind data, and some of the deposition algorithms from air to surface soil and surface water rely on precipitation data. The meteorological and related inputs needed for TRIM.FaTE are listed in the adjacent text box (vertical wind velocities are also needed when modeling multiple air layers). Meteorological data at any (or various) time intervals can be used in TRIM.FaTE (*e.g.*, hourly wind speed and direction data). Preprocessors are available to convert the available meteorological data to the format required for TRIM.FaTE. For example, TRIMet is a data preprocessor developed for use with TRIM.FaTE to process the necessary meteorological data and convert them into a single, specifically formatted, meteorological input file.

METEOROLOGICAL INPUTS

- horizontal wind speed
- horizontal wind direction
- air temperature
- precipitation rate
- mixing height
- day/night
- beginning and end of litter fall
- frost date

5.4.4.2 Other Environmental Setting Data

Other environmental setting data are needed to define the characteristics of the biotic and abiotic compartment types that TRIM.FaTE uses to estimate the transport and transformation of chemical mass in the system. For example, data on atmospheric dust load are needed for TRIM.FaTE to estimate dry deposition of airborne particles to soils and surface water; data on sediment porosity (*i.e.*, water content) are required to estimate mass transfers between a sediment compartment and its overlying surface water compartment. In addition, some data are also required to define properties of links between compartments, such as the fraction of total surface runoff from one soil compartment that enters into an adjacent soil or water compartment. Input data values can be provided to TRIM.FaTE as point estimates, or, when using the stochastic

sampling feature for uncertainty analyses, as distributions (with appropriate associated characteristics such as mean and standard deviation). 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 DEFINING TIME STEPS

The final inputs necessary to begin a TRIM.FaTE simulation are the time steps. The simulation time step specifies a minimum frequency at which the model will calculate transfer factors and chemical mass exchange between (and transformation within) compartments.³ The output time step (defined by a combination of the simulation time step and the number of simulation steps per output)

determines the points in time at which the amount of chemical in each compartment will be reported as an output as moles, mass, or concentration. Post-processors may be used to aggregate these results over specified averaging periods. For example, the results using an output time step of one hour may be averaged to produce the mean daily or monthly concentrations of the pollutant in each compartment. Refer to Section 3.2 for a more detailed discussion of basic timing issues and Section 5.6 for more information on analysis of results.

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)

5.5 SIMULATION IMPLEMENTATION

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 by the model to the algorithm library to determine the transfer factors that mathematically describe the potential exchange of chemical mass across an interface between two compartments or a compartment and a sink. 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 is 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).

³ As described in Section 3.5.1, the model also calculates the chemical inventory at each time point when a new value is encountered for any inputs.

The basic TRIM.FaTE outputs are described in the adjacent text box. The concentration estimates in the abiotic compartments and uptake rates (*i.e.*, doses) for 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.

A separate part of the application of TRIM.FaTE at a site involves analysis of uncertainty and variability for a simulation. The concepts and processes involved with that analysis are discussed in Chapter 6, Treatment of Uncertainty and Variability.

TYPES OF OUTPUTS

TRIM.FaTE provides several different types of output to a user. The main TRIM.FaTE outputs are the moles, mass, and concentration in each compartment at each reporting time step. TRIM.FaTE can also output all algorithms used, all input values, and transfer factors for each transfer of mass. In addition, TRIM.FaTE can output certain intermediate calculated values, such as the calculated chemical mass moving across the interface between two volume elements, that can be used for evaluating the performance of the model.

5.6 ANALYSIS OF RESULTS

After 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 100 compartments for 30 years, with simulation and reporting time steps of one hour, the model would produce nearly 79 million values each for moles, mass, and concentration ($3 \times 100 \times 30 \times 8,760$). Even using a reporting time of once per day (*i.e.*, 24-hour reporting time step) would result in over three million output values. 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, different users will have different needs for the model's output. 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, and long-term time trends of environmental concentrations.

TRIM.FaTE also includes tools that facilitate analysis of results by summarizing and condensing output data through spatial, tabular, and graphical methods. Examples of three tools currently implemented in TRIM.FaTE are presented here.

- The **Averager** can generate averages of TRIM.FaTE outputs in any multiple of the output time step as well as in monthly and annual increments. It can also limit the compartments included in the averaged file by excluding selected results columns (each column represents the results for a single compartment). These functions are useful for reducing the size of output files for further off-line analysis in a separate program (*e.g.*, spreadsheet or other quantitative analysis program).
- The **Graphical Results Viewer** presents model results (moles, mass, or concentration) for each compartment type on a map of the parcels by using different colors to represent incremental gradations in the results for a specific chemical. Results can be presented

for any time increment that is output by the model or generated using the Averager. The results can also be animated over a time series (*e.g.*, to show changes in monthly average concentration over the course of a multi-year run).

- The **Aggregator** can produce tables in HTML, text, or comma-delimited formats that combine columns of output data in different ways for producing combined or comparative statistics. Functions available for combining results columns include sum, average, difference, ratio, and percent difference. For example, the user can use this tool to combine columns for similar chemicals (*e.g.*, to calculate total mercury for a particular compartment type) or to compare two columns (*e.g.*, to compare results for two PAHs and calculate differences in concentration).

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 (USEPA 1999). Additional background on how this method was selected is provided in Appendix B of the TRIM Status Report (USEPA 1999). 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 (e.g., taking more precise measurements of people's heights does not reduce the natural variation in heights). However, it can often be accounted for by a more detailed model formulation (e.g., modeling peoples' heights in terms of age will reduce the unexplained variability due to variation 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.FaTE. The first stage, consisting of sensitivity analyses that are comparatively easy to implement, identifies influential parameters and generates an importance-ranking of parameters. The results of this stage are useful for narrowing down the number of parameters to be analyzed in the second-stage uncertainty and variability analysis and are also useful in evaluating model structure and modeling assumptions. 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.

6.1 SENSITIVITY ANALYSES

The sensitivity analysis provides a quantitative characterization of the sensitivity of the model results to variations in the model input parameters. A ranking of sensitivity results can be used to provide a first-order determination of the most influential parameters that will need to be included in the detailed uncertainty analysis. Assessment of whether it is reasonable that parameters would have the influence they do in the model can also aid in evaluating model structure and modeling assumptions.

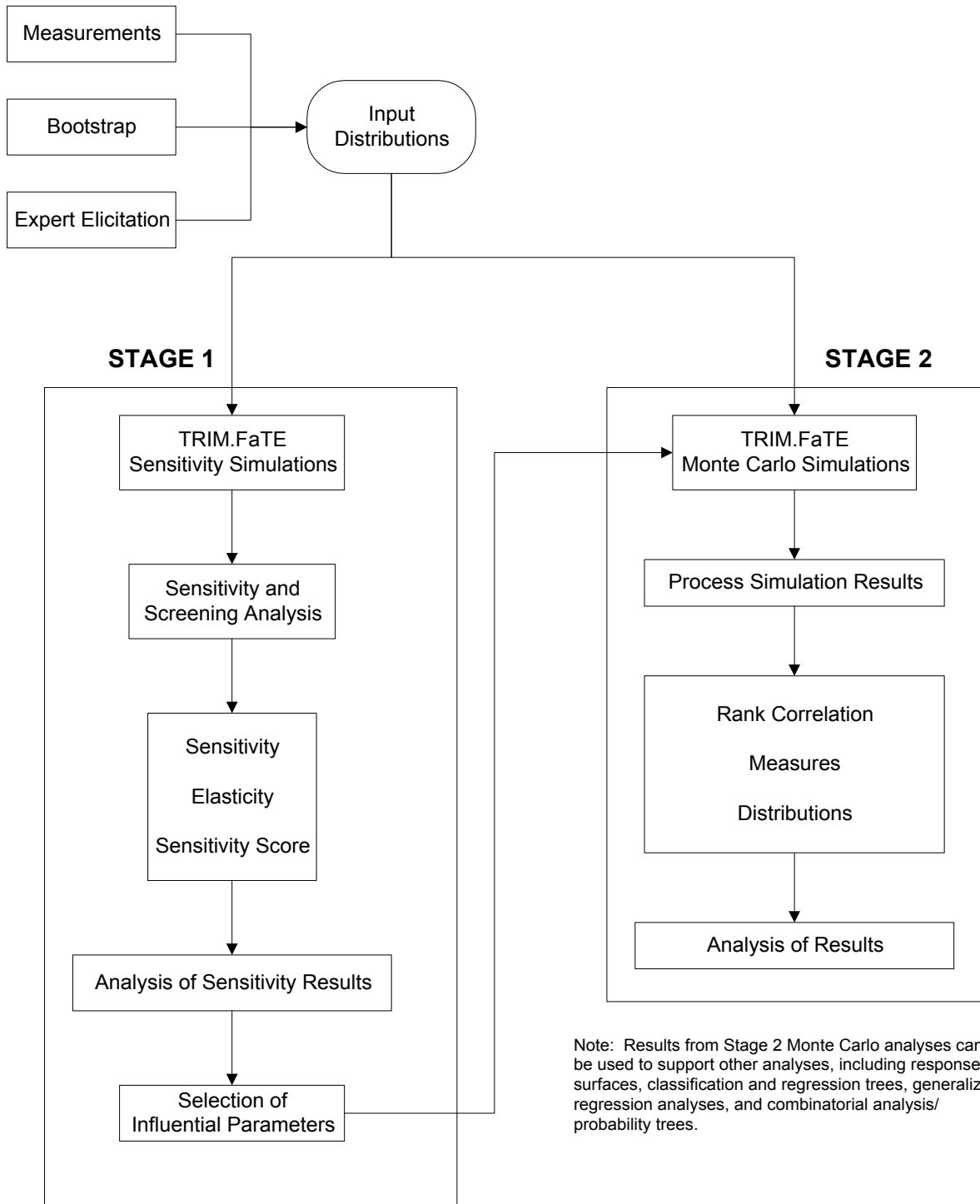
The TRIM.FaTE sensitivity feature allows the user to choose a set of parameters to vary, the compartments in which to vary them, and the compartments and chemicals for which the results are of interest. A parameter can be varied in parallel across all compartments of a specific type (*e.g.*, vary the organic carbon content in surface soil simultaneously for all surface soil compartments, where the varying parameter values would match across all surface soil compartments) or independently in specific compartments (*e.g.*, vary organic carbon content in surface soil separately for each compartment). One simulation of the user's design (*e.g.*, a 5-year dynamic run, or a steady-state analysis) is completed per selected parameter for comparison to the base simulation of the same design. All parameter values in that simulation would match the values in the base simulation except for the selected parameter which is set equal to a new value.

In the current version of TRIM.FaTE, the parameters to be varied must be constants or time-varying values such as meteorological data (*i.e.*, parameters that are specified by formulas in the model cannot be varied). The amount by which each selected parameter is varied (represented by p) is specified by the user, and may be a small fixed percentage (*e.g.*, one to ten percent) of the nominal parameter value or 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 (*e.g.*, the range from the 10th to the 90th percentile). A simulation for each parameter is required for this analysis; thus, 2,000 simulations would be needed to examine 2,000 parameters.

For the selected compartment and chemical outputs of interest, the system will calculate the sensitivity score for each parameter based on a specified result (*e.g.*, the average concentration values for the last year of the simulations). Thus, the user may run simulations of the TRIM.FaTE model with the parameters being varied singly, with the model results summarized to show the sensitivity to parameters and to identify the most influential parameters.

The results of a sensitivity analysis are applicable to a particular location and for the range of conditions (*i.e.*, parameter space) simulated, and may not apply to conditions outside of this. To generate more broadly applicable sensitivity results, the sensitivity analysis can be performed for a number of different "nominal" base simulations representing distinct modeling regimes (*e.g.*, summer and winter time periods, wet and arid locations).

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



Varying parameters so that they are both larger and smaller by $\pm p$ (*i.e.*, varying by $\pm p$ instead of just $+ p$) doubles the number of simulations required to complete the analysis, but allows the user to calculate the local nonlinearity of the effect of varying a parameter on the model results (*i.e.*, the nonlinear impact of varying parameters around a given value, for values close to the original value). These results are reported as second order terms in the sensitivity measures to show the extent of local nonlinearity for parameters. Non-local nonlinearities (*i.e.*, the nonlinear effects of wider variations of a parameter value) are quantified by increasing $\pm p$ to be in the range of 10 to 100 percent of the nominal values or spread of the parameters.

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 automatically computed in sensitivity analyses are the *sensitivity*, the *elasticity*, and the *sensitivity score*. The user can set up sensitivity simulations to calculate the *nominal range sensitivity* if desired. 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 $\frac{\partial y}{\partial p}$, 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 , keeping all other parameters fixed, and is referred to as a “local” measure.

We calculate the sensitivity by:

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

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

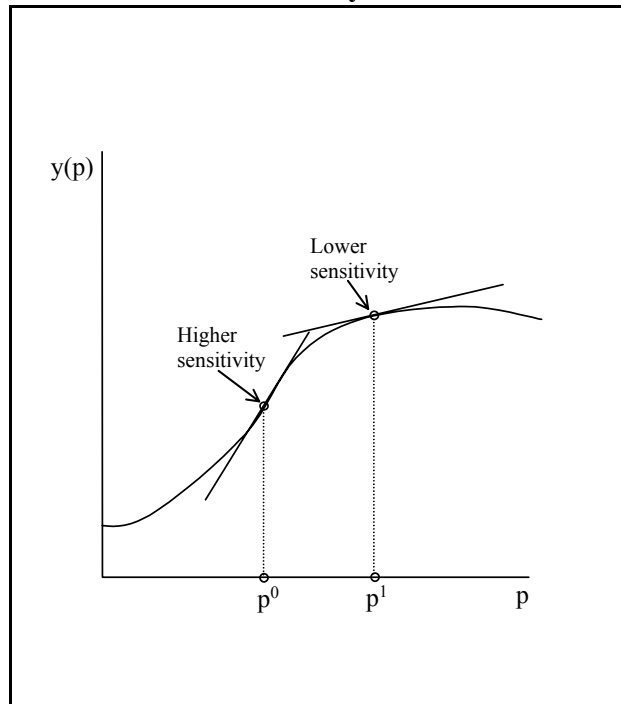
$$y = y(p^0 + \Delta p) - y(p^0) \quad (15)$$

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:

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

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 . The sensitivity to a parameter can be quite different at different values p^0 of the parameter. It can be useful to vary both Δp and p^0 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 :

$$Elasticity = \frac{\Delta y}{y^0} / \frac{\Delta p}{p^0} \quad (17)$$

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:

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

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).

6.2 THE MONTE CARLO APPROACH FOR UNCERTAINTY AND VARIABILITY ANALYSES

A Monte Carlo approach with Latin Hypercube Sampling (LHS) is available within TRIM.FaTE 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 can treat 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.

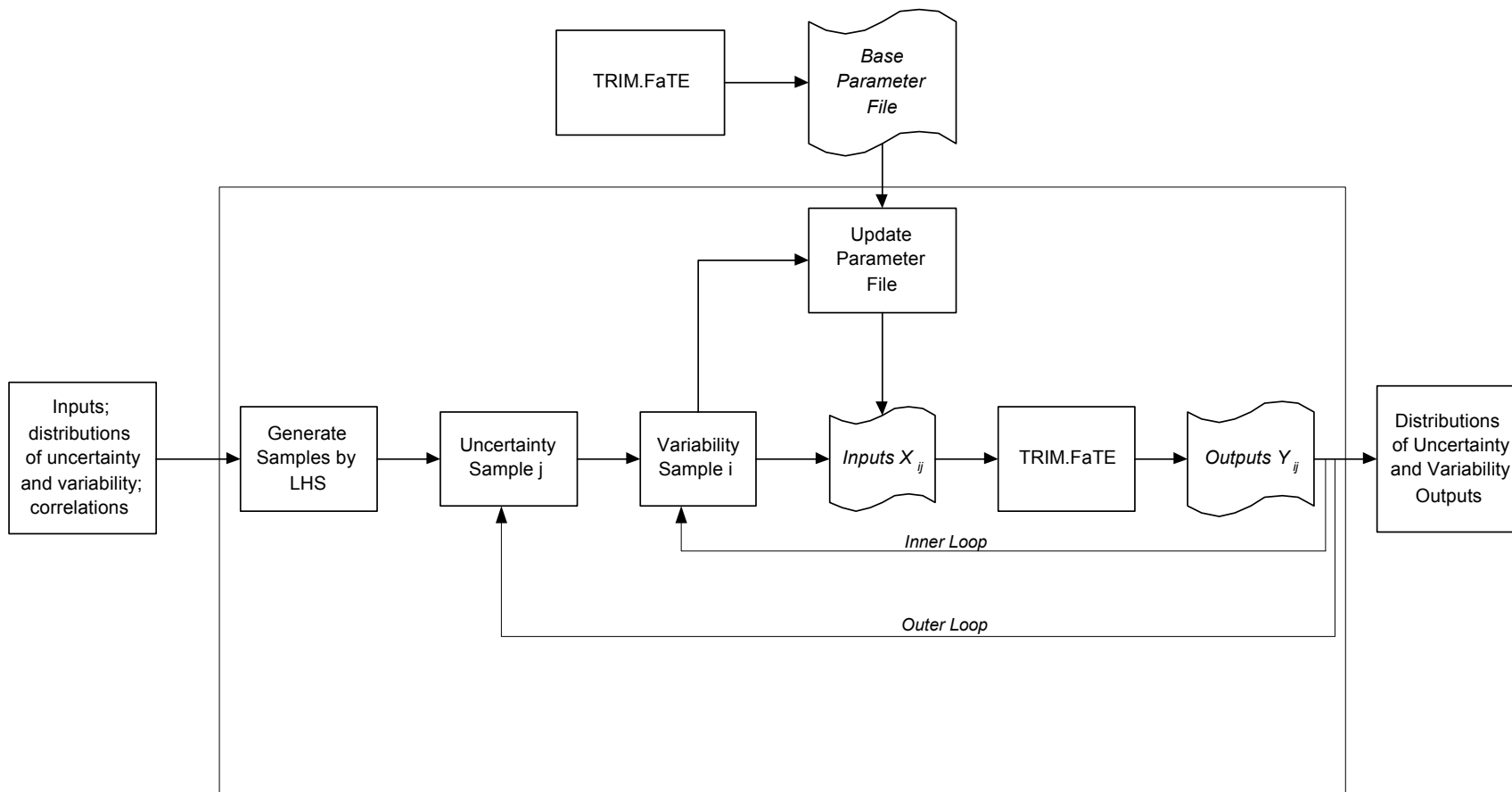
A significant limitation results from the fact that the analysis of uncertainty and variability requires estimates of parameter distributions that reflect both uncertainty and variability individually, and information on the distributions for parameters is not available for most parameters. Estimates of dependencies (*i.e.*, correlations) between parameters would enable a more detailed analysis to be performed, although this is of lesser importance. However, 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 by developing distributions for the parameters to which the model shows the greatest sensitivity. Distributions are not needed for all parameters.

6.2.1 TWO-STAGE MONTE CARLO DESIGN

Two-stage Monte Carlo designs are used to characterize uncertainty and variability separately. This is not currently implemented in TRIM.FaTE, and is being considered for a future version. 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 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 (*e.g.*, mean, percentiles, variance). For each of these statistics, there are N_u values, corresponding to the N_u uncertainty samples. These are then used to calculate a cumulative distribution function for each statistic, representing the uncertainty distribution for that statistic.

Figure 6-3
Two-stage Monte Carlo Approach



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. In general, distributions can be specified as parametric forms of probability distribution functions (PDFs) or cumulative distribution functions (CDFs), as nonparametric PDFs or CDFs, or as sets of data points from which samples are drawn. At the present time the distributions supported by TRIM.FaTE are the uniform, normal, lognormal and triangular distributions. Future enhancements to TRIM.FaTE will include an expansion of the types of distributions which can be specified by the user.

Distributions for parameter variability and for parameter uncertainty are required for those parameters to be analyzed; TRIM does 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.

Both the simple random sampling and LHS techniques are available in TRIM.FaTE. The preferred sampling technique is LHS, which employs a stratified random sampling without replacement scheme that is very efficient for sampling, especially for multiparameter models (Iman and Shortencarier 1984, Iman and Helton 1987, Helton and Davis 2000). 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. This is being considered for inclusion in a future version of TRIM.FaTE.

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. These techniques are being considered for a future version of TRIM.FaTE.

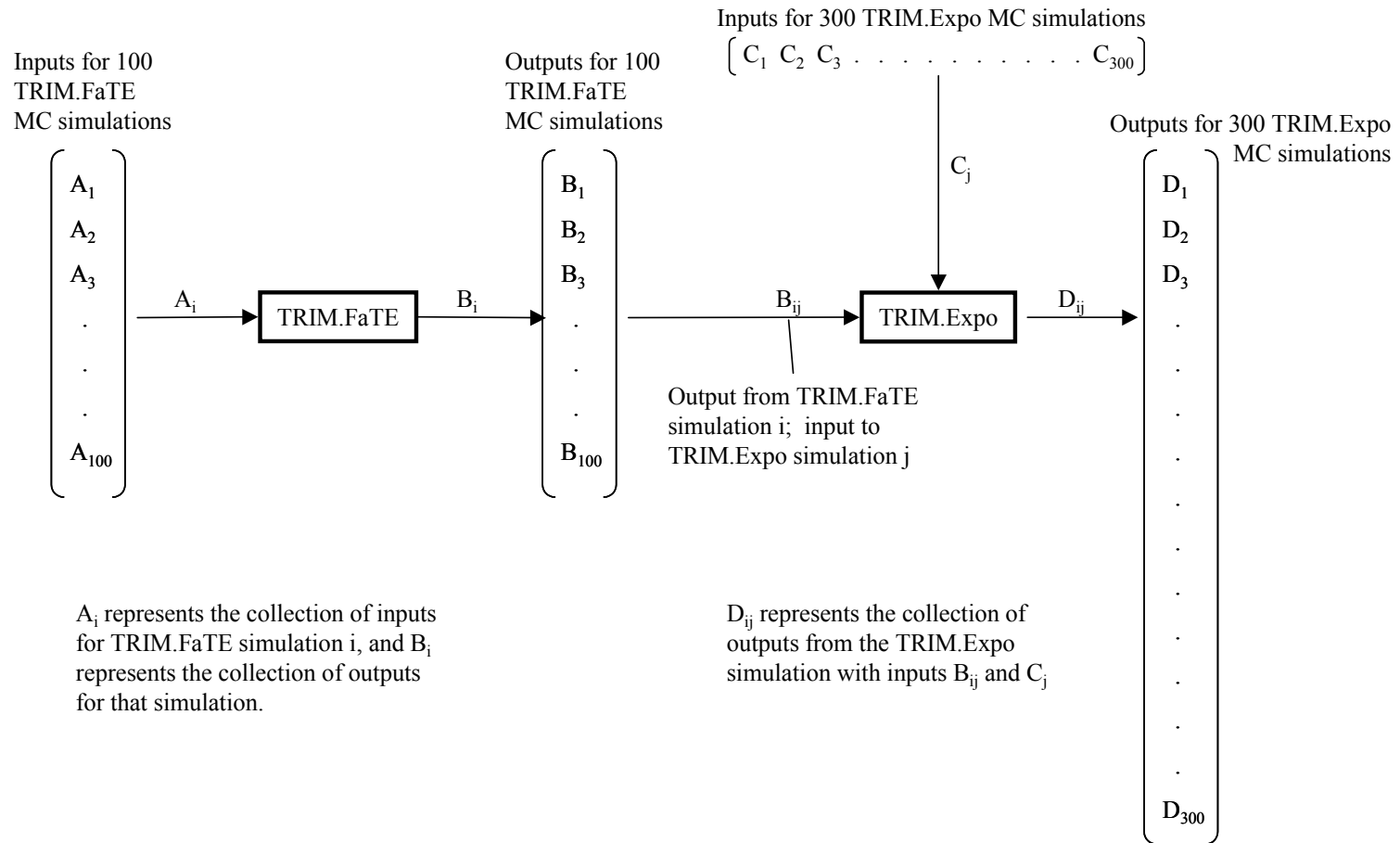
6.2.5 TRACKING INFORMATION BETWEEN MODULES

There are two levels at which tracking of information related to uncertainty analysis occurs; the first is within each TRIM module, and the second is from one TRIM module to the next. 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. This is accomplished by maintaining a record of the input parameter values used for each Monte Carlo simulation of a TRIM module. Simulations of one module are randomly selected for input to Monte Carlo simulations for a succeeding module, while keeping track of the input values for all simulations.

For example, take the first module to be TRIM.FaTE and the following module to be TRIM.Expo. TRIM.Expo takes as inputs some of the results generated by TRIM.FaTE, in addition to other input parameters. Suppose that 100 Monte Carlo simulations of TRIM.FaTE are performed and, following this, TRIM.Expo is going to be run for 300 Monte Carlo simulations. Figure 6-4 provides an illustration of this example. For each of the TRIM.Expo Monte Carlo simulations, one of the TRIM.FaTE simulations is randomly selected and the results of this simulation used for input to TRIM.Expo. There are other input parameters also input to TRIM.Expo, and some of these might be sampled from uncertainty and/or variability distributions as part of the Monte Carlo process. Using the notation of Figure 6-4, suppose the i^{th} TRIM.FaTE simulation is selected for the j^{th} Monte Carlo simulation of TRIM.Expo. For this simulation, TRIM.FaTE inputs $\{A_i\}$ result in outputs $\{B_i\}$ which are then input to TRIM.Expo. The other inputs to the j^{th} Monte Carlo simulation of TRIM.Expo are denoted as $\{C_j\}$, and the results of this simulation are denoted as $\{D_j\}$. Then, each of the 300 simulations of TRIM.Expo are tagged with the indices i_j and j to respectively track the corresponding TRIM.FaTE and TRIM.Expo input values, for $j = 1$ to 300. The index I takes values from 1 to 100, but is indexed by j so that the TRIM.FaTE inputs used for the j^{th} TRIM.Expo simulation are tracked.

The same process would be used for a module following TRIM.Expo, where the 300 TRIM.Expo simulations would be tagged by i_j , $j = 1$ to 300.

Figure 6-4
Example of Propagation of Uncertainty and Variability Between TRIM Modules



A_i represents the collection of inputs for TRIM.FaTE simulation i , and B_i represents the collection of outputs for that simulation.

D_{ij} represents the collection of outputs from the TRIM.Expo simulation with inputs B_{ij} and C_j

Care must be taken to ensure that the model input values are consistent in sequences of runs. For example, if there is an input to TRIM.FaTE which is also an input to TRIM.Expo, then the value for the TRIM.Expo simulation should be the same as the TRIM.FaTE input value. Similar consistency constraints should be imposed if joint variables are highly correlated or related by a functional relationship.

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. Consequently, the more detailed analyses may have to restrict their scope to small numbers of parameters being jointly varied.

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.

Uncertainty analyses may be conducted running TRIM.FaTE in a steady-state mode, which requires drastically less processing time than the dynamic modeling mode. In the steady-state mode, TRIM.FaTE calculates single values for chemical moles, mass, and concentration for each compartment. These values approximate the steady-state levels that the chemical would reach if the dynamic form of the model was run for a long enough period of time to allow all chemical mass inputs and outputs to balance for each compartment (*i.e.*, to reach a steady-state).

6.2.7 SPATIAL AND TEMPORAL RESOLUTION AND AGGREGATION

Estimation of the effects of spatial and temporal aggregation on uncertainty and variability could be accomplished by sensitivity analyses of Monte Carlo results. For analysis of spatial aggregation, the user could set up a small number 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 output distributions for the scenarios would show the impact of the aggregation on uncertainty and variability for the scenarios modeled. Similarly, the effects on model output uncertainty of temporal aggregation could be assessed by comparing uncertainty results from scenarios with different levels of temporal aggregation.

6.2.8 SPECIFICATION OF PROBABILITY DISTRIBUTIONS 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. A

distribution for variability and a distribution for uncertainty is required for each parameter. As described in Section 6.2.1, both variability and uncertainty distributions are used a two-stage Monte Carlo analysis.

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 one or a small number of descriptive statistics, such as the sensitivity score, or the 10th, 50th, and 90th percentiles of a distribution. In addition to summary measures, ways of presenting the results include graphs of distributions of model outputs, tree diagrams, other graphs, and tables of statistics.

Results from Monte Carlo simulations are collected in a data file which can be accessed with other analysis software, such as graphical and statistical software, to analyze and present the results of the uncertainty and variability analysis. In the future, the overall TRIM framework or TRIM.Risk may be used to generate these results:

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

The first three of these are produced from results of the sensitivity simulations; the remainder can be produced from the Monte Carlo results.

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APPENDIX A

GLOSSARY

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APPENDIX A GLOSSARY

Abiotic Compartment Type	A compartment type consisting primarily of a non-living environmental medium (<i>e.g.</i> , 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 (<i>e.g.</i> , bald eagle, benthic invertebrate), or in the case of terrestrial plants, portions of living organisms (<i>e.g.</i> , stems, leaves), for which TRIM.FaTE calculates chemical masses and concentrations (see also compartment type).
Boundary Condition	A user-defined setting that establishes the concentration of a chemical on the external (<i>i.e.</i> , non-modeled) side of the modeled domain; chemical mass can enter a compartment across this interface via advective processes.
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 (<i>e.g.</i> , molecular weight, diffusion coefficient in air) are defined.
Compartment	The TRIM.FaTE modeling unit that contains chemical mass. Chemical mass is transported between and transformed within compartments; a specific compartment is characterized by its physical and spatial composition and its relationship to other compartments.
Compartment Type	A specific kind of compartment, such as an air compartment type or a racoon compartment type. Compartment types are distinguished from each other by their basic properties and the way they exchange chemical mass with other compartment types.
Composite Compartment Type	A group of different compartment types that are consistently interconnected. Individual compartments within a composite compartment require the presence of other compartments.

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.
Initial Condition	The user-defined chemical concentration in a compartment at the beginning of a scenario; represents concentrations in environmental media just before a source begins to emit chemicals in the modeled scenario.
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 (<i>e.g.</i> , emission rate, half-life, biomass).
Parcel	A planar (<i>i.e.</i> , 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.
Phase	The physical state of material within a compartment; in TRIM.FaTE, the various phases in which a chemical exists within a compartment are assumed to be in equilibrium with respect to chemical partitioning.

Source	Within TRIM.FaTE, a chemical source that is emitted directly to the primary abiotic compartment within which the source is located (e.g., a stack at a facility).
Project	A computer framework for saving one or more scenarios and all of the data properties for the scenarios that pertain to a single site (<i>i.e.</i> , bounded modeling region).
Reporting Time Step	The user-specified time interval at which the model results (<i>e.g.</i> , compartment moles) are saved and reported in output files by the model.
Scenario	A specified set of conditions (<i>e.g.</i> , 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 recalculates iteratively throughout the simulation period) a new inventory of compartment masses and concentrations.
Sink	A special kind of compartment type that accounts for chemical mass no longer available for transport or uptake within a scenario. There are three types of sinks: advection sinks, flush rate sinks, and degradation/reaction sinks.
Source	An external component that introduces chemical mass directly into a compartment.
Transfer Factor (T-factor)	A quantitative factor in units of inverse time that describes, for a first-order transfer between two compartments, the instantaneous flux of modeled chemical per amount of the chemical in the sending compartment.

TRIM.FaTE	The TRIM Environmental Fate, Transport and Ecological Exposure module that accounts for movement of a chemical through a comprehensive system of discrete compartments that represent possible locations of the chemical in the physical and biological environment and provides an inventory, over time, of a chemical throughout the entire system.
TRIM.Expo	The TRIM Exposure-Event module that measures human exposures by tracking population groups referred to as “cohorts” and their inhalation and ingestion through time and space.
TRIM.Risk	The TRIM Risk Characterization module that characterizes human exposures or doses with regard to potential risk using the corresponding exposure- or dose-response relationships.
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 an abiotic compartment and provides a frame of reference for one or more biotic compartments. This term is introduced to provide a consistent method for organizing objects that have a natural spatial relationship.

APPENDIX B

**INTEGRATING EXTERNAL MODELS OR MEASURED DATA INTO
TRIM.FaTE**

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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:

$$\frac{d\vec{N}}{dt} = A\vec{N} + \vec{s} \quad (1)$$

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

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

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:

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

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:

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

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

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:

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

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

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

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

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

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 $n_1(t) = M$:

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

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):

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

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 k th compartment/chemical pair is to be constant (say with value M_k), then one puts zeros in the k th row and k th column, and adds the term $M_k a_{nk}$ to the n th 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:

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

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
PROTOTYPES I - IV

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APPENDIX C

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”). These prototypes were developmental applications of the TRIM.FaTE modeling framework that were used to test the model as additional phases, compartment types, processes, algorithms, and other aspects of the TRIM.FaTE methodology were added to the model. Four early prototypes (*i.e.*, I through IV) were developed for preliminary testing purposes. Section 1 of this appendix 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. More documentation of Prototypes I - IV, including a detailed description of the testing performed using Prototype IV, is presented in the initial TRIM.FaTE Status Report (U.S. EPA 1998a) and Technical Support Document (U.S. EPA 1998b).

Based on the lessons learned from testing and application of Prototypes I - IV and the 1998 comments by EPA’s Science Advisory Board, EPA developed Prototype V, the first application of TRIM.FaTE at an actual site for a metal contaminant (*i.e.*, mercury). For detailed information regarding testing and application of Prototype V, the reader is referred to the 1999 TRIM.FaTE Status Report (U.S. EPA 1999a) and Technical Support Documents (U.S. EPA 1999b,c).

C.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):

$$dy/dt = F(t,y), y(t_0) = y_0$$

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

$$y(t) = [y_1(t), y_2(t), \dots, y_n(t)].$$

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.

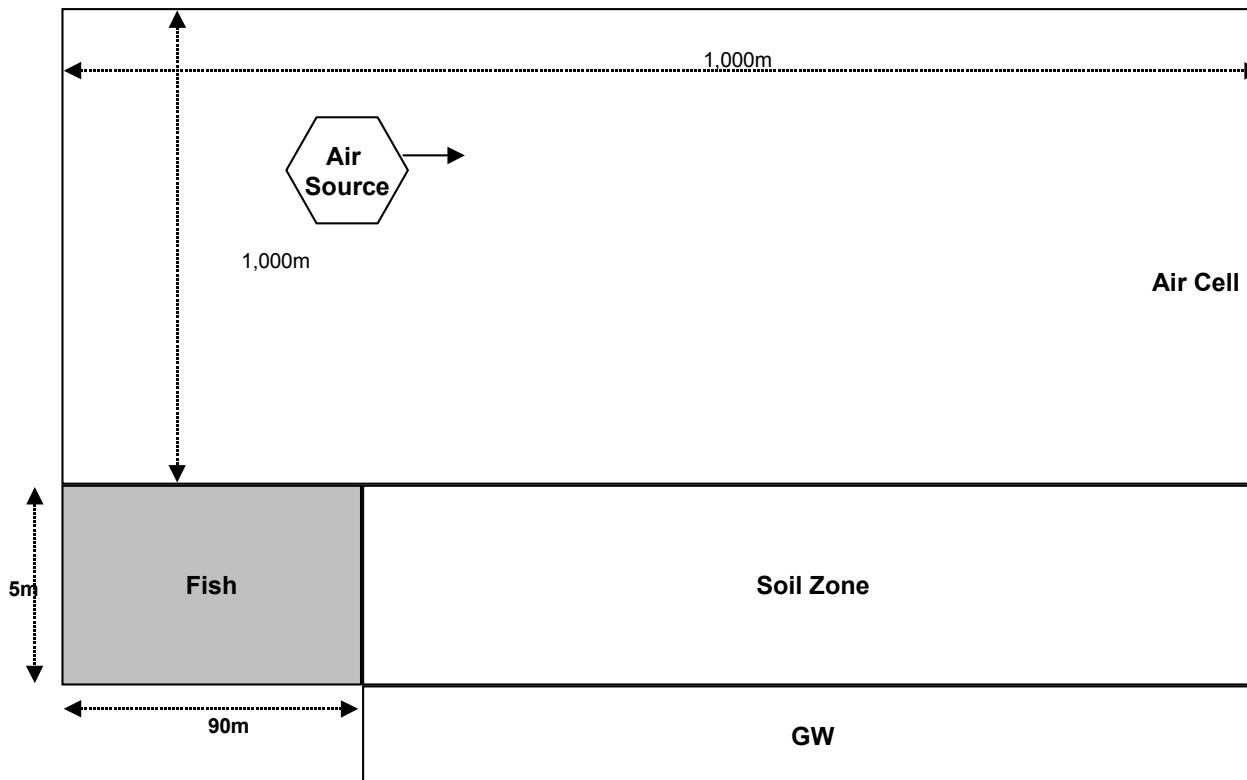
C.2 PROTOTYPE DEVELOPMENT

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.

C.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 C-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).

Figure C-1
Conceptual Site Model for Prototype I



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.

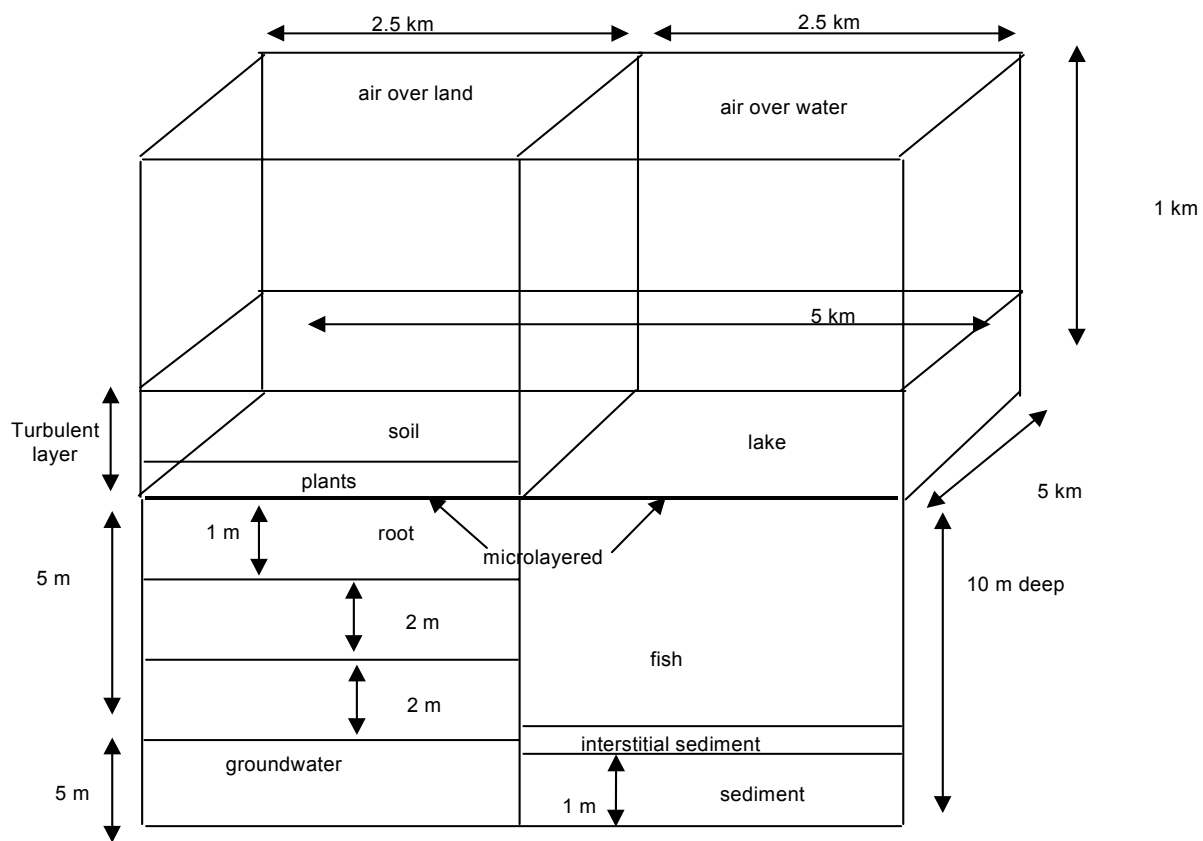
C.2.2 PROTOTYPE II

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 C-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 partitioning 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.

Figure C-2
Conceptual Site Model for Prototype II



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 simple approximations to model transport in ground water.

C.2.3 PROTOTYPE III

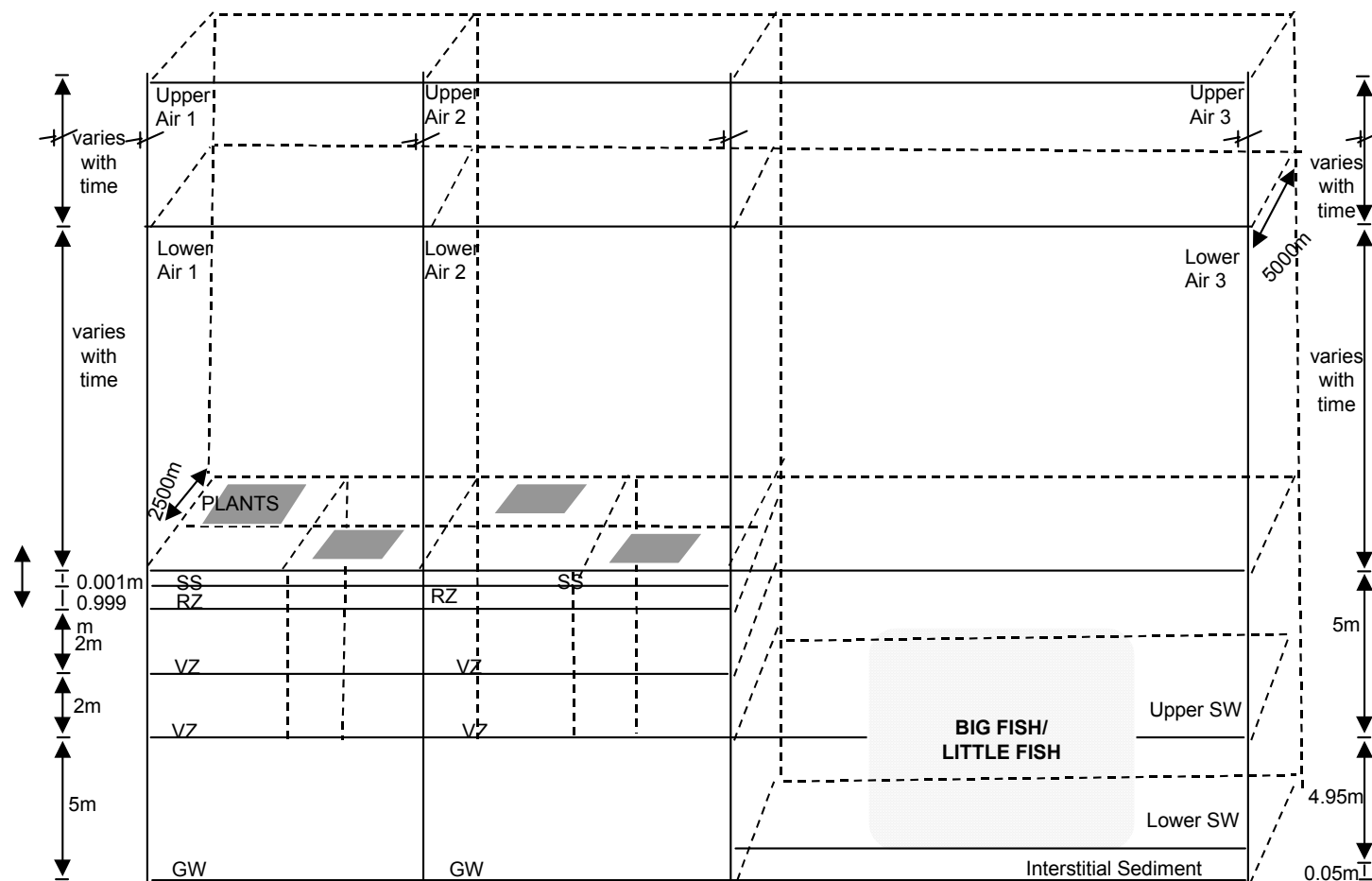
Prototype III (P3) focuses on code and input data structure refinements because the code and input data are significantly more complex than either P1 or P2. P3 was developed both to incorporate lessons learned from P2, which has a refined set of abiotic algorithms, and to set up the TRIM.FaTE model for 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 C-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 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:

- C Addition of terrestrial earthworm, kingfisher, and mouse compartment types;
- C Addition of aquatic food-web system;
- Addition of macrophyte compartment type;
- C Addition of compartments with varying heights for air;
- C Division of soil compartments horizontally;
- C Introduction of “thermoclines” and refinement of mixing for surface water;
- C Refinement of plant algorithms;
- C Refinement of soil diffusion algorithms;
- C Addition of erosion in the soil compartment types;
- C Refinement of ground water algorithm;
- C Introduction of flexible code design; and
- C 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

Figure C-3
Conceptual Site Model for Prototype III



algorithms as previously stated and implied that the prototype was appropriate for application to a more complicated test case.

C.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. A detailed description of the compartment layout used, the abiotic and biotic compartment types modeled, and model evaluations carried out for P4 is included in the 1998 TRIM.FaTE Status Report (U.S. EPA 1998a) and Technical Support Document (U.S. EPA 1998b).

C.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.

C.3.1 ABIOTIC COMPARTMENTS

In P1 (Figure C-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 C-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 C-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 C-1.

C.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 C-2.

Table C-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 C-2
 Biotic Compartments Modeled**

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

C.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 C-3 shows examples of generalized links applied in P1 through P4. This table is generic and can be used in conjunction with Tables C-1 and C-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 C-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 C-3. Sinks refer to the compartments of pollutant mass leaving the modeled ecosystem through a reaction or physical process(es).

Table C-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

C.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.

C.4.1 TRANSFORMATION OF PAHs BY PLANTS

C.4.1.1 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 C-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 C-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

C.4.1.2 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 ($k = 0.0156 \text{ hr}^{-1}$). 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:

$$\ln k = -1.355 - 1.279(1/T) + 0.831(\ln(I)) + 0.816(\ln[\text{H}_2\text{O}]),$$

where:

I = the average solar intensity ($\text{cal/cm}^2/\text{min}$)
 [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 $<0.00069 \text{ hr}^{-1}$ 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.

C.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 C-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 1 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.*, $A_a = A_w = A_s = A_f$. 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).

C.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 C-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 D

TRIM.FaTE COMPUTER FRAMEWORK

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APPENDIX D

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;
- Specify 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 and Monte Carlo studies; and
- Export and process results.

The development of the TRIM.FaTE framework began with the creation of a series of prototypes. These prototypes served as test beds for evaluating approaches and allowed changes to be quickly implemented and tested. The lessons learned from Prototypes I through V were incorporated into Version 1.0 of the TRIM.FaTE framework 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. The Version 1.0 framework has served as the basis for all subsequent versions. The current version, Version 2.5, was released in July 2002 and includes expanded analysis tools and stochastic modeling capabilities.

This description of the TRIM.FaTE computer framework generally covers both the prototypes and Version 2.5 with indications where necessary that descriptions apply to only one of the implementations. As the software architecture and implementation for Version 1.0 and all subsequent versions are very similar, only the Version 2.5 will be described in this chapter. Additional information about the architecture and design of TRIM.FaTE Version 1.0 can be found in Fine et al. (1998a,b).

D.1 SOFTWARE ARCHITECTURE

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

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.

As the prototypes and Version 2.5 have different architectures, they are described separately in this section.

D.1.1 ARCHITECTURE OF THE PROTOTYPES

The prototypes were 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 was constructed in a hierarchical fashion: first a parcel was created, then volume elements were added “to” the parcel, and then compartments were added to the volume elements. Links were created manually or automatically determined based on the spatial adjacency information of the project.

When a run was initiated, the needed transition matrices, source term vectors, and initial condition vector were constructed from the modeled system. This process utilized 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 were used in successive calls to the differential equation solver (*i.e.*, LSODE), after which the predicted chemical mass in each compartment was available.

An expression evaluator was 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 were calculated from properties of the chemical and the soil compartment). The expressions themselves were stored as strings, using an object-oriented syntax consistent with the overall object model used. These expressions were “compiled” when a run was performed, with the objects needed to calculate each expression obtained for subsequent calculation. This allowed flexible naming of variables and the creation of numerous

intermediate terms that helped provide insight into the finer details of a particular run. Further, it significantly improved the quality of output reports that could be produced. For example, detailed reports could be generated that showed 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 and subsequent versions.

D.1.2 VERSION 2.5 ARCHITECTURE

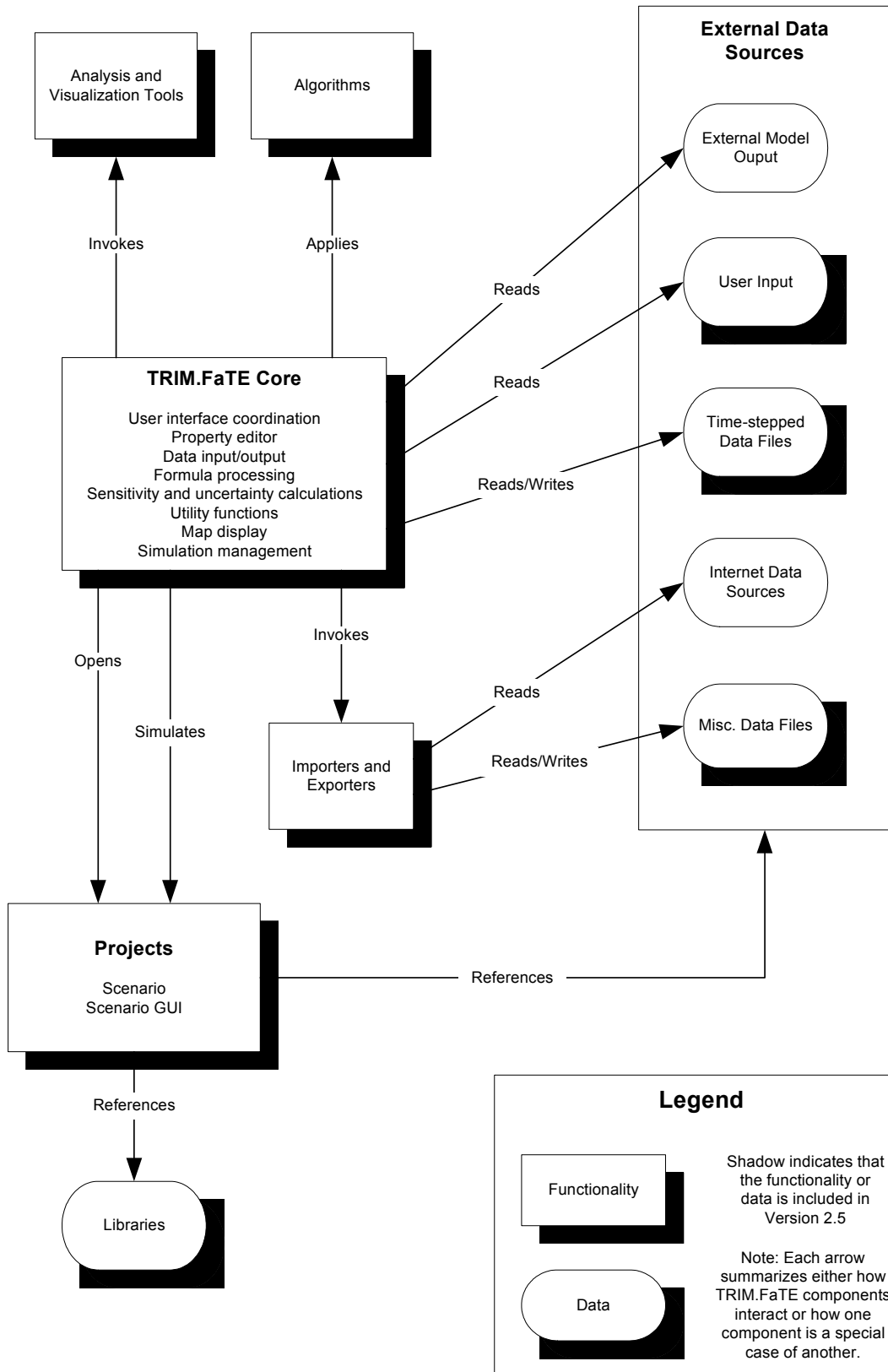
As shown in Figure D-1, the TRIM.FaTE computer system architecture is complex yet flexible. The architecture components used to describe TRIM are classified as those that primarily provide (1) functionality (rectangles), and (2) those that primarily provide data (ovals). However, each of the components except for external data sources provide both functionality and data. The architectural components that are implemented to some degree in Version 2.5 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 D-1 are described below. Note that this framework is used only for TRIM.FaTE. The remaining modules will be integrated together into EPA’s Multimedia Integrated Modeling System (MIMS) (Fine et al. 2002).

D.1.2.1 TRIM.FaTE Core

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

- 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 a parameter or attribute (*e.g.*, molecular weight) that describes an entity used by a model, such as a compartment or volume element. Properties include air temperature, scavenging coefficients, and chemical reaction rates.
- Interpretation of formulas used to describe property values. TRIM.FaTE allows users to write formulas using a simple language for conveying expressions, developed for TRIM.FaTE.
- Calculation of sensitivity and uncertainty.
- Utility functions used by TRIM.FaTE, such as routines to assist with common graphical user interface (GUI) and geometric operations.

Figure D-1
TRIM.FaTE Computer System Architecture



- Utility functions used by TRIM.FaTE, such as routines to assist with common graphical user interface (GUI) and geometric operations (*e.g.*, computing parcel overlaps and adjacencies, low-level routines used to represent points, lines, and polygons such as those used to define parcels and volume elements).
- Spatial presentation (“mapping”) of TRIM.FaTE compartment results with respect to volume elements. Future versions will be able to display arbitrary supplemental information supplied by the user, such as soil types. The mapping tool will also allow users to specify the X-Y extent of TRIM.FaTE volume elements.
- Coordination of simulation functions, including management of algorithms that compute chemical transfer coefficients between and transformation coefficients within conceptual compartments and controls that start and stop simulations, display error messages, and manage complex sets of simulations.

D.1.2.2 Project

All information pertinent to an environmental study is stored in a “project.” Each project is responsible for displaying the information it contains and allowing the user to change the information, in some cases relying on a TRIM.FaTE Core functionality such as the property editor. A project can contain one or more “scenarios,” where each scenario contains a complete description of a model run (or set of related runs), a description of the outdoor environment being simulated, populations being studied, and model parameters, such as the simulation time step.

D.1.2.3 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. In addition, many of the characteristics of and relationships between compartments are defined using formulas that do not change for a given simulation. 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.

D.1.2.4 External Data Sources, Importers, and Exporters

It will be common for TRIM.FaTE users to access or create data sets beyond TRIM.FaTE 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.FaTE provides several methods for accessing external information. The TRIM.FaTE Core accepts user inputs and will read and write data in files in the standard TRIM.FaTE format. These files are currently delimited ASCII text files that can be imported into spreadsheets. In the future, output directly to a database will be considered.

TRIM.FaTE is modular and allows new importers and exporters to be developed quickly and easily. Current data importers read data sets created outside of TRIM.FaTE, create TRIM.FaTE objects as needed, and set appropriate TRIM.FaTE properties. For example, an importer could read files containing measurements of surface air temperature and set properties in ground-level TRIM.FaTE air domains. Data exporters provide TRIM.FaTE 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 and HTML formatted files that allow the user to view links, transfer factors, and other information for a time step of a specific scenario.

D.1.2.5 Analysis and Visualization Tools

Version 2.5 includes several analysis and visualization tools. The first group of tools, which includes the Graphical Results Viewer and the Food Web Viewer, are used to display results and simulation setup details graphically. The second group of tools, which includes the Averager, the Aggregator, and the Transposer, are post-processing tools used to process TRIM.FaTE moles, mass, and concentration output files. In addition, simulation results can be easily exported to Excel or other analysis packages. In the future, TRIM.FaTE may include additional analysis and visualization capabilities.

D.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 units that contain internal data (*e.g.*, the boundaries of a volume element) and operations on that data (*e.g.*, compute volume). Additionally, 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.FaTE's view of the environment (with volume elements that contain compartments) and the development of associated graphical user interfaces are well suited for an object-oriented treatment.

TRIM.FaTE is being developed in an iterative manner. The major components and responsibilities of a class of objects are understood before implementation, but some details are worked out as implementation proceeds. During implementation, the design is modified as needed. The object-oriented, open-ended structure of TRIM is intended to make future changes and additions a relatively simple process. For Version 2.5 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 were used. As time permits, operations that cause noticeable speed or resource problems will be optimized.

D.3 IMPLEMENTATION LANGUAGE

Due to the different objectives of the framework prototypes and Version 2.5, different development languages were chosen. The rationale for each choice is described below.

D.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, to which all members on the team had access (for early prototypes);
- Object-oriented features of language, while limited¹, simplify a dynamic, iterative architecture development cycle; and
- Straightforward to call needed Fortran codes (*e.g.*, differential equation solver, linear equation solver, triangulation).

D.3.2 VERSION 2.5

The Version 2.5 computer framework was developed primarily, but not entirely, in the Java programming language. Some parts of TRIM.FaTE, such as the differential equation solver, 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.

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.

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.
- 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.

D.4 EMBEDDED FUNCTIONS

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.

D.4.1 ADVECTIVE TRANSPORT BETWEEN AIR COMPARTMENTS

The advective transport 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.

D.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 2.5 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 2.5.

D.4.3 AREA OF VOLUME ELEMENTS

The area of volume elements is also used frequently (e.g., for deposition and resuspension transfers). It is a simple calculation in the source code that uses the X-Y coordinates of a volume element to calculate the horizontal area of the volume element. This function is called in the volume element property “area.”

D.4.4 VOLUME OF VOLUME ELEMENTS

The volume of volume elements is used in nearly every algorithm involving an abiotic compartment. It is a simple calculation in the source code that uses the X-Y coordinates and height of a volume element to calculate the volume of the volume element. This function is called in the volume element property “volume.”

D.4.5 BOUNDARY CONTRIBUTION

This function computes the advective contribution from a boundary of the modeling system to an air compartment. It requires as inputs the boundary concentration (in grams per cubic meter), wind speed (in meters per second), and wind direction (in degrees clockwise from north). This function is called in the boundary air compartment property “boundaryContribution.”

D.4.6 OTHER MATHEMATICAL FUNCTIONS

In addition to the TRIM-specific functions described above, TRIM.FaTE also includes the following standard mathematical functions that can be used by the user in writing algorithms and/or defining object properties.

- $\text{abs}(x_1)$ - absolute value of x_1
- $\text{exp}(x_1)$ - exponential of x_1
- $\text{ln}(x_1)$ - natural logarithm of x_1
- $\text{log10}(x_1)$ - log base 10 of x_1
- $\text{max}(x_1, x_2, x_3, \dots, x_n)$ - maximum of values $x_1 \dots x_n$
- $\text{min}(x_1, x_2, x_3, \dots, x_n)$ - minimum of values $x_1 \dots x_n$
- $\text{mod}(x_1, x_2)$ - modulo of x_1 relative to x_2
- $\text{sqrt}(x_1)$ - square root of x_1

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16. ABSTRACT <p>This report is part of a series of documentation for the Total Risk Integrated Methodology (TRIM). TRIM is a time series modeling system, with multimedia capabilities, designed for assessing human health and ecological risks from hazardous and criteria air pollutants. The detailed documentation of TRIM's logic, assumptions, equations, and input parameters is provided in comprehensive technical support documents for each of the three TRIM modules, as they are developed. This report 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.</p>		
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