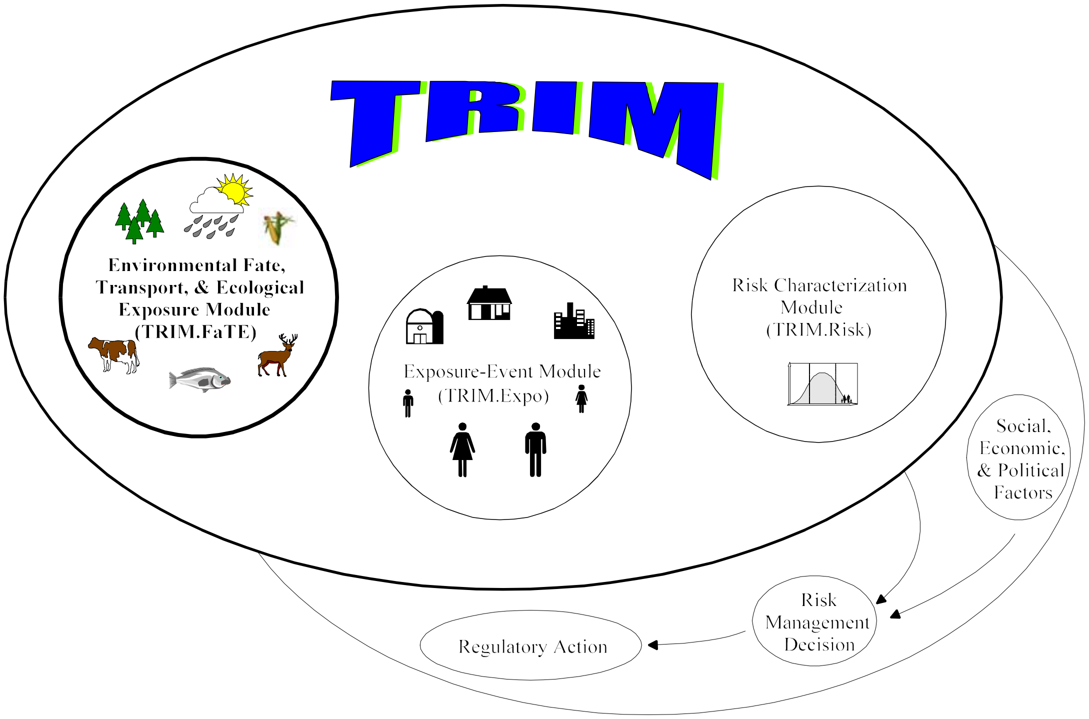
UNITED STATES ENVIRONMENTAL PROTECTION AGENCY

Evaluation of TRIM.FaTE

Volume I: Approach and Initial Findings



EPA-453/R-02-012
September 2002

Evaluation of TRIM.FaTE

Volume I: Approach and Initial Findings

BY:
Randy Maddalena, Deborah Hall Bennett, and Thomas E. McKone
Lawrence Berkeley National Laboratory, Berkeley, California
Interagency Agreement #DW89786601

Bradford F. Lyon, Rebecca A. Efroymson, and Daniel S. Jones
Oak Ridge National Laboratory, Oak Ridge, Tennessee
Interagency Agreement #DW89876501

Alison Eyth
MCNC Environmental Modeling Center, Research Triangle Park, North Carolina
Contract #GS-35F-0067K

Mark Lee, Margaret E. McVey, David Burch, Josh Cleland, and Baxter Jones
ICF Consulting, Fairfax, Virginia
Contract #s 68-D6-0064, 68-D-01-052

Prepared for:
Terri Hollingsworth, EPA Project Officer & Work Assignment Manager
Deirdre Murphy, Technical Lead
Emissions Standards Division

U.S. Environmental Protection Agency
Office of Air Quality Planning and Standards
Emissions Standards & Air Quality Strategies and Standards Divisions
Research Triangle Park, North Carolina

DISCLAIMER

This document has been reviewed and approved for publication by the U.S. Environmental Protection Agency. It does not constitute Agency policy. The opinions, findings, and conclusions expressed are those of the authors and are not necessarily those of the Environmental Protection Agency. Mention of trade names or commercial products is not intended to constitute endorsement or recommendation for use.

[This page intentionally left blank.]

PREFACE

This document, *Evaluation of TRIM.FaTE*, *Volume 1: Approach and Initial Findings,* is part of a series of documentation for the overall Total Risk Integrated Methodology (TRIM) modeling system. Subsequent evaluation analyses may be presented in subsequent volumes, while the detailed documentation of TRIM's logic, assumptions, algorithms, and equations is provided elsewhere in comprehensive Technical Support Documents (TSDs) and/or user's guidance for each of the TRIM modules.

This report describes a set of evaluation analyses performed on the TRIM.FaTE model primarily during 2000, with some spanning into 2002.

Comments should be addressed to Dr. Deirdre Murphy, U.S. EPA, Office of Air Quality Planning and Standards, C404-01, Research Triangle Park, North Carolina, 27711; murphy.deirdre@epa.gov.

[This page intentionally left blank.]

TABLE OF CONTENTS

Appendices

[This page intentionally left blank.]

1. INTRODUCTION

TRIM.FaTE is a predictive environmental fate and transport model designed to support decisions on programmatic policy and regulation for multimedia air pollutants. These decisions can have far-reaching human health, environmental, and economic implications. It is important that an assessment of how well the model is expected to perform the tasks for which it was designed is incorporated within the model development process. In other words, the trustworthiness of models used to determine policy or to attest to public safety should be ascertained (Oreskes et al. 1994). This report describes the model evaluation activities performed to date to assess TRIM.FaTE's quality and acceptability. In short, it describes the progress made to date in fulfilling the Evaluation Plan laid out in Chapter 6 of the November 1999 *TRIM Status Report* (U.S. EPA 1999a).

The Evaluation Report is composed of two volumes. This volume, Volume I, presents conceptual, mechanistic, and structural complexity evaluations of various aspects of the model (e.g., inputs, process models). Volume II (bound separately) presents performance evaluation of the model as a whole, focusing on initial case study application.

This first chapter of Volume I provides background information on model evaluation and describes the general approach of the TRIM.FaTE evaluation. Chapter 2 describes conceptual model evaluation activities for TRIM.FaTE. Chapter 3 describes mechanistic evaluation of individual TRIM.FaTE process models and algorithms. Chapter 4 describes structural and complexity evaluation of TRIM.FaTE. Chapter 5 identifies literature references cited in this report. Background information related to evaluations is provided in two appendices to this volume.

1.1 BACKGROUND

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

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

Over the last 10 years, the Agency has been considering model acceptance or model use acceptability criteria for selection of environmental models for regulatory activities. The Agency's efforts in this area are a result of EPA's Science Advisory Board (SAB) recommendations in 1989 that "EPA establish a general model validation protocol and provide sufficient resources to test and confirm models with appropriate field and laboratory data" and that "an Agency-wide task group to assess and guide model use by EPA should be formed" (U.S. EPA 1989). In response, EPA formed the Agency Task Force on Environmental Regulatory Modeling (ATFERM). This cross-agency task force was charged to make "a recommendation to the Agency on specific actions that should be taken to satisfy the needs for improvement in the way that models are developed and used in policy and regulatory assessment and decision-making" (Habicht 1992). In its March 1994 report, ATFERM recommended the development of "a comprehensive set of criteria for model selection (that) could reduce inconsistency in model selection and ease the burden on the regions and states applying the models in their programs," and they drafted a set of "model use acceptability criteria" (U.S. EPA 1994a).

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

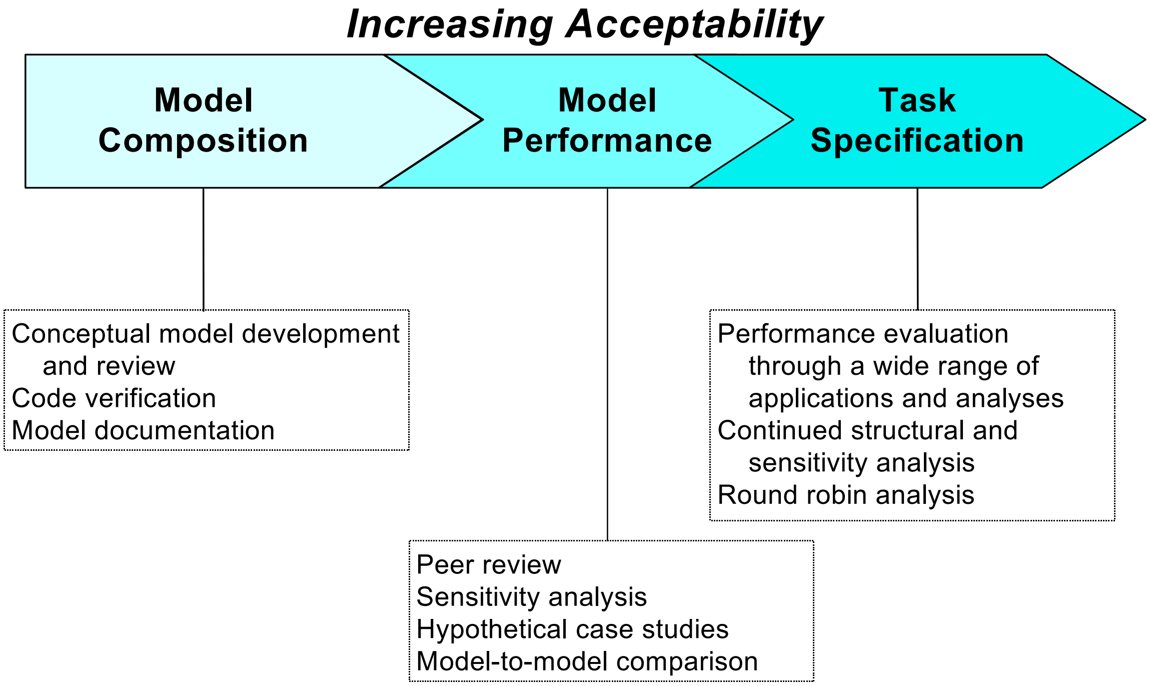
In their May 1998 review of TRIM.FaTE, SAB recognized the challenge in developing a methodological framework for evaluating a model such as TRIM.FaTE. Further, SAB suggested that "novel methodologies may become available for quantitatively assuring the quality of models as tools for fulfilling specified predictive tasks" (U.S. EPA 1998d). Comments regarding the complexity of mercury environmental chemistry, made by SAB in their December 1999 review (U.S. EPA 2000), led to additional evaluation activities that include focus on organic chemicals (e.g., benzo[a]pyrene). At that time, SAB also commented on the need for continual evaluation. In developing and implementing the evaluation plan for TRIM.FaTE, the Agency has attempted to incorporate the essential ingredients for judging the acceptability of TRIM.FaTE for its intended uses, while retaining the flexibility to accommodate and evaluate new methods that become available or changes in direction indicated by knowledge gained through the evaluation process.

1.2 TYPES OF MODEL EVALUATION

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

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

Figure 1-1
Schematic Representation of the Model Evaluation Process



The evaluation activities performed to date for TRIM.FaTE correspond to different (but overlapping) types of model evaluation activities:

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

The first three evaluation activities primarily focus on the information that goes into the model (e.g., theory and data); how this information is synthesized (e.g., process models, algorithms, and assumptions); and how the finished model is set up (e.g., appropriate level of complexity). The fourth evaluation activity focuses mainly on the information that comes out of the model (e.g., comparing overall model outputs to various kinds of benchmarks). Detailed methods and results of the first three evaluation types are presented in subsequent chapters of this volume. The initial performance evaluation activities for TRIM.FaTE are presented in Volume II.

The model evaluation plan for TRIM.FaTE was designed at the output to be flexible. Results from the TRIM.FaTE evaluation efforts have posed new questions and led to additional review, analysis, and testing, not all of which is described here. The various evaluation activities performed on TRIM.FaTE increase the experience and understanding that will ultimately lead to a judgment about its quality, reliability, relevance, and acceptability. The activities that are currently part of the consensus building process for TRIM.FaTE are described in the following sections. At this time, there has been substantial progress on a number of these activities (e.g., code verification, model documentation, peer review, mechanistic evaluation of individual process models and algorithms). Other evaluation activities (e.g., complexity analyses, overall performance evaluation) are continuing and will continue with new applications and various analyses.

EVALUATION THROUGHOUT MODEL DEVELOPMENT

As noted in the text, model evaluation is being performed in conjunction with model development. Earlier evaluation activities were performed using the most current Prototype (i.e., I through V) of TRIM.FaTE available at the time. These evaluation activities are fully applicable to TRIM.FaTE Version 1.0, which was built from the same simulation algorithms and data as Prototype V. Version 1.0 is also the focus of model evaluation activities described here, and Version 2.0 is the focus of much of the mercury test case (see Volume II of the Evaluation Report); later versions of TRIM.FaTE will be used as evaluation activities and model development continue.

1.3 GENERAL APPROACH OF THIS EVALUATION

The evaluation of TRIM.FaTE is an iterative process, starting with simpler analyses and proceeding to more-complex studies. Early model analyses, especially those mechanistic evaluations focusing on one fate and transport aspect of TRIM.FaTE, have used limited time periods, simplified modeling layouts (e.g., a single, square modeling compartment composed of surface soil, surface water, and air volume elements), and simplified assumptions (e.g., fixed concentrations in abiotic media). More-advanced layouts were constructed for some intermediate evaluation activities (e.g., temporal and spatial complexity analyses). In order to test the whole model in a realistic setting, the mercury case study described in this section (and in more detail in Volume II) was used. Various parts of this case study setup were used in most of the evaluation activities described in both volumes of the Evaluation Report.

1.3.1 Chemical Selection

As part of the evaluation process for TRIM, EPA must test TRIM.FaTE with both organic and inorganic pollutants because of their distinctly different multimedia fate and transport properties. The EPA selected PAHs for an initial organic chemical test case, and the methodology and results of that testing were reported in the *1998 TRIM Status Report* (U.S. EPA 1998b). For the evaluations of the current version of TRIM.FaTE, benzo(a)pyrene and mercury were selected. Benzo(a)pyrene was used in some analyses in order to test an organic compound. The Agency selected mercury as an inorganic chemical for testing TRIM.FaTE because of its fate and transport properties (e.g., transformation to multiple chemical species), the concern for multipathway exposure (particularly through ingestion of fish), and the potential health effects associated with exposure. In some instances (e.g., some air evaluation activities), elemental mercury was used with the assumption of no transformation.

MERCURY

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

1.3.2 TRIM.FaTE Mercury Case Study

As a part of the evaluation activities for TRIM.FaTE, OAQPS has developed a case study data set for mercury at a chlor-alkali plant in the U.S. This case study data set has been used in sensitivity analyses and in mechanistic and structural evaluations, which have improved understanding of the most important model processes and inputs and of the effects of varying the model's spatial and temporal resolution. After gaining an understanding of and confidence in the model's structure and performance, OAQPS will proceed to fuller spatial and temporal case study simulations. The TRIM.FaTE case study outputs will be compared with outputs from other models applied to the site, as well as biotic and abiotic mercury measurements available for the case study area. The case study site and conditions also have served as the basis for extensive testing and troubleshooting of TRIM.FaTE. This section provides summary information on the mercury case study, including information on selection of the test site and an overview of the evaluation activities. In the future, EPA may perform additional case studies and apply TRIM.FaTE to other chemicals (e.g., dioxins) and other locations.

1.3.2.1 Case Study Site Selection

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

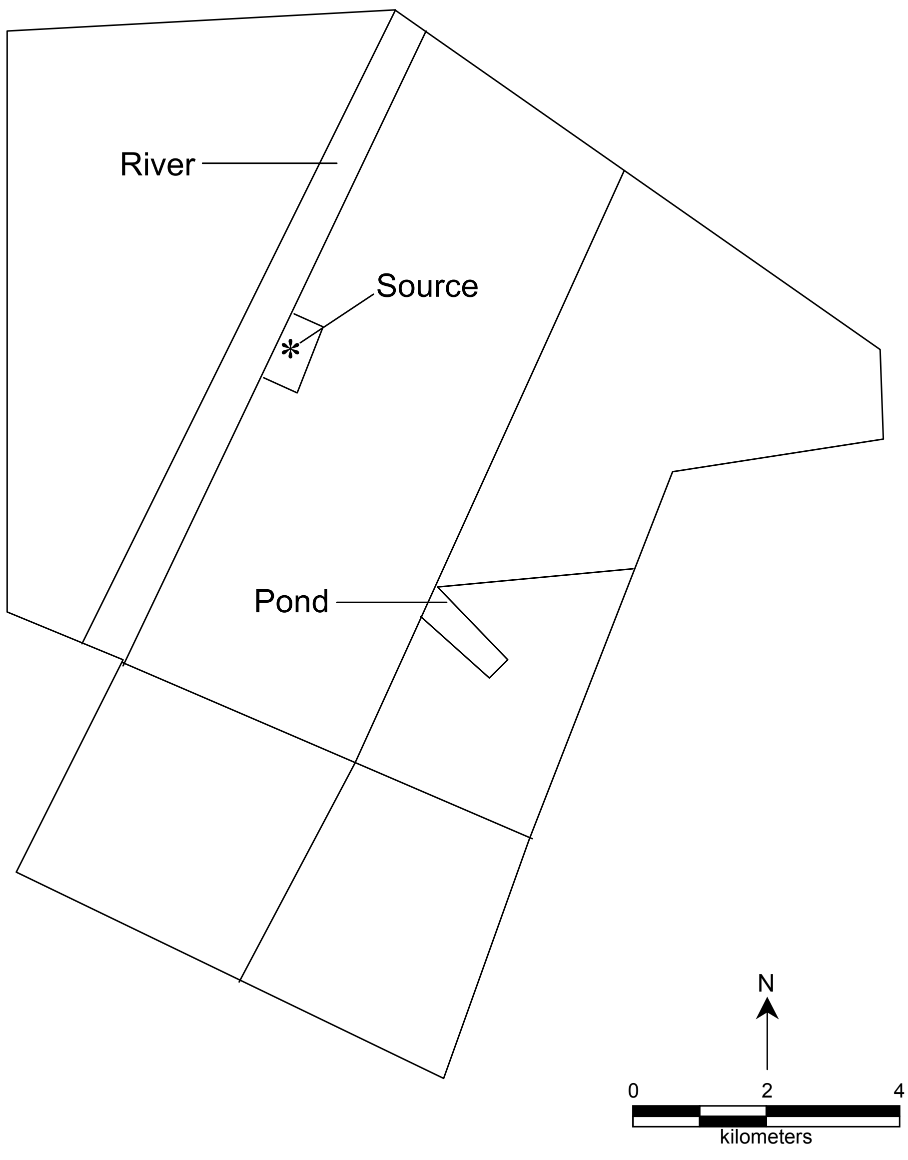
Chlor-alkali plants were selected for further assessment in the TRIM.FaTE case study because they are a substantial source of mercury air emissions and are not yet regulated for HAP emissions. In addition, these plants are more likely than other major mercury emission sources to pose localized health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

The Agency selected a single chlor-alkali plant for the mercury case study after evaluating data availability for several sites. At the time of the site selection, 14 chlor-alkali plants were in operation in the United States. Mercury air emission estimates were available for all 14 plants; however, data on mercury levels in environmental media and biota were available for only two of the plants. Fish tissue, water quality, and air quality data had been collected for one of the two plants, but ultra-clean techniques were not used for collecting and analyzing the water samples. For the second plant, air quality, soil, fish tissue, sediment, and additional biotic data had been collected and analyzed. In addition, accumulation of mercury in environmental media and biota near the second plant was possible because the plant has been in operation since 1967. Because the data set for the second plant was more complete, of higher quality, and readily available for use, that chlor-alkali plant was selected for the mercury case study. A schematic map of the site area showing delineation of the simple set of parcels used for many of the evaluation activities is provided in Figure 1-2. (For a general discussion of the process of defining parcels, volume elements, and compartments for a TRIM.FaTE application, see Chapter 5 of TRIM.FaTE TSD Volume I).[1] Maps showing the full, more complex parcel layouts used for the overall performance evaluation are included in Volume II.

---

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

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



---

[2] This diagram shows the initial set of surface water (i.e., river, pond) and soil (i.e., all other) parcels for the TRIM.FaTE mercury case study site; the air parcels are slightly different.

1.3.2.2 Overview of Evaluation Activities

As part of the TRIM.FaTE model evaluation, several different types of analyses that correspond with different types of evaluations (i.e., mechanistic and data quality, structural, performance) are being performed using the case study data set. These analyses are described in general below and in more detail in subsequent chapters and in Volume II. The model input values developed for the TRIM.FaTE mercury study are documented in an appendix of Volume II.

Evaluating the quality of the input data for a given model application is an iterative process. A literature search is completed to determine the value and identify any available information on the predicted uncertainty or variability associated with that value. The current values resulting from our search are listed in an appendix to Volume II. Then, a sensitivity analysis is performed for all of the parameters to evaluate how varying an input value influences the model output. If a model input is very uncertain and significantly influences the model output, more research may be completed to refine that input value.

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

For example, one mechanistic evaluation performed was a comparison of the TRIM.FaTE air component with a commonly used air dispersion model, the Urban Airshed Model (UAM) available at http://www.epa.gov/scram001/. Specifically, the air concentrations from UAM were compared to the concentrations estimated for the air compartments in TRIM.FaTE to provide insight into how the methodology for modeling transport and fate in TRIM.FaTE compares to a grid model with a track record of application and acceptance.

Another type of evaluation being performed using the TRIM.FaTE mercury case study data set is an assessment of the influence of the structural representation of the system being modeled. Some of the key assumptions in any TRIM.FaTE application involve determination of the time step for input data averaging, the background and boundary concentrations of chemicals of interest, the spatial representation (i.e., grid layout) of the modeled system, and the compartment types selected for modeling. Examples of structural evaluation, some of which have been performed and are reported here, include the following:

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

- **Understanding the effect of spatial configuration,** by comparing results obtained using spatial layouts of varying complexity and resolution; and

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

Model performance evaluation can include comparisons of model outputs to outputs from other models and to available measurement data for a specific site. Both of these types of performance evaluations are being or have been performed as part of the TRIM.FaTE mercury case study discussed in Volume II.

[This page intentionally left blank.]

2. CONCEPTUAL MODEL EVALUATION

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

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

Examples of conceptual model evaluation activities include:

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

2.1 INITIAL ACTIVITIES

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

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

- Extensive model documentation has been presented:

    - TRIM Status Reports have been published in 1998 (U.S. EPA 1998b) and 1999 (U.S. EPA 1999a);

    - Presentations have been made at scientific meetings including the Society of Environmental Toxicology and Chemistry (SETAC) annual meetings in 1997 (McKone et al. 1997a; Zimmer et al. 1997; Efroymson et al. 1997), 1998 (Vasu et al. 1998), 1999 (Efroymson et al. 1999), and 2000 (Murphy et al. 2000; Lyon et al. 2000; Maddalena et al. 2000; Efroymson et al. 2000; Bennett et al. 2000; Burch et al. 2000a; Hetes and Langstaff 2000; Fine et al. 2000; Bennett et al. 2000b); the Society for Risk Analysis (SRA) in 1997 (Vasu et al. 1997; Guha et al. 1997; Lyon et al. 1997; Bennett et al. 1997; McKone et al. 1997b; Johnson et al. 1997); and the International Societies of Exposure Analysis and Environmental Epidemiology (ISEA/ISEE) in 2002 (Murphy et al. 2002).

  - A detailed Technical Support Document for TRIM.FaTE is available (U.S. EPA 2002a and U.S. EPA 2002b).
  - Aspects of TRIM have been published in peer-reviewed journals (Palma et al. 1999; Efroymson and Murphy 2001).
- Two reviews by the SAB have been published (U.S. EPA 1998a; U.S. EPA 2000).

As refinements to TRIM.FaTE are made and as new applications are performed, conceptual model evaluation will continue. These evaluations will continue to be reported in peer reviewed journals and will be subject to additional SAB consultation and review.

2.2 DOCUMENTATION

Previously published TRIM.FaTE documentation include Status Reports and the TRIM.FaTE Technical Support Document.

2.2.1 Status Reports

The first TRIM Status Report was published in March 1998 (U.S. EPA 1998b). This report focused on the first developmental phase of TRIM, including the conceptualization of TRIM and the implementation of the conceptual approach through the development of TRIM.FaTE. Many aspects of the conceptual evaluation are described in the first Status Report, including the initial goals and objectives of the TRIM project, the conceptual framework for TRIM.FaTE (including a review of currently available models and tools), development of the first prototype versions of TRIM.FaTE, and the limited testing and model evaluation analyses that were completed on these prototypes.

A second TRIM Status Report was published in November 1999 (U.S. EPA 1999a). This report summarized work performed on TRIM during the second developmental phase, including the refinement of the initial TRIM.FaTE module following the 1998 SAB review of TRIM. Details regarding TRIM.FaTE capabilities and the algorithms implemented in TRIM.FaTE, as well as the plan for the evaluation described in the current document, were included. Descriptions of the exposure and risk characterization modules of TRIM (i.e., TRIM.Expo and TRIM.Risk) were also included in the 1999 Status Report.

2.2.2 TRIM.FaTE Technical Support Document

The TRIM.FaTE Technical Support Document is composed of two volumes (U.S. EPA 2002a; U.S. EPA 2002b). The first volume provides a description of the terminology, model framework, and functionality of TRIM.FaTE. Volume II presents detailed descriptions of the algorithms used in the TRIM.FaTE module.

In addition to SAB review (see Section 2.3), an internal draft of the Technical Support Document, along with the Status Reports, were subjected to formal review by representatives from the major program offices at EPA and an EPA Models 2000 review team.

2.3 SCIENCE ADVISORY BOARD REVIEWS

To date, two reviews of TRIM have been completed by the Environmental Models Subcommittee of the Executive Committee of SAB. The first review, undertaken in May 1998 (U.S. EPA 1998a), focused on the conceptual approach for TRIM and the prototype of TRIM.FaTE that was available at that time. Six charge questions related to TRIM and TRIM.FaTE were posed to SAB. Responses to each question and recommendations to EPA for improvements in the next versions of TRIM modules and TRIM.FaTE in particular were summarized in a December 1998 report by SAB (U.S. EPA 1998a).

Overall, in its first review, SAB found the development of TRIM and the TRIM.FaTE module to be conceptually sound and scientifically based. The SAB recommended that the TRIM team (1) seek input from users before and after the methodology is developed to maximize its utility; (2) understand the potential uses of TRIM to guard against inappropriate uses; (3) provide documentation of recommended and inappropriate applications; (4) provide training for users; (5) test the model and its subcomponents against current data and models to evaluate its ability to provide realistic results; and (6) apply terminology consistently.

The second SAB review of TRIM took place in December 1999 and focused on the TRIM Status Report (U.S. EPA 2000), the review draft of the two volumes of the TRIM.FaTE Technical Support Document (U.S. EPA 1999c; U.S. EPA 1999d), and a separate draft Technical Support Document developed for the TRIM.Expo module (U.S. EPA 1999b). Three charge questions related to the overall TRIM system and three questions regarding the TRIM.FaTE module in particular were posed to SAB, along with several questions regarding other TRIM modules. The SAB's responses and comments are summarized in a final report dated May 2000 U.S. EPA 2000. In this report, SAB described EPA's TRIM development efforts as being "innovative and effective, given the significant challenges and the relatively new and rapidly evolving state of science for multimedia fate, transport, exposure, and risk models." Specific recommendations were proposed for the charge questions.

[This page intentionally left blank.]

3. MECHANISTIC AND DATA QUALITY EVALUATION

This chapter presents the results of the mechanistic and data quality evaluation of TRIM.FaTE during 1999 and 2000. Summaries of the initial shakedown evaluation of TRIM.FaTE and the computer and software evaluations are included. This chapter also includes descriptions of the evaluations of a number of the individual process models that comprise TRIM.FaTE.

3.1 BACKGROUND

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

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

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

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

Examples of mechanistic and data quality evaluation activities performed on TRIM.FaTE include:

- Computer code verification;
- Verification of generic algorithms adapted for and used within a model;
- Literature review to determine the extent of prior process model testing;
- Peer review of model components;
- Mass or molar balance checks;
- Performance evaluation of new and existing individual process models and of multiple process models in a linked system (e.g., compare with existing models or with measurements, when available);
- Comparison of alternative process models (e.g., equilibrium versus bioenergetic model for fish bioaccumulation of mercury);
- Data acquisition and evaluation (e.g., data quality or reliability relative to the other inputs and assumptions), and development and documentation of default input data;
- Distribution development for input data to support probabilistic analysis; and
- Generic sensitivity analysis to help identify parameters that are most influential on model results, as well as potential data limitations (i.e., model inputs that need further refinement or that are potential sources of uncertainty in the analysis).

One of the features of TRIM.FaTE that aids in mechanistic and data quality evaluation (as well as in other types of evaluation) is its web-based output functions. There is an option to create a “full-recursive output,” which documents the mass flow, as well as the associated transfer factors, to and from each compartment. Mass and molar balance checks are incorporated in the model for non-transforming organic compounds and mercury to allow for the quick assessment of model performance under a range of conditions. The equation for each transfer factor can be viewed on a separate web page, and any calculated quantities used in that equation can then be viewed on additional pages. In this manner, checks can be made to ensure that the equations are input properly, and that the computer code is correctly calculating intermediate values. Analyses have been conducted on various parts of the code using this feature.

3.2 SELECTION OF CHEMICALS FOR EVALUATION RUNS

Prior to conducting detailed evaluations of the process models within TRIM.FaTE, numerous preliminary model runs were performed in a "debugging" mode. Given the amount of information produced in a full run, a new approach to evaluating performance was adopted in order to evaluate whether the model was producing results that were logical, internally consistent, and reasonable. Thus, a screening set of hypothetical chemicals was developed and used to conduct a systematic probe of the model across the range of applicable fate scenarios.

3.2.1 Methods

The environment in its simplest form can be divided into solid, aqueous, and gaseous phases. The relative solubility of a chemical in each of these phases is indicative of how a chemical will partition when released to the environment. The octanol/water partition coefficient (K_{ow}) and the non-dimensionalized Henry's Law constant (K_{aw}) provide a general means to characterize the relative solubility of a chemical in the three primary environmental phases (Cole and Mackay 2000; Cousins and Mackay 2000).

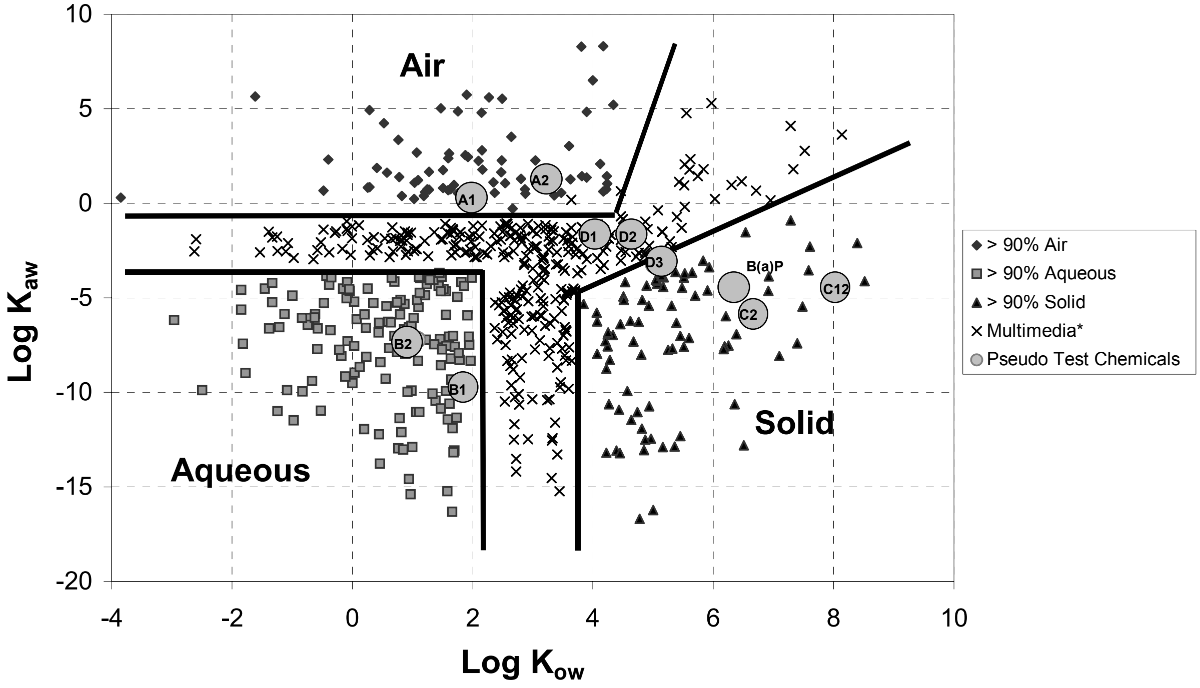
Crystal Ball software (Decisioneering 1996) and existing data on several hundred chemicals were used to construct correlated probability distributions for the primary physical-chemical properties used in TRIM.FaTE. A simple Monte Carlo sampling scheme was then used to draw 500 random combinations from the correlated distributions. The 500 candidate chemicals were then run through an existing mass balance model (McKone 1993a,b,c) to evaluate their partitioning behavior. The results are plotted in Figure 3-1, where each physical-chemical property combination is defined by a unique pair of K_{ow} and K_{aw} values.

Single-medium chemicals are arbitrarily defined as those that have more than 90 percent of their mass in a single medium. Multimedia chemicals are defined as those having not more than 80 percent of their mass in a single medium. Chemicals with between 80 percent and 90 percent of total mass in a single medium were excluded from selection. The 500 candidate chemicals were classified according to their partitioning behavior. Two chemicals were then selected at random from each single-medium pollutant class, and three chemicals were selected from the multimedia pollutant class. The resulting nine test chemicals made up the initial shakedown evaluation set for TRIM.FaTE.

3.2.2 Results and Discussion

The test set was particularly useful during diagnostic evaluations. Having a general understanding of the expected fate of a chemical provides insight into possible reasons for unexpected model outcomes. For example, intermedia transfer for the single-medium gas-phase pollutants occurs typically by diffusion and, to a lesser extent, washout from the atmosphere during rain events. If TRIM.FaTE results during an initial evaluation are suspect for the single-medium gas-phase chemicals, then the focus of the diagnostic evaluation can be placed on a relatively small number of algorithms. This approach was used with TRIM.FaTE by running the model with only a subset of the available compartment types to focus on a particular algorithm or set of algorithms. For the TRIM.FaTE evaluation phase, the test set of chemicals was used to evaluate the soil algorithms, the plant algorithms, and the general biotic algorithms. The general test set will continue to be used for both initial evaluations and diagnostic evaluations for the process models in TRIM.FaTE and for the model as a whole.

Figure 3-1
Single-Medium and Multimedia Chemical Regions for 500 Hypothetical Chemicals



* Multimedia is defined as having not more than 80 percent of total mass in any single medium. Chemicals with between 80 percent and 90 percent of total mass in any single medium were excluded from selection.

3.3 COMPUTER/SOFTWARE EVALUATIONS

This section provides an overview of computer/software evaluations for the successive developmental versions of TRIM.FaTE. Section 3.3.1 describes evaluations of prototypes I through V. Section 3.3.2 describes evaluations of TRIM.FaTE Version 1 through 2.5, the first production versions of the model. Section 3.3 describes audits of the algorithm and compartment sections of the TRIM.FaTE library.

3.3.1 Evaluation of the Prototypes

The TRIM Computer Framework started as a series of prototypes. Prototypes I-IV were implemented using a combination of Microsoft Visual Basic™, FORTRAN, and Microsoft Excel™ software. Prototype V, the final prototype, was written in Visual Basic 5 and used an Access database to store information about the model configuration and input parameters. Prototype V was used for many of the initial mechanistic evaluations of TRIM.FaTE.

Each of the prototypes used the Livermore Solver for Ordinary Differential Equations (LSODE) (Radhakrishnan and Hindmarsh 1993) to solve the system of linear ordinary differential equations that represent the transfer of chemical mass between compartments and transformation of chemical mass within compartments. LSODE is a FORTAN program freely available via several online numerical algorithm repositories. Early on, the use of LSODE in TRIM.FaTE was evaluated by comparing its results to solutions of some small systems for which the exact solution was known. Additional checks regarding mass balance preservation indicated that the numerical solutions had the proper properties. Tests with matrices as large as 1000 x 1000 were successful. Thus, LSODE was determined to be an appropriate tool for use in TRIM.FaTE.

Prior to specific process model evaluations, the user interface of Prototype V was evaluated to determine possible modifications that could make it easier to use. Changes made to Prototype V as a result of this evaluation included:

- More efficient methods to set up the program and view results (in addition to HTML results) under the "results" tab of the "setup run/view results" menu selection. This included HTML output with an extra page of summary biotic masses and population sizes for each compartment in order to check implications of the input biota population densities. A page showing how each chemical is distributed between biotic and abiotic compartments and within the biota was added;

- A new option to send the resulting concentrations in user-selected compartments within volume elements to Excel plots; and

- Changes/additions to the biotic import sheet, including the ability to perform an "all biotic" and "all abiotic" run. These changes/additions led to automatic creation of biotic sinks, which improved run time efficiency.

Performance improvements were also made in Prototype V. For example, multiple calls within the same run were adjusted to decrease run-time (i.e., optimization passes). These optimization passes included the ability to re-use the previously generated transition matrix structure (as long as compartments are the same as in the previous run). Prototype V was set up to generate links automatically (such that fewer output excretion links would occur for animals and cross-composite container links would not occur which, for example, would prevent roots of coniferous forest from hooking up to the stem of grasses/herbs). Further, a run option was added to use a multiplier to preserve the mercury molar mass.

To facilitate the various model comparisons being considered, run options were made available to omit certain types of links (e.g., soil to soil, soil to water, abiotic to abiotic diffusion, biotic to abiotic diffusion). One-step disable/re-enable "all biota" was created. Extra result pages (to make the model more amenable to post-processing) were made available to show concentrations, average concentrations, and compartment-averaged cumulative fluxes. Because certain links could be omitted, it was possible to analyze the net flux to the soil from the air and thus evaluate the change in chemical mass due only to exchange with the atmosphere.

3.3.2 Overall Evaluation of Versions 1 Through 2.5

TRIM Version 1, which was written in Java, was the first production version of the computer framework after Prototype V. TRIM Version 1 contained an implementation of TRIM.FaTE that provided similar capabilities to Prototype V. TRIM Version 2 included TRIM.FaTE and interfaces to the TRIM Expo inhalation programs APEX and HAPEM. In versions after TRIM 2.5, the APEX and HAPEM interfaces will instead by provided by the Multimedia Integrated Modeling System (MIMS). MIMS will provide a means of connecting and running all the TRIM modules: FaTE, Expo, and Risk.

The implementation of TRIM.FaTE in TRIM Version 1 was evaluated by comparing its results to those from Prototype V for a variety of scenarios. The first evaluations used simple systems of abiotic compartments (e.g., air only, air/soil/water). Later evaluations used systems with hundreds of biotic and abiotic compartments. At the conclusion of the evaluation, the results of Prototype V and Version 1 were indistinguishable when the models used the same configuration and input parameters. Like the prototypes, Version 1 also used LSODE to solve systems of linear ordinary differential equations. Many of the optimizations that were added to Prototype V during the process evaluation were implemented in Version 1. Optimizations specific to the Java implementation were also added. In addition to benefitting from specifically coded optimizations, the performance of the TRIM computer framework will continue to improve with advances in the Java programming language and the availability of faster computer hardware.

Initial applications demonstrated that Version 1 had some difficulties running on Windows 95 and Windows 98 computer systems. These difficulties were primarily a result of the fact that TRIM.FaTE was developed using Java on Windows NT and was not designed to address the memory management limitations associated with Windows 95 and Windows 98. On Windows NT, overall usage of memory by TRIM was reasonable for the size of the application and stayed relatively constant while the program was running. However, on Windows 95/98 the management of memory was far less efficient. That is, instead of memory usage remaining fairly constant, it continued to grow while the program was used until it exceeded the available amount of RAM, at which time the computer began to slow down significantly until it ultimately halted execution of TRIM. It was not possible to determine whether the memory problems were due to Java in particular or Windows 95/98 in general. As a result of these memory issues, Version 1 of TRIM.FaTE can only be used for small scenarios on Windows 95/98. To run Version 1, at least a 400 MHz processor with 256 MB of RAM running Windows NT or 2000 is recommended.

The Spring 2000 release of the TRIM computer framework (Version 1.1) included some restrictions that made long-term (e.g. 30 year) studies difficult to run. The model required that all time-varying data such as meteorology be read in to memory, and that all output results fit in memory. This restricted the size and duration of scenarios that could be run with Version 1.1. These restrictions are removed in TRIM Versions 1.3 and beyond. In these later versions, time-varying data are read in from files on an as-needed basis and multiple variables can be read in from the same file. In addition, outputs are written to disk as they are produced instead of being stored in memory and then exported to disk. The Spring 2001 release of the TRIM computer framework (Version 2.0) has a sensitivity analysis feature included in it. The results of the sensitivity analysis produced by TRIM Version 2.0 will be compared qualitatively and quantitatively to the results obtained using Prototype V. TRIM Version 2.5, released in July, 2002, includes support for Monte Carlo simulations, and visualization tools (e.g. a food web viewer and a results viewer that shows compartment concentrations in their volume elements with other geographic-oriented data).

3.3.3 Algorithm and Compartment Audit

A comprehensive audit of the master TRIM.FaTE library was performed, with follow-up investigation and resolution of discrepancies encountered. This follow-up has continued into 2002. The purpose of this audit was to verify that the equations, constants, and units in the master library are accurate and consistent with the TRIM.FaTE documentation, and that the current set of input parameters are implemented as intended.

3.3.3.1 TRIM.FaTE Libraries

The majority of the information describing chemical transport and transformation in TRIM.FaTE is contained within files referred to as libraries. A library, which can be viewed by the user and customized as needed or particular scenarios, is similar to a database in that it contains data for a number of related objects in a single file. In particular, libraries consist of properties and their associated values grouped by compartments (e.g., air, surface water, water column herbivore, white-tailed deer). These properties can be defined as constants, booleans (i.e., true/false values), or as formulas.

For a typical compartment, these properties include both constants (e.g., depth of a soil compartment) and formulas (e.g., a function to calculate the wet deposition rate of particles in air). The algorithms contain the equations that describe (1) how pollutant mass is transported between compartments and (2) how pollutants are transformed within compartments over time. TRIM.FaTE is unique among models in that the algorithms that define the transport and transformation of pollutants in the environment are stored in a data file that can be edited by the user using the TRIM graphical user interface (GUI). Thus, the user has direct access to these algorithms, and would not need programming skills to make adjustments/corrections to them. Examples of the properties associated with transport and transformation algorithms are provided in Tables 3-1 and 3-2, respectively.

Chemicals and sources are similar to compartments in that they also consist of a set of constant and formula properties that describe their characteristics. For a more detailed description of the TRIM computer architecture, refer to the TRIM.FaTE TSD Volume I (U.S. EPA 2002a).

Table 3-1
Example of Transport Algorithm Properties (Ingestion of Arthropod by Mouse)

Property Name	Value
Category	Ingestion
ChemicalCategory	All
DoesTransformChemical	False
DoesTransportChemical	True
Enabled	True
IsDefaultForCategory	True
ReceivingCompartmentCategory	Mammal/Mouse
SendingCompartmentCategory	Insect/Arthropod
TransferFactor	ReceivingCompartment.PopulationSize * ReceivingCompartment.BW * TheLink.FractionSpecificcompartmentDiet * ReceivingCompartment.FractionDietSoilArthropod * ReceivingCompartment.FoodIngestionRate * ReceivingCompartment.Chemical.AssimilationEfficiencyFromArthropods / SendingCompartment.TotalMass

Table 3-2
Example of Transformation Algorithm Properties (Methylation by Birds)

Property Name	Value
Category	Transformation
ChemicalCategory	Same
DoesTransformChemical	True
DoesTransportChemical	False
Enabled	True
IsDefaultForCategory	True
ReceivingChemicalName	Methylmercury
ReceivingCompartmentCategory	Bird
SendingChemicalName	Divalent Mercury
SendingCompartmentCategory	Bird
TransferFactor	SendingCompartment.Chemical.MethylationRate

3.3.3.2 Audit Scope

The audit of the TRIM.FaTE library compared the formulas, constants, and units contained within the compartments and algorithms to the TRIM.FaTE documentation to confirm that:

- All formulas and constants in the library are included in the TRIM.FaTE documentation (i.e., no omissions);
- All formulas and constants in the library are consistent with the documentation (i.e., no typos or translation errors);
- The units used in the library are internally consistent (i.e., each formula using a particular variable assumed the same units for the variable) and consistent with the documentation; and
- The most recent updates to the formulas and constants are reflected in the library and in the TRIM.FaTE documentation.

The formulas and their units were compared with the TRIM.FaTE documentation presented in the 1999 draft *TRIM.FaTE TSD Volume II: Description of Chemical Transport and Transformation Algorithms*. The constants were compared with the data tables provided in Appendix C of the 1999 TRIM.FaTE Status Report.

Note that this audit only reviewed the TRIM.FaTE documentation to confirm formulas, constants, and units used in the library. It did not include an exhaustive review of the documentation. In many cases, the TSD Volume II presents detailed derivations of formulas and alternative algorithms and methods for characterizing compartments and mass transfer between compartments that were not presented in the library. This audit only reviewed those parts of the documentation that were required to verify a part of the library. Furthermore, there are several "built-in" constants (e.g., π) used by the TRIM.FaTE library that are not actually included in the library, but in a separate constants file. These constants were not verified as part of this audit.

This audit did not include review of the main TRIM.FaTE code responsible for calling the algorithms and identifying the sending and receiving compartments to which an algorithm is to be applied, which is in part specified by the user. This audit focused solely on the content of the TRIM.FaTE library and did not review the application of the library. A review of this implementation is the subject of the mercury test case (see Volume II of this report).

3.3.3.3 Audit Methods

TRIM.FaTE is designed to estimate the transport and transformation of chemical mass between and within both abiotic and biotic media, and a large number of constants and formulas are required to describe these processes. The version of the TRIM.FaTE library assessed in this audit contained 177 named algorithms describing the transfer of contaminant mass between compartments and 47 compartment types (7 abiotic and 40 biotic). Many of the named algorithms related to food ingestion are repeated many times, differing only with respect to the identities of the pollutant and the receiving compartment (i.e., the species named as the consumer). For example, the "Ingestion of Arthropod" algorithm was included 20 times in the algorithm library to represent four species of animals that consume soil arthropods and five different pollutants (i.e., 4 x 5 = 20). The algorithms for transfers between abiotic media can be repeated to represent different chemicals (e.g., applied to two organic compounds, applied to three mercury species, or applied to all chemicals). Most algorithms include one or more formulas, but some simply refer to variables named within one of the compartments. Within each compartment type, there are a number of different constants and formulas.

The audit began with a review of the chemical transport and transformation algorithms and their associated properties as compared with Volume II of the 1999 draft TSD (U.S. EPA 1999d). Because many of the formulas presented in the TRIM.FaTE documentation are divided between the algorithm and compartment sections of the library, however, a systematic audit of the compartments was also needed.

When comparing formulas in Volume II of the TSD to the library, the units for each variable described in the TSD and the units assigned to the variable in the library were examined to ensure that the units were consistent and that all unit conversions (e.g., grams to kilograms) that might be needed in the library were present. Because the units for the library variables were not defined for all variables in the "Variable Definition" file, an audit of the units for each variable was also conducted. After that audit, the audit of the algorithms was completed.

The comparisons were documented and discrepancies explained in some detail. These comments were then sent to the experts responsible for developing, refining, or implementing different components (e.g., air, biota, surface water and sediments) of the TRIM.FaTE model for their review and recommendations on how to address the discrepancies. Their comments and recommendations were incorporated into the detailed audit documentation, which was then distributed again to the experts for review. For some of the discrepancies, several rounds of review were required to establish a solution (i.e., a change in the library, a change in the documentation, or changes in both). Finally, as some of the recommended library changes were actually implemented, a few new discrepancies were uncovered. These were also resolved by the expert(s) familiar with the compartments or transfers at issue. The resolution and its basis were documented and reflected in the final TSD Volume II (U.S. EPA 2002b).

3.3.3.4 Findings/Results

This audit of the algorithms and compartments resulted in a number of changes being made to both the library and TRIM.FaTE documentation. A summary of the changes is presented in Appendix I-A and the TRIM.FaTE Algorithm and Compartment Audit (ICF Consulting 2002); refer to the audit report for detailed review comments on each algorithm and compartment.

Algorithm Audit

To facilitate the evaluations and discussions, the named algorithms contained in the library were numbered consecutively from 1 to 177. The chemicals to which each algorithm was applied (e.g., two organic compounds) was noted, as well as how many different receiving compartments were represented (e.g., three species of mammals). Thus, if a named algorithm applied to two chemicals and three species of mammals, there were six instances of that named algorithm in the algorithm library. The first instance of each named algorithm was evaluated.

The audit of the algorithm library revealed several types of discrepancies between the TRIM.FaTE library and documentation that required changes to one or the other or both (ICF Consulting 2002). Several general types of changes are described below.

- The majority of the changes required did not change the output of the library. Draft TSD Volume II indicated that the food ingestion algorithms should include an assimilation efficiency of the contaminant by the receiving animal compartment. Assimilation efficiencies were included for fish, but not for birds and mammals. Assimilation efficiencies for contaminants from general "food" (i.e., fish, birds, or mammals), arthropods, worms, and plants have been added to the appropriate ingestion algorithms and compartments (the assimilation efficiency is a function of both the food type and the consumer species). Assimilation efficiencies of the contaminant from soil and from water also were added to those algorithms and to the bird and mammal compartments. As a default, the values of all assimilation efficiencies have all been set to one (1) in the animal compartments. As stated in Volume II of the 1999 draft TSD, "if rate constants for excretion and chemical transformation are determined with respect to the mass of a contaminant that is taken up in the diet rather than the mass that is assimilated, the dietary assimilation efficiencies may be ignored." The rate constants used to-date were determined on the former basis (i.e., mass of contaminant taken up in the diet, not mass assimilated). However, to allow for future runs using different rate constants and to match the documentation of the ingestion algorithms, the assimilation efficiencies were added.

- Some of the changes involved changing the algorithm properties to ensure that the algorithm name described the transfer in the algorithm in the correct direction (or vise versa). For example, the demethylation algorithms called for the methylation rate instead of the demethylation rate (Algorithm numbers 26 through 30). The demethylation algorithms now call for the demethylation rate from the appropriate compartments.

- Some of the changes involved restricting the chemicals to which some of the algorithms applied. Some algorithms were intended for use with only divalent or both divalent and elemental mercury, yet were applied to all mercury species, including methylmercury (e.g., Algorithms 46, 47, 173, 174, 175). The way these algorithms were restricted to specific chemicals prior to the audit was by setting rate constants to 0 for those chemicals to which the algorithm should not apply.

To streamline the TRIM.FaTE library and reduce runtime, the new method removed the algorithms that did not apply.

- Some of the algorithms reflected an older library that had not been updated according to the mass transfer formulas developed for the draft TSD Volume II (e.g., Algorithms 32, 38, 54, 55, 147). These algorithms have been updated.

- Some of the documentation in the draft TSD Volume II reflected older versions of a mass transfer formula that had not been updated, although the library had been updated (e.g., Algorithms 40, 46, 47, 149). The final TSD has been updated to be consistent with the formula.

- Some of the mass transfer formulas in the algorithm library apparently had not been documented in the draft TSD. Very few of the ingestion algorithms were specified in the documentation; instead, the documentation provided one very long formula describing all transfers into and out of an animal (e.g., Algorithms 63 to 65 and many of the remaining ingestion algorithms). Other mass transfer formulas also were missing from the draft TSD (e.g., Algorithm 2, 150, 134). The mass transfer formulas have been added to the final TSD.

- Some of the documentation of mass transfer equations in the draft TSD, Volume II, were in error through typographical error, omission of variables, or other mistakes (e.g., TSD Equation 5-36 for Algorithm 148, TSD Equation 7-41 for Algorithm 155, and TSD Equations 2-39 and 2-40, which incorrectly represented the single equation that should have been included). These errors and omissions have been corrected in the final TSD.

- A few of the changes related to mistakes in unit conversions in the library (e.g., Algorithms 33 and 159).

- Wet and dry depositions of particles from air to the surface of plant leaves were missing from the algorithm library (e.g., new Algorithms 48b, 177b), even though the mass that would have been deposited to the plant surfaces was removed from the mass that fell to the soil. Also, the ingestion of particles on the leaf surface by herbivores consuming the leaves was not represented in the library or in the draft TSD. The algorithm library and documentation have been updated based on these findings.

As a consequence of discovering algorithms that were missing altogether from the algorithm library, we assembled the algorithm names in a table, pairing those that described a mass transfer in one direction and in the reverse direction. Those results are provided in Appendix I-A. Using that table, it was possible to identify additional algorithms that perhaps should be included and to confirm with the model developers that those algorithms were not included in the model for a reason. The final TSD Volume II has been prepared with the intent to provide an exact crosswalk between equations in the library and the TSD.

Compartment Audit

The audit of the compartment properties section of the TRIM.FaTE library revealed several types of discrepancies with the TRIM.FaTE documentation that required changes to one or the other or both (ICF Consulting 2002). Several general types of changes are described below.

- The majority of the changes resulting from the audit of the compartments involved documenting properties (i.e., formulas and constants) for PAHs that are contained in the library. The summary of input data included in Appendix C of the 1999 TRIM.FaTE Status Report had only included values for mercury species.

- There were a number of errors identified in the compartments resulting from improper translation of equations from the documentation into the library. Some of these mistakes were as simple as incorrect unit conversions impacting a single property, while others were logic errors impacting a number of properties. These logic errors were typically introduced by representing a single equation from the documentation with several simpler equations in the library. All such errors have been corrected.

- As for the algorithm library, we also identified and corrected compartment properties that had been updated in the documentation but not in the library, as well as formulas that had been updated in the library but not in the documentation.

- There were a few properties in the compartments that were no longer being used, having been replaced with newer formulas. We removed these properties to improve computational efficiency and to prevent future confusion for users reviewing the library.

- Finally, as a result of our review, we identified a few formulas that were incorrect in both the library and documentation. In these cases, the expert team reviewed the environmental processes in question and developed new formulas. Corresponding library changes were then implemented.

3.3.3.5 Audit Summary and Conclusions

The audit of the algorithm and compartment sections of the TRIM.FaTE library identified some mistakes in both the library and the documentation of the library. Although difficult, the exercise was extremely important to ensure that the model library is coded correctly and that the documentation of TRIM.FaTE clearly and accurately represents the formulas in the model. Moreover, many suggestions for clarification of the mass transfer formulas in TSD Volume II were provided by the experts. This evaluation strengthened both the TRIM.FaTE model library and documentation.

3.4 TESTING OF INDIVIDUAL PROCESS MODELS

Tests were designed and performed to evaluate individual process models, as well as for approaches and algorithms developed specifically for TRIM.FaTE. Examples of process models identified for evaluation include the particle/plant leaf algorithms, the soil flux model, and the air transport algorithms.

When different models are available for the same process (e.g., bioaccumulation in fish), model-to-model evaluations may be performed at a process model level to test the overall performance of TRIM.FaTE using different input algorithms. As one example of this, EPA has evaluated both an equilibrium-based approach and a bioenergetics approach to model bioaccumulation in fish.

Input data acquisition and the careful evaluation of model inputs are ongoing. To date, the majority of effort has focused on compiling an initial set of model inputs for a small set of test chemicals (i.e., phenanthrene, benzo(a)pyrene, various mercury species) and environmental settings (U.S. EPA 1998e).

3.5 AIR PROCESS MODEL EVALUATION

For the air process model evaluation, the TRIM.FaTE air transport module was compared to the Urban Airshed Model (UAM) and the Industrial Source Complex (ISC) Model. These comparisons are presented in Sections 3.5.1 and 3.5.2, respectively.

3.5.1 Comparison with the Urban Airshed Model

This section presents the approach and results of runs to compare the TRIM.FaTE air transport module with the UAM transport module.

3.5.1.1 Approach and Model Setup

As part of the evaluation of the air transport module of TRIM.FaTE, a simple "air-only" TRIM.FaTE run was set up and quantitatively compared with the transport module of the UAM, an existing grid model used by EPA and others to estimate dispersion of air pollutants.[3] The source included in all runs emitted gaseous mercury at a constant rate of 1.514E-2 g/s. Mercury emissions were 100 percent elemental, and no chemical transformation/degradation was included. No background mercury concentrations were included and only dispersion (i.e., no deposition) was considered.

Two grid layouts comprised of equal-sized square parcels were selected for this comparison (modeled region 27.76 km on a side; total area approximately 770 km^2):

---

[3] As this comparison was based on a simple scenario (i.e., simple terrain, no chemical transformation, etc.), the results are not necessarily indicative of all of the differences between the air module of TRIM.FaTE and UAM. It is possible that more complex scenarios would lead to more marked differences in model output.

- 5 x 5 (25 square parcels)
- 9 x 9 (81 square parcels)

Figure 3-2 presents configurations for both of these grid layouts. For both grids, two vertical layers were included. Layer 1 was defined as the lower layer, extending vertically from ground level to the mixing height. Layer 2 extended from the mixing height to 1,864 m above ground level (or 1,000 m above the highest mixing height for the meteorology data used in this analysis). Scenario descriptions for each model and key model characteristics are described below.

One UAM run was completed for each grid layout. Surface meteorology data for UAM were obtained from the National Weather Service (NWS) Hourly U.S. Weather Observation (HUSWO) database; values for January 1990 for the chlor-alkali test site were used. Upper air meteorology data were obtained from the NWS Radiosonde database for the same site and time period. Before a run is initiated, UAM preprocesses these two sets of data to account for vertical heterogeneity in wind speed and wind direction values. This preprocessing results in different input data sets for the lower and upper layers (i.e., the layer 1 data are not identical to the HUSWO data, and the layer 2 data are not identical to the radiosonde data); however, as a result they best represent the average winds for both layers. The vertical wind speed (i.e., between layers 1 and 2) is estimated internally by UAM based on mass continuity and changes in compartment size that result from the changing mixing height. Average hourly concentrations were calculated by UAM for 1 month for each compartment of each layer. These results were averaged to obtain the monthly average for each compartment.

Figure 3-2
Grid Configurations
(source parcels are shaded)

5x5

1	2	3	4	5
6	7	8	9	10
11	12	13	14	15
16	17	18	19	20
21	22	23	24	25

9x9

1	2	3	4	5	6	7	8	9
10	11	12	13	14	15	16	17	18
19	20	21	22	23	24	25	26	27
28	29	30	31	32	33	34	35	36
37	38	39	40	41	42	43	44	45
46	47	48	49	50	51	52	53	54
55	56	57	58	59	60	61	62	63
64	65	66	67	68	69	70	71	72
73	74	75	76	77	78	79	80	81

For TRIM.FaTE, a set of four runs was completed for each grid layout resulting in eight total TRIM.FaTE runs. These four runs were obtained by using two sets of meteorology data and two sets of vertical wind speed data as follows:

Horizontal meteorology data sets:

(1) NWS HUSWO database, values for January 1990 for the chlor-alkali test site (referred to in the context of these analyses as the "original meteorology data").

(2) Data for January 1990 for the chlor-alkali test site *after* preprocessing by UAM to account for vertical heterogeneity (referred to below as "UAM meteorology data").

Vertical wind speed data sets:

(1) Vertical wind speed equal to zero (i.e., no transfer from lower layer to upper layer).

(2) Vertical wind speed calculated by UAM (extracted from UAM and then input into TRIM.FaTE).

These four sets of TRIM.FaTE runs were completed to evaluate the effects of the various meteorology data and vertical wind speed input combinations. However, the TRIM.FaTE run completed using UAM meteorology data and vertical wind speed from UAM was considered to be the most similar to UAM with regard to input data. Therefore, results from this run were used for the model-to-model comparisons.

3.5.1.2 Results

Several key UAM and TRIM.FaTE model characteristics should be considered when comparing the results of these two models:

- UAM calculates mass transport in the horizontal and vertical directions via three mechanisms: advection, dispersion, and diffusion.
- TRIM.FaTE explicitly models advective transport, only models diffusion by assuming equal mixing of pollutant concentrations within a compartment, and does not model dispersion.
- TRIM.FaTE does not have a vertical sink and thus does not lose system mass across the vertical boundaries. For the UAM runs in this analysis, vertical transport out of the top of the modeled domain was not allowed.

Effect of Meteorological Data and Vertical Velocity Input Data for TRIM.FaTE

Overall, concentration patterns were similar for all TRIM.FaTE runs for each grid layout. The following effects were observed:

- As expected, a vertical velocity of 0 resulted in higher concentrations for layer 1 because no mass was transported to layer 2. Layer 1 concentrations were about 1.5 to 3 times larger relative to runs with a vertical velocity.[4]

- Using the "original meteorology data" resulted in slightly higher concentrations for some compartments in layer 1 but did not appear to introduce major differences into the overall pattern of concentrations.

The general patterns for a given model were similar for both the 5 x 5 grid and the 9 x 9 grid, with the denser grid providing greater resolution. Comparison of the different grid results did not appear to provide any additional information regarding the model comparison. Observations listed below for layer 1 and layer 2 are generalized (i.e., not specific to one grid layout); quantitative results provided with this summary reflect the results for the 5 x 5 grid.

Layer 1 Comparison (UAM vs. TRIM.FaTE with UAM Meteorology Data)

TRIM.FaTE and UAM layer 1 results followed the same basic pattern across all compartments (see Figure 3-3). Table 3-3 presents the percent differences between the average results from the two models. On average, the concentrations estimated using UAM were approximately 22 percent higher than those estimated using TRIM.FaTE. For the southwest quadrant of the grid, the TRIM.FaTE concentration was noticeably less than the UAM concentration. For compartments in the other three quadrants (NW, NE, and SE), the TRIM.FaTE concentrations were generally equal to or higher than the UAM concentrations (see Figure 3-4). Mass bias toward the axes of the grid (i.e., a "pipeline effect") was observed in both TRIM.FaTE and UAM layer 1 results; however, the bias was slightly less pronounced in the UAM results. For more details regarding this effect, see Section 4.2.

---

[4] To verify that the vertical transport algorithms in TRIM.FaTE were operating properly, an additional run was made for each grid layout with the vertical velocity set to zero. We compared the results of these scenarios to the results of similar scenarios with only one vertical layer. As expected the results for the one vertical layer scenarios were identical to the results for the two vertical layer/zero vertical velocity scenarios.

Figure 3-3
TRIM.FaTE and UAM Concentrations, Layer 1, 5 x 5 Grid

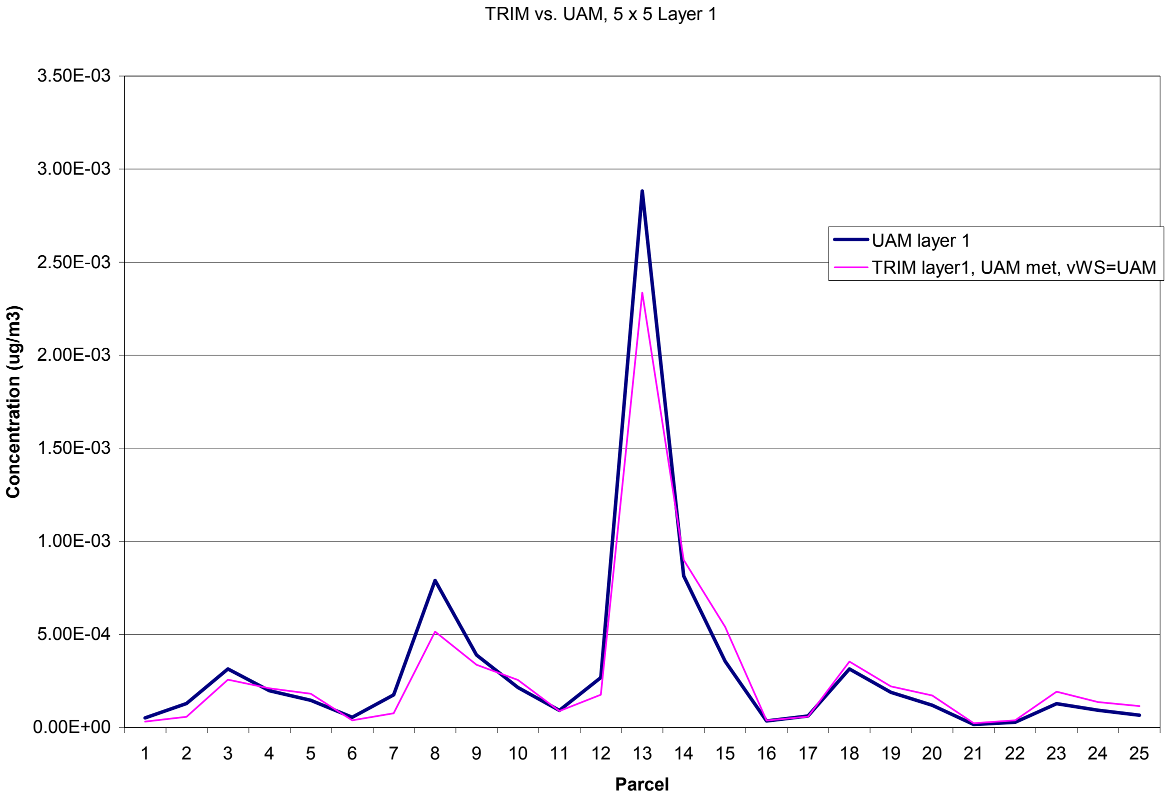
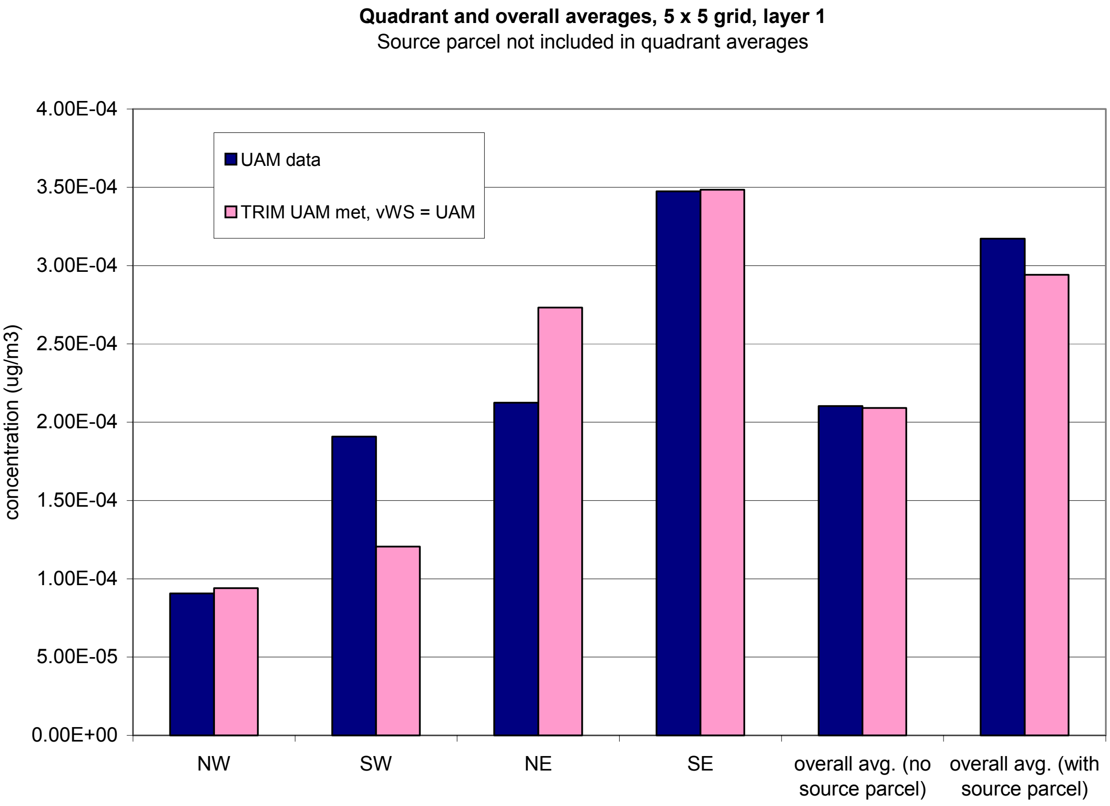


Table 3-3
Percent Difference ((UAM-TRIM.FaTE)/UAM), Layer 1, 5 x 5 Grid

Parcel	% Diff	Parcel	% Diff	Parcel	% Diff	Parcel	% Diff	Parcel	% Diff
1	38%	6	29%	11	3.9%	16	-7.1%	21	-43%
2	55%	7	57%	12	34%	17	5.2%	22	-36%
3	18%	8	35%	13	19%	18	-12%	23	-50%
4	-6.5%	9	13%	14	-10%	19	-17%	24	-48%
5	-24%	10	-18%	15	-52%	20	-43%	25	-74%

Figure 3-4
Quadrant Averages, Layer 1, 5 x 5 Grid



Overall, TRIM.FaTE and UAM seemed to agree more closely in the quadrants that are predominantly upwind (NW) and downwind (SE) of the prevailing winds. The largest compartment concentration differences between TRIM.FaTE and UAM were primarily located in the compartments comprising the boundary of the grid; at these locations, TRIM.FaTE concentrations were larger than UAM results. This effect may have resulted in part from differences in how the two models treat mass flow beyond the grid boundaries. The UAM has a set of boundary cells encompassing the entire perimeter of the modeling domain. Mass from the modeling domain can flow into these cells or mass from these cells can flow back into the modeling domain, depending on the direction of the wind. TRIM.FaTE, on the other hand, was run without boundary cells and thus mass leaving the modeling domain was deposited in sinks and was not available to be transported back into the modeling domain. The impact of adding boundary cells to a TRIM.FaTE run is discussed in Section 4.2.1.3.

If the compartment results for the 5 x 5 grid for each model are ranked by concentration, the rankings are close (within two ranks) for most of the compartments and match for 8 of the 25 grid compartments. The largest rank difference is six (e.g., 12th highest concentration vs. 18th), calculated for two compartments.

UAM results were regressed on TRIM.FaTE results to obtain a rough estimate of correlation. For the 5 x 5 grid, the R-square value for this regression was 0.9697. For the 9 x 9 grid, the R-square value was 0.9643. Thus, increasing grid resolution did not appear to result in a higher correlation between the two models.

Layer 2 Comparison (UAM vs. TRIM.FaTE with UAM Meteorology Data)

For layer 2, the concentration patterns for the two models were relatively similar overall but there were noticeable differences for some compartments. UAM results were larger than TRIM.FaTE results for all compartments but one (see Figure 3-5 and Table 3-4). Concentration gradients across these compartments were generally somewhat different for UAM and TRIM.FaTE, especially in the eastern half of the grid. Regression of UAM results on TRIM.FaTE resulted in an R-square value of 0.8219, which is smaller than the corresponding value obtained for layer 1. Note that for both models, the level 2 results are roughly an order of magnitude lower than the level 1 results.

Figure 3-5
TRIM.FaTE and UAM Concentrations, Layer 2, 5 x 5 Grid

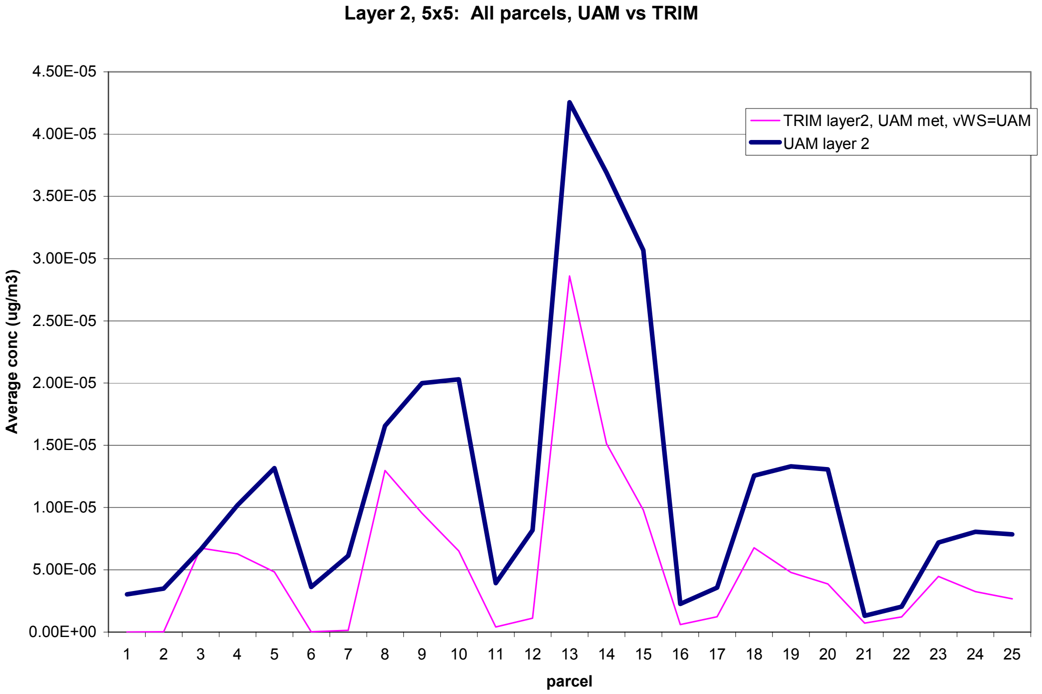


Table 3-4
Percent Difference ((UAM-TRIM.FaTE)/UAM), Layer 2, 5x5 Grid

Parcel	% Diff	Parcel	% Diff	Parcel	% Diff	Parcel	% Diff	Parcel	% Diff
1	99.9%	6	99.2%	11	90%	16	73%	21	45%
2	99.0%	7	97%	12	86%	17	65%	22	41%
3	-1.3%	8	22%	13	33%	18	46%	23	38%
4	38%	9	52%	14	59%	19	64%	24	60%
5	63%	10	68%	15	68%	20	70%	25	66%

The observed differences between TRIM.FaTE and UAM for layer 2 could be the result of lower net mass transport to layer 2 in TRIM.FaTE compared to UAM. This effect may be due to differences in the advection algorithms. In addition, quicker mass transport out of the grid for layer 2 could occur in TRIM.FaTE (i.e., mass more quickly advected to the sinks). The differences could also be due to UAM's inclusion of both vertical dispersion and diffusion. TRIM.FaTE does not include vertical dispersion and only includes vertical diffusion in that mass transported vertically by advection is assumed to spread evenly throughout the receiving compartment.

Summary

For the regular grids examined in these analyses, UAM and TRIM.FaTE predicted similar average monthly air concentrations across the entire grid for layer 1. Patterns for layer 2 were less similar, but concentrations for UAM and TRIM.FaTE were generally within an order of magnitude and often within a factor of 2 or 3 of each other (UAM values were consistently higher). It is important to note that these results were obtained using identical meteorology data that had been preprocessed by UAM. Additionally, it should be stressed that this evaluation was carried out with a focus on using identical input data for UAM and TRIM.FaTE (where possible) in order to compare model operation. Also, these results may be different for other seasons, as this evaluation was done in January when advection strongly dominates over diffusion. For other locations and times diffusion may be as important as advection and the differences between the models may be different. Overall, UAM and the air component of TRIM.FaTE seem to produce comparable results for simple, single-vertical-layer scenarios. However, based on the differences between the estimated concentrations in layer 2, TRIM.FaTE may not be appropriate for modeling pollutants that are transported significant distances by aloft winds and dispersion processes.

3.5.2 Comparison with the Industrial Source Complex Model

TRIM.FaTE also was compared to an EPA dispersion model widely used in regulatory applications, the Industrial Source Complex Model (Short Term), version 3 (ISCST-3). The fate and transport algorithms in ISC are based on Gaussian dispersion equations that are solved for a given set of temporal and spatial circumstances. ISC is not a mass-balanced model, whereas

TRIM.FaTE is mass-balanced, as are grid models in general. Thus, this evaluation was carried out to obtain a rough comparison with an air model currently used by EPA for regulatory purposes. As ISC is used as part of EPA's Multimedia, Multi-pathway, Multi-receptor Exposure and Risk Assessment (3MRA) model (http://www.epa.gov/athens/research/projects/3mra/), the model-model comparison aspect of the mercury test case (Volume II) will include some comparison of ISC output to TRIM.FaTE's air output.

3.6 EVALUATION OF MERCURY SPECIATION IN AIR AND SOIL

This section evaluates the mercury parameter values (e.g., reduction and oxidation rates in air and soil) that affect mercury speciation in air and soil. Specifically, the parameter values chosen for relevant air and soil processes are presented, and simulations are performed to determine whether predicted speciation in soil and air is consistent with observed background levels.

Section 3.6.1 describes the properties and behavior of mercury relevant to the air and soil processes model. Section 3.6.2 presents the methods of the evaluation, including the chosen parameter values. The results and conclusions of the evaluation are presented in Section 3.6.3 and Section 3.6.4, respectively.

3.6.1 Mercury Species and Transformations in Air and Soil

Mercury is emitted to the atmosphere both in elemental (Hg^0) and divalent (Hg^{2+} or Hg(II)) forms and is found in both species in the atmosphere. Once emitted into the environment, these species can be transformed to another species or deposited to other environmental media.

Background concentrations of mercury in air are 1 to 3 ng/m^3 in the Southern Hemisphere and 2 to 4 ng/m^3 in Northern Hemisphere (Slemr and Langer cited in Lin and Pehkonen 1999). More than 90 percent of atmospheric mercury is elemental, and some estimates are as high as 95 to 97 percent. The predominant oxidation reactions transforming gaseous elemental mercury to divalent mercury are with O_3 and H_2O_2. Because of such transformations, the half-life of elemental mercury in the atmosphere is between 0.5 and 2 years (U.S. EPA 1997). Although significant transformation of elemental to divalent mercury may occur in aqueous media, all transformation of elemental to divalent mercury in TRIM.FaTE is included in the general atmospheric transformation rate.

Most divalent mercury released to air is removed from the environment on the local or regional scale (i.e., relatively close to the source). Divalent mercury is extremely reactive and may be transformed back to the elemental form or other species. It may be gaseous, but often is associated with particles. Some of the gaseous forms of divalent mercury in the atmosphere may originate from evaporation from clouds. Divalent mercury often is found as $HgCl_2$, $Hg(OH)_2$, or compounds of other halides, which collectively are referred to as reactive gaseous mercury (RGM). All these forms are very water soluble, often 105 times more soluble than elemental mercury (Lindberg and Stratton 1998). RGM can be rapidly reduced back to Hg^0, at least in the aqueous phase (Pleijel and Munthe 1995a and 1995b). All of these transformations make it difficult to quantify source distribution (Lindberg and Stratton 1998). Because of its reactivity, RGM is thought to exist in ambient air at very low concentrations. There are consistent dial and diurnal cycles of RGM, with the peak concentrations occurring at midday and sharply dropping off at night (Lindberg and Stratton 1998).

In ambient air, concentrations of particulate mercury are on the order of picograms per cubic meter, but concentrations as high as a few nanograms per cubic meter have been measured in urban/industrial areas (Lu and Schroeder 1999). Although particulate mercury usually is a very small fraction of total atmospheric mercury, it plays an important role in the mercury deposition patterns (Lu and Schroeder 1999). Munthe (1993) found that a large fraction of mercury in rainwater was bound to particles, indicating the importance of understanding the dynamics involved with the particulate phase.

Mercury deposition rates generally are much higher for the divalent species than for the elemental species. Because divalent mercury is more water soluble and more likely to partition to particles than elemental mercury, what little elemental mercury is transformed to divalent mercury is quickly deposited to soil, particularly during rain events. In addition, atmospheric divalent mercury near moist soil will partition out of the atmosphere and into the moist soil (U.S. EPA 1997).

Once deposited to surface soil, each of the mercury species can diffuse or be advected to lower soil zones, react into another species, or diffuse back into the air. Mercury speciation in soil is highly variable, and it is difficult. However, mercury in soil generally would be expected to be predominantly in the divalent form (e.g., Biester and Scholz 1997).

There is limited information on how deep mercury is found in soils, and even less information is available on mercury speciation in subsurface soil. One study (DiGiulio and Ryan 1987) on peat soils found little change in mercury at soil depths up to one meter. Another study (EPRI 1998) found similar mercury concentrations in the 0- to 2-cm and 5- to 10-cm horizons.

3.6.2 Methods

Information presented in Section 3.6.1, as well as other available information on the environmental chemistry of mercury, was used to select preliminary default values for parameters included in the TRIM.FaTE air and soil process models. Model simulations using a simple hypothetical scenario then were performed to evaluate whether the preliminary parameter values produced realistic predictions of mercury speciation in soil. Specifically, the goal of the evaluation was to identify a set of parameter values that resulted in 90 to 98 percent divalent mercury in the surface soil compartment. An iterative series of simulations was performed with varied parameter values until this goal was achieved. Because mercury deposition is substantially affected by precipitation, all simulations were run both with and without precipitation included in the input meteorological data.

The model configuration for this evaluation consisted of air, surface soil, root zone soil, and vadose zone soil compartments. Mercury was introduced into the system via a constant background air concentration blowing into the system (i.e., no discrete source was included).

Mercury speciation in background air was assumed to be 98 percent elemental and 2 percent divalent. Model runs were completed for a constant precipitation case and a no precipitation case.

3.6.3 Results

The final parameter values are presented in Table 3-5. For the scenario used in this evaluation, the final parameter values result in 98.2 percent divalent mercury in surface soil with and without precipitation. These results are slightly higher than the goal of this evaluation, which was 90 to 98 percent divalent mercury in surface soil.

Table 3-5
Concluding Values of Particular Air and Soil Parameters

Parameter Name	Default Value	Comments
Percent of divalent mercury in background air	2%	Based on mercury speciation observed in various studies.
Oxidation rate in air	0.0038/day	Corresponds to a half-life of 6 months.
Reduction rate in air	0/day	None.
Oxidation rate in soil	0/day	Although transformation rates in soil are unknown, they are thought to be small. Thus, the default value was set to zero.
Reduction rate in soil	0/day	Although transformation rates in soil are unknown, they are thought to be small. Thus, the default value was set to zero.
Damkohler depth in soil	8 cm	The Damkohler depth is based on the expected steady state soil concentration profile and is used to help define the transfer factors between the various soil layers. The default value was based on constant measurements down to this depth. However, it may be too small.

Predicted mercury concentrations in the three soil compartments are presented in Table 3-6, and mercury speciation results are presented in Table 3-7. When simulations with the final parameters were run without precipitation, no divalent mercury was predicted in the root zone and vadose zone. This finding is reasonable, because without precipitation the divalent mercury deposited from the air would remain tightly bound to soil particles in the surface soil compartment. The lack of moisture, as well as the relatively rapid transformation rates from divalent to methyl and elemental mercury, would make diffusion of divalent mercury from surface soil to deeper soil compartments unlikely. Under conditions of constant average precipitation, mercury speciation in the root zone soil appears to be reasonable (see Table 3-7).

Mercury concentrations in surface soil are more important to the overall model results than mercury concentrations in root and vadose zone soils, because human and ecological risks are much more likely to result from exposure to surface soil than exposure to subsurface soil. In this evaluation, very little elemental mercury was predicted in surface soil either with or without precipitation. This result is reasonably consistent with field data (Biester and Scholz 1997), which indicate that one to two percent elemental mercury generally would be expected in surface soil. However, it is possible that the field data are based on experimental samples that included an amount of root zone soil where considerable elemental mercury is found.

3.6.4 Conclusions

This evaluation developed default air and soil process parameter values for mercury. For the scenarios used in this evaluation, TRIM.FaTE simulations with these parameters resulted in predicted mercury concentrations and speciation in surface and subsurface soils that are consistent with field data and other available information on the fate of mercury in soils. No refinements to the air or soil process models were made based on this evaluation.

Table 3-6
Predicted Total Mercury Concentrations in Soil Compartments, With and Without Precipitation

Soil Compartment	Mercury Concentration (ng/g bulk)	
	No Precipitation	Constant Average Precipitation (0.001 m/day)
Surface	23.3	42.6
Root Zone	0.0017	0.12
Vadose Zone	0.0019	0.03

Table 3-7
Predicted Mercury Speciation in Soil Compartments, With and Without Precipitation

Soil Compartment	Mercury Species	Percent of Total Mercury	
		No Precipitation	Constant Average Precipitation (0.001 m/day)
Surface	Elemental	0.0%	0.1%
	Divalent	98.2%	98.2%
	Methyl	1.8%	1.8%
Root Zone	Elemental	100.0%	24.6%
	Divalent	0.0%	74.1%
	Methyl	0.0%	1.3%
Vadose Zone	Elemental	100.0%	99.7%
	Divalent	0.0%	0.3%
	Methyl	0.0%	0.0%

3.7 SEDIMENT AND SURFACE WATER

The sediment module in TRIM.FaTE is treated as a well-mixed compartment of specified depth that exchanges mass (by both physical and chemical processes) with the overlying water. The compartment is composed of water and solids. Chemical fate processes include diffusive and advective exchange in both directions across the water-sediment interface and loss from the sediment due to “burial.” Burial is the process of freshly deposited material accumulating at the surface and preventing the deeper layer of sediment from interacting with the overlying water. The structure provides a well-mixed cap over a sink. Chemical transformation is also included in the sediment compartment.

The current model structure does not specifically include bioturbation, although it is implicitly included by specifying the depth of the “surface mixed sediment layer” (Schwarzenbach et al. 1993). Bioturbation may lead to increased mixing of both sorbed and dissolved contaminants in the sediment, but not enough is currently known about the process to include it as a separate input to the model at this point. Several other processes (e.g., ground water infiltration, nepheloid layer interactions, relationships or correlation among sedimentation, erosion, and water current) are not explicitly modeled in the sediment module as currently implemented in TRIM.FaTE. Users are advised to evaluate whether the lack of these processes limits the utility of TRIM.FaTE to their particular applications.

For mercury species, the algorithm for air/surface water diffusion/volatilization is equivalent to the "Volatilization Option 4" that is used in the Water Quality Analysis Simulation Program (WASP) (Ambrose et al. 1995). Sediment/surface water diffusion is modeled using the same two-resistance model used in CalTOX (CalTOX 1993). The TRIM.FaTE TSD Volume II (Chapter 4) provides more detailed background information on the sediment and surface water algorithms included in TRIM.FaTE.

3.7.1 Purpose of Evaluations

Initial model runs resulted in predicted mercury speciations in surface water that were inconsistent with the literature. In particular, the fraction that was elemental mercury was on the order of 75 percent; by comparison, the results obtained in the 1997 *Mercury Study Report to Congress* indicated that the fraction should be less than 10 percent (U.S. EPA 1997). Thus, a more in-depth evaluation of the surface water and sediment components of the currently implemented algorithms was conducted. The two primary focus areas of this evaluation were: (1) identification of modifications to mercury-dependent parameters in order to achieve predicted concentrations and speciation consistent with that achieved in the 1997 *Mercury Study Report to Congress*, and (2) evaluation of the general surface water and sediment dynamics.

3.7.2 Model Setup and Assumptions

The basic modeling configuration for the sediment and surface water evaluations was a small rectangular watershed adjacent to a surface water body (depth 3 m), with a single air compartment over the soil and water. A single sediment layer (depth 0.02 m) was located below the surface water. Both a flush sink (based on a flush rate of 0.5/yr) and a sediment burial sink were included in this scenario. The burial rate is calculated from the resuspension velocity, deposition velocity, and suspended sediment concentration in the water body so as to result in zero net deposition of sediment to the sediment bed. Note that the outputs of interest in this run were the predicted steady-state concentrations in surface water and sediment. The wind speed was constant for a given run; for various runs, wind speeds were set to 2 m/s, 4 m/s, and 6 m/s.

In order to simplify the focus of this evaluation, the concentrations were fixed in the soil and air compartments for the model runs at approximate "background" values and speciations. In air, a concentration of 1 ng/m^3 (98 percent elemental, 2 percent divalent) was assumed. The air concentration is the midpoint reported for rural areas in the 1997 *Mercury Study Report to Congress*. A total mercury soil concentration of 102 ng/g was assumed, with 98 percent considered to be divalent, 2 percent considered to be methylmercury (to be consistent with the *Mercury Study Report to Congress*) and 0.01 ng/g considered to be elemental. The value assumed for elemental mercury was based on the assumption of only a small fraction of total mercury present in the elemental form. A precise estimate of what this fraction should be was considered unnecessary for the current effort.

Erosion and runoff were calculated based on an input areal soil erosion rate of 0.000289 kg/m^2/day, from an average for soils in the test case state, and a runoff rate of 0.001009 m^3[water]/m^2[area]-day.

3.7.3 Results

Table 3-8 summarizes the changes made to default input parameters and modifications to algorithms themselves as a result of this evaluation. The modeling results obtained using these changes are summarized in the subsequent table (Table 3-8).

The predicted concentrations are within the range of measured values as indicated in the 1997 *Mercury Study Report to Congress*. Similarly, the predicted speciations of divalent and methylmercury are also consistent with those obtained in the *Mercury Study Report to Congress* (see Table 3-9). There are few data available regarding the fraction that is elemental mercury, but the values here are consistent with the result obtained in the 1997 *Mercury Study Report to Congress* using the IEM-2M model.

3.7.4 Conclusion

By making appropriate changes to various inputs and algorithms (including fixing a units conversion error in one algorithm), realistic concentrations of elemental, divalent, and methylmercury in surface water and sediment were obtained using fixed values for soil and air concentrations that are typical of uncontaminated areas. It was also determined in this evaluation that the wind speed assumed over the water body is an influential factor in the predicted elemental mercury concentration in surface water; indeed, the predicted elemental mercury concentration in the surface water is essentially inversely proportional to the wind speed assumed. It is noted, however, that usually very little of the mercury in surface water is present as elemental mercury (U.S. EPA 1997).

3.8 EVALUATION OF THE TRIM.FaTE PLANT MODULE

Two evaluation phases have been completed for the plant module in TRIM.FaTE:

- A compositional audit, where the overall plant model was evaluated against the original conceptual design; and
- An algorithm audit, where the transfer factors (T-factors) for each of the interfacial transfer processes were evaluated independently and in concert with the other equations in the plant module.

3.8.1 Compositional Audit

The evaluation of the conceptual model described in Section 2 of this report is extended here to provide a more detailed look at the plant module. This section presents results of a compositional audit where the original conceptual design of the plant module is reviewed and the code in Prototype V is evaluated to verify that each component of the conceptual model is included.

Table 3-8
Changes Made to Sediment and Surface Water Values as a Result of Sediment/Surface Water Runs

Term Changed	Units	Change Made	Comment
Dynamic Water Viscosity; calculated property of surface water	kg/m-s	Added additional units conversion term to equation	The “dynamic water viscosity” was an intermediate term that contained a missing units conversion term. The equation used is from IEM (and EXAMS and WASP) water viscosity = 10^(-3.0233 + 1301/(998.333+8.155*(Domain.Temperature_C -20) + 0.00585*(Domain.Temperature_C -20)^2.0)) The units in IEM (and EXAMS) are g/cm-sec. In TRIM, it is being treated as kg/m-sec. The conversion factor was originally input as 1 but should be (converting from g/cm-s to kg/m-s) 0.1 [= (100 cm/m) * (1 kg / 1000 g)]. Previous water viscosity = 10^(-3.0233 + 1301/(998.333+8.155*(Domain.Temperature_C -20) + 0.00585*(Domain.Temperature_C -20)^2.0)) New water viscosity = Constants.Convert_g_per_cm_to_kg_per_m * 10^(-3.0233 + 1301/(998.333+8.155*(Domain.Temperature_C -20) + 0.00585*(Domain.Temperature_C -20)^2.0)) where “Convert_g_per_cm_to_kg_per_m” is a new constant = 0.1.
Default Suspended Sediment Settling Velocity; input property of surface water	m/day	Changed default value to 0.5 m/day from 13 m/day	The deposition velocity was originally set to 13 m/d (this is a default value from CalTOX for California). Typical values in the literature are around 0.5 m/d depending on particle size and wind/turbulence. Note: Subsequent evaluation resulted in further change to this value to match that from U.S. EPA 1997 (2m/day).
Default Suspended Sediment Concentration; input property of sediment	kg [sediment]/m^3 [water column]	Changed default value to 0.015 from 0.8 kg/m^3	The suspended sediment concentration was originally set to 0.8 kg/m^3 which converts to 800 mg/L (default value from CalTOX). Typical values for lakes and streams are around 15 mg/L. Much lower values may be relevant for many lakes.
Default Sediment Resuspension Velocity; property of sediment	m/day (note that this is the velocity of the moving solids, not a volumetric velocity)	Changed default value to 6.28E-6 m/day from 1.37E-05 m/day	Information on resuspension rates was unavailable, but using the input of solid from soil (erosion), neglecting dry deposition from air and assuming the mass of particles flowing into and out of the pond are about equal, the accumulation rate in the pond was estimated to be around 0.0026 kg(solid)/m^2/d, which was consistent with reported values in the literature. With this value, the resuspension velocity was estimated to be 6.28E-6 m/d with a benthic solids concentration of 780 kg/m^3 (based on 30 percent solids in bulk sediment). A value of 0.65 is used in U.S. EPA 1997.
phi (Sediment Porosity); property of sediment	m^3 [pore space]/m^3 [compartment]	Changed default value to 0.7 from 0.2	Based on professional judgment under the assumption that the fraction of sediment that is water will be much larger than 0.2.

Term Changed	Units	Change Made	Comment
Benthic Solids Concentration of Sediment; property of sediment	kg[sediment]/m^3 [compartment]	Changed to a calculated parameter instead of being an input parameter	The benthic solids concentration is a function of the sediment porosity and the sediment density; the previous default input was actually calculated in this way outside of the model, and hence was consistent with the default porosity and sediment density. However, it would not remain consistent if either had changed. The new equation implemented is: Benthic Solids Concentration = Compartment.rho * (1 - Compartment.phi) where Compartment.rho is the sediment density (kg[sediment]/m^3[sediment]), and Compartment.phi is the porosity of the sediment compartment.
Default K_d in Soil, elemental mercury; property of soil	ml/g	Changed default value to 10 from 0.1 ml/g	The previous value was based on previous test runs performed. Evaluation runs indicated that an increase to the value was appropriate, as the lower value resulted in a substantial flux of elemental mercury to the water body. The value used in the 1997 *Mercury Study Report to Congress* (1,000) has also been used subsequently.
K_d in surface water, elemental mercury; property of surface water	ml/g	Changed default value to 10 from 0.1 ml/g	This value was changed in order to be consistent with change made in surface soil; runs indicated that this did not impact the results in surface water significantly. The value used in the 1997 *Mercury Study Report to Congress* (1,000) has also been used subsequently.

Table 3-9
Summary of Predicted Steady-State Concentrations in Surface Water and Sediment

Species	Surface Water Concentration (ng/L)	Sediment Concentration, ng/g (ng/g dry weight; see note)
Elemental	0.45	0.33 (0.6)
Divalent	5.38	116 (219)
Methyl	0.11	0.27 (0.5)

Notes:

Assumed fixed concentrations in air (1 ng/m^3 total mercury, 98 percent elemental and 2 percent divalent). Assumed mercury concentration in soil of 102 ng/g, with 98 percent divalent, 2 percent methylmercury, and a 0.01percent elemental mercury. Assumed constant wind speed over surface water of 4 m/s.

Sediment concentration is calculated as (mass of sorbed chemical in sediment compartment)/(mass of dry sediment in sediment compartment). For each species, over 99 percent is sorbed in the sediment compartment. The mass of dry sediment was calculated as :

Benthic Solids Concentration (kg[sediment]/m^3[compartment]) * Compartment Volume (m^3[compartment])

The benthic solids concentration was calculated as:

Benthic Solids Concentration (kg[sediment]/m^3[compartment]) = Sediment Density (kg[sediment]/m^3[sediment]) * (1 - Porosity)

where the default sediment density of 2,600 kg/m^3 and porosity of 0.7 were used in the run.

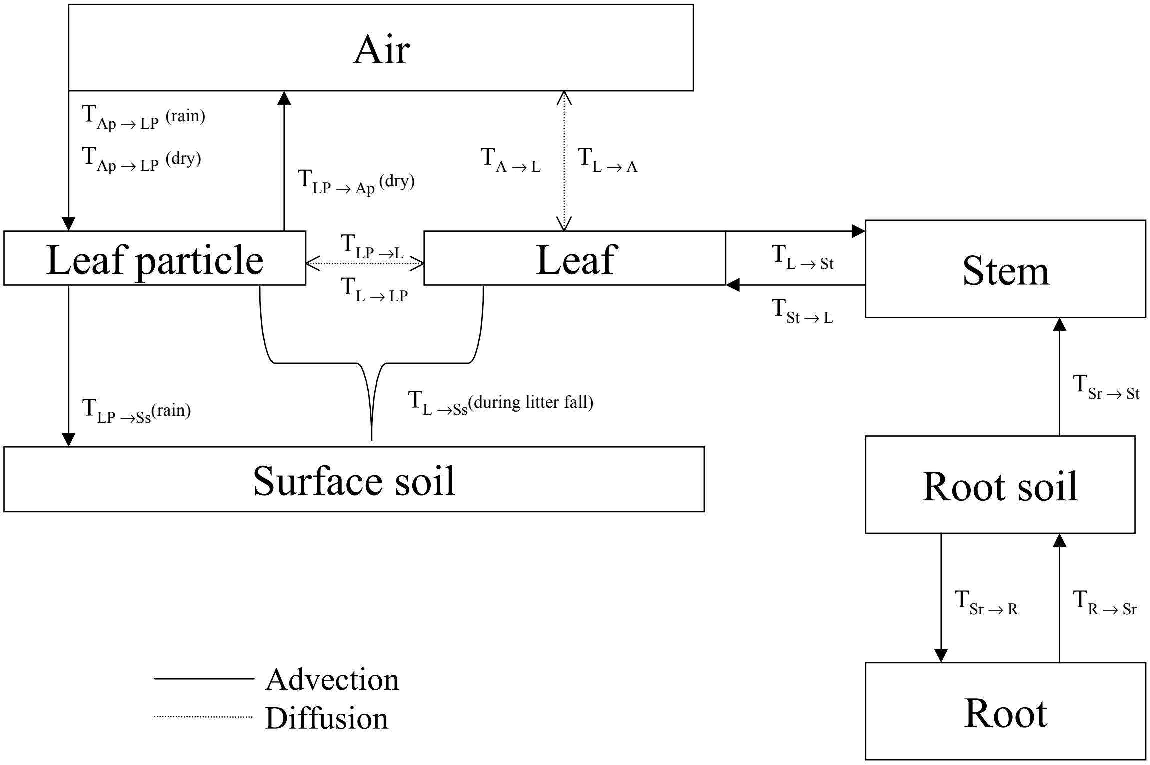
3.8.1.1 Conceptual Design of the Plant Module

The TRIM.FaTE plant module includes four homogeneous compartment types: root, stem, leaf and particles-on-leaf. These compartment types interact, as illustrated in Figure 3-6, with three environmental compartment types: air, surface soil, and root-zone soil. Vegetation also interacts with various animal compartment types through food-chain transfers but these are described and evaluated elsewhere (see Sections 3.9 and 4.3). The linked structure and exchange processes for the vegetation compartments are summarized in Table 3-10 along with descriptions of each transfer factor.

The mass transfer processes (gains and losses) in the plant module include both diffusion and advection. Mass can also be gained or lost through chemical reaction or metabolism in each compartment. Although the compartments are fully coupled, some of the interfaces are limited to unidirectional transfers (litter fall, soil-to-stem transfer). In addition, several of the transfer processes are toggled (on/off) during a simulation depending on rain (wet vs. dry deposition), season (litter fall to soil over a predefined period) or time of day (temporal response of stomata).

During rain events, the transfer from air to vegetation occurs by rain scavenging of both gas-phase chemical and particle-bound chemical followed by interception and retention of the advecting phase (raindrops) by the leaf. Particles and gases are also scavenged by vegetation through dry deposition processes when it is not raining. Particle-bound chemical is washed from the particle-on-leaf compartment to surface soil during rain and is blown into the air when it is not raining.

Figure 3-6
Schematic of the Plant Module



Diffusive exchange of gas-phase chemical is included for transfer between air and leaf. The boundary layer approach is used with air-side and vegetation-side resistance modeled in series (Mackay 1991; Schwarzenbach et al. 1993). The vegetation-side resistance combines cuticular and stomatal uptake in parallel and the stomata is modeled in series with the mesophyll for certain mercury species based on evidence reported by Shi-Hua (1982).

Transfer of chemical between the leaf and the particles on leaf is modeled with a simple first-order rate constant that is specified by the user. Litter fall is also modeled as a first-order process that transfers a specified percentage of leaf mass, along with particles on the leaf, to surface soil over a specified period of time (30 days for deciduous trees, several hundred days for grasses and herbs, several years for conifers).

Transfer through the root and stem is modeled in TRIM.FaTE as an advective process where the moving phase is either pore-water, xylem, or phloem fluid. Measurements of the uptake of chemicals into vegetation from soil have been described by Stem-Concentration-Factors (SCFs) and Transpiration-Stream-Concentration-Factors (TSCFs) for the stem/soil relationship, and by Root-Concentration-Factors (RCFs) for the root/soil relationship. The TSCF is used to predict the concentration in the advecting phase (xylem fluid), which is then used along with an estimated SCF to model the dynamic uptake in stem. The leaf is then modeled in series with the stem. The RCF and the time required to reach 95 percent of the root/soil equilibrium value are used to model dynamic uptake into roots (Burken 1998; Briggs et al. 1982; Briggs et al. 1983).

Table 3-10
Intended Gain/Loss Structure of TRIM.FaTE Vegetation Compartments

Compartment Type	Gains from		Losses to	
	Name	Source/description	Name	Target/description
Particle-on-leaf	$T_{L \rightarrow LP}$ $T_{A \rightarrow LP}$	Leaf (F) pseudo diffusion Air (A) dry particle deposition wet particle deposition	$T_{LP \rightarrow Ss}$ $T_{LP \rightarrow L}$ $T_{LP \rightarrow A}$ $T_{1 \rightarrow 2}$	Surface soil (F,A) wash-off and litter fall Leaf (F) pseudo diffusion Air (A) blow-off of particles Reaction (F)
Leaf	$T_{LP \rightarrow L}$ $T_{St \rightarrow L}$ $T_{A \rightarrow L}$	Leaf particle (F) pseudo diffusion Stem (A) xylem flow Air (D,A) wet gas deposition dry gas deposition	$T_{L \rightarrow Ss}$ $T_{L \rightarrow LP}$ $T_{L \rightarrow St}$ $T_{L \rightarrow A}$ $T_{1 \rightarrow 2}$	Surface soil (A) litter fall Leaf particle (F) psuedo diffusion Stem (A) phloem flow Air (D,A) diffusion Reaction (F)
Stem	$T_{L \rightarrow St}$ $T_{Sr \rightarrow St}$	Leaf (A) phloem flow Root soil (A)	$T_{St \rightarrow L}$ $T_{1 \rightarrow 2}$	Leaf (A) xylem flow Reaction (F)
Root	$T_{Sr \rightarrow R}$	Root soil (A) water uptake	$T_{St \rightarrow Sr}$ $T_{1 \rightarrow 2}$	Root soil (A) senescence Reaction (F)

Notes: D indicates diffusive transfer, A indicates advective transfer, and F indicates user supplied first-order rate constant.

3.8.1.2 Reconciling the Conceptual Model and the Code

The evaluation of the code in Prototype V of TRIM.FaTE identified a number of discrepancies between the intended and actual model code. These discrepancies and the steps taken to reconcile the differences are listed in Table 3-11.

Table 3-11
Summary of Results from the Compositional Audit of Prototype V

Identified Discrepancy	Reconciliation
Dry particle deposition from air to vegetation missing from code	Implemented appropriate algorithm from TSD
Wet particle deposition from air to vegetation missing from code. Algorithm in TSD for wet deposition of particle (Eq. 7-9) is same as that for gas (Eq. 7-7)	Developed algorithm for wet deposition of particles for inclusion in code and TSD
Transfer from leaf to air and leaf to soil for particle-on-leaf [a] results in "double-counting" blow-off	Removed transfer to soil of blow-off
Mesophyll resistance missing from stomatal diffusion pathway	Developed and implemented algorithm for mesophyll resistance in air-leaf diffusion
Limited basis for mass transfer rate between particles-on-leaf and leaf	Used best engineering judgment to specify value
Not clear whether litter fall loss should be linear or exponential	Future analysis of different litter fall models
Current method for soil-root-stem continuum may impact dynamic mass balance predictions[b]	Further evaluation (e.g., via use of alternative model)

[a] TRIM.FaTE includes a particle-on-leaf compartment to provide more relevant exposure estimates for chemicals that are predominantly particle bound. However, little information is available for characterizing the particle-on-leaf compartment. Best engineering judgment is used to estimate mass transfer rates for the particle-on-leaf compartment.

[b] TRIM.FaTE is a dynamic model, but the state of the science for vegetation root uptake decouples the soil-to-root transfers from the soil-to-stem transfers. Structurally, the soil-root-stem-leaf continuum allows stem and root to simultaneously approach equilibrium with the root-zone soil. Theoretically this could allow the stem (and subsequently the leaf) to approach equilibrium faster than it would if modeled in series with the root. It is unclear how this model assumption impacts the dynamic mass balance.

3.8.2 Algorithm Audit

In the algorithm audit each T-factor in the plant module was audited for its technical quality (correct derivation) and its relevance (appropriate for modeling tasks that TRIM.FaTE is designed to address). The T-factors were grouped by compartment interface across which they transfer mass. The TRIM.FaTE plant module includes eight interfaces:

1. Particle-on-leaf ↔air;
2. Particle-on-leaf→surface soil;
3. Particle-on-leaf↔leaf;
4. Leaf↔air;
5. Leaf→surface soil;

6. Leaf↔stem;
7. Root-zone soil→stem; and
8. Root-zone soil ← root.

The arrows in the interface names indicate the directions of mass transfer allowed by the transfer factors. Table 3-12 presents the findings of the algorithm audit and the changes made or planned for each finding.

Table 3-12
Summary of Results from the Algorithm Audit

Finding	Recommendation
Particle-on-Leaf ↔ Air Interface	
Dry deposition not normalized to bulk air compartment	Included appropriate partition coefficient to normalize T-factor to lower air compartment type
Dry particle deposition rate specific for certain chemical class	Applied a more general default value (500 m/d) and placed an explanatory note in users' manual
Particle blow-off from leaf to air forces concentration in moving phase to equal concentration in receiving compartment particles	Developed estimate for volume of particles on leaf and related T-factor to concentration in sending compartment
Wet particle deposition T-factor to vegetation missing	Developed and included algorithm based on wet deposition to soil of particles
Particle-on-Leaf → Surface Soil	
Default value used for wash-off rate is suspect (much too rapid)	Used a 14-day half-life (wash-off rate of 0.05/day) for removal of particles-on-leaf to soil
Best judgment for litter fall rate seems appropriate, but should be evaluated on case-by-case basis	Included comment in users' manual and TSD Vol II suggesting evaluation of default assumptions using sensitivity analysis
Particle-on-Leaf ↔ Leaf Interface	
Data lacking for specified rate constant	Included comment in users' manual and TSD Vol II suggesting evaluation of default assumptions using sensitivity analysis

Finding	Recommendation
Leaf ↔ Air Interface	
Incorrect washout ratio for gasses	Changed $Z_{pure\_air}/Z_{Total\_air}$ in the wet deposition of gas algorithm to $Z_{pure\_water}/Z_{Total\_air}$
Wet interception fraction model significantly under-predicts interception	Further evaluation of cumulative rain (rather than rain rate) for estimating interception
Mesophyll resistance missing from the stomatal uptake pathway for certain mercury species	Developed and parameterized mesophyll resistance model to add in series to air-stomata pathway
Air-side boundary layer thickness model difficult to parameterize	Replaced equation with lognormal distribution having a mean of 5.0E-4 and CV of 1
Natural log (ln) of K_{ow} used to predict cuticle conductance but original model was log base 10 (log)	Changed natural log to log base 10 in estimate of cuticular conductance
Model for air-stomata transfer over-predicts transfer when relative humidity (RH) is greater than 80 percent	Placed upper limit on conductance based on empirical evidence or use alternate algorithm from Reiderer (1995) or Nobel (1999)
Leaf → Surface Soil	
Best judgment for litter fall rate seems appropriate, but should be evaluated on case-by-case basis	See particle-on-leaf → surface soil (above)
Leaf ↔ Stem Interface	
Model for estimating xylem flux over-predicts relative to reported values	Evaluate options of applying an upper limit or replacing algorithm
K_{ow} correction exponent for leaf and stem are suspect	Additional literature review to evaluate default value
Model for estimation of stem/xylem partition coefficient does not agree with published model (Briggs et al. 1983)	Evaluate calibration of prototype model or replacement with Briggs et al. (1983) model
Root-Zone Soil → Stem Interface	
Estimated transpiration stream flux in excess of reported values	See Leaf ↔ Air Interface
Alternate models exist for transpiration stream concentration factor (TSCF)	Evaluate combining existing models or incorporating uncertainty into prediction

Finding	Recommendation
Root-Zone Soil ← Root Interface	
Default value for time to equilibrium very rapid	Evaluate incorporating uncertainty in the input

3.8.3 Future Activities for Evaluation of the Plant Module

With the conceptual and mechanistic evaluations of the plant module completed, the next steps will be to evaluate the actual performance of the module. Recent data for a class of organic chemicals will be used to evaluate the deposition of pollutants to above-ground vegetation and to compare the relative importance of particle-bound and gas-phase deposition processes.

3.9 CONCENTRATIONS AND FLOWS THROUGH TERRESTRIAL WILDLIFE

This evaluation examines the reasonableness of predicted concentrations and flows of contaminants in terrestrial wildlife compartments. The evaluation focuses on four aspects of the TRIM.FaTE's design and performance:

- Algorithm coding (e.g., are all links included, are units correct, are biomasses of different trophic levels reasonable);
- Differences in Hg concentrations among trophic levels;
- Relative input and output fluxes; and
- Reasonableness of concentrations compared to soil and plant concentrations and relative to values found in the literature.

As a result of preliminary simulations which illustrated the impact of unrealistically high deer and vole biomass input values, biomass estimates typical for forested areas in the northeastern United States were used in this evaluation

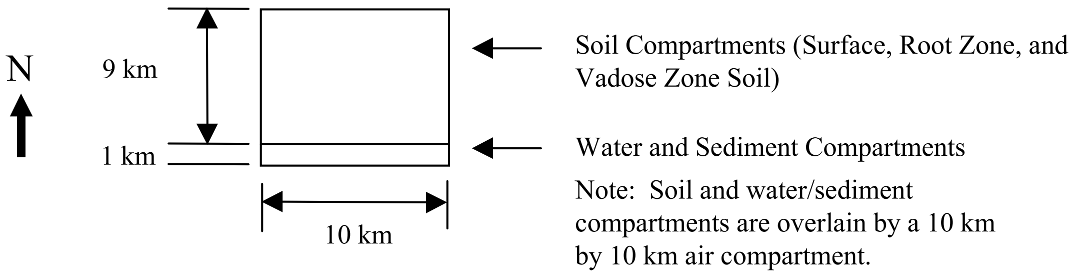
Section 3.9.1 describes the model setup for this evaluation. Section 3.9.2 presents the results of the evaluation. Conclusions are presented in Section 3.9.3.

3.9.1 Model Setup

The model setup for this evaluation included single soil (with surface and root zone components), air, and surface water (with sediment) volume elements. The configuration and dimensions of the abiotic compartments are shown in Figure 3-7. Groundwater and vadose zone compartments were omitted. All wildlife biotic compartment types available in the TRIM.FaTE library were included in the model setup; the grasses/herbs vegetation type was the only plant compartment included. Constant meteorology data were used. The temperature was set at 25 degrees Celsius, wind speed at two m/s, and there was no precipitation.

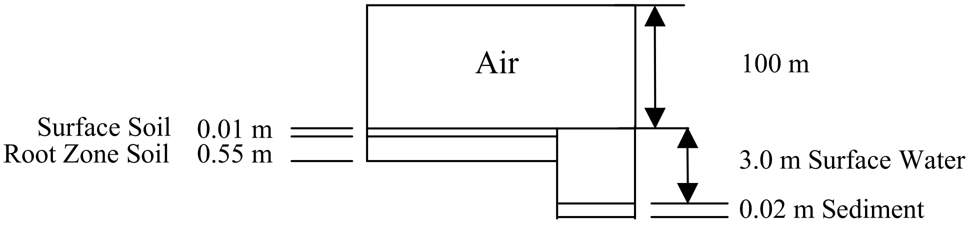
Figure 3-7
Modeling Configuration for Evaluation of Concentrations and Flows through Terrestrial Wildlife

Horizontal Compartment Dimensions



Note: Soil and water/sediment compartments are overlain by a 10 km by 10 km air compartment.

Vertical Compartment Dimensions



Note: Not to scale

The model setup did not include a source term. Instead, static concentrations in the abiotic compartments, which are shown in Table 3-13, were the source of mercury to the system. The simulation period for the evaluation was five years.

Table 3-13
Mercury Concentrations in Abiotic Compartments in the Terrestrial Wildlife Evaluation

Mercury Species	Fixed Concentration in Environmental Media				
	Surface Water (mg/L)	*Sediment (g/m^3 or mg/L)*	*Root Zone Soil (g/m^3 or mg/L)*	*Surface Soil (g/m^3 or mg/L)*	*Lower Air (mg/L)*
Elemental	1.0E-8	2.3E-8	1.0E-8	2.6E-5	1.0E-9
Divalent	9.0E-7	2.3E-4	1.0E-4	2.6E-1	2.0E-11
Methyl	1.0E-7	4.6E-6	2.0E-6	5.2E-3	7.4E-9[a]

[a] Concentration not fixed.

3.9.2 Results

The reasonableness of the terrestrial wildlife algorithm coding can be evaluated based on the distribution of mercury mass between abiotic and biotic compartments at the end of the simulation period, the final concentrations of mercury in the various biotic compartments, and fluxes of mercury among compartments.

Table 3-14 shows the distribution of mass of various species of mercury in a few biotic and abiotic compartments at the end of the simulation period. The total mass of mercury is dependent on the size of the compartment as well as the chemical transfer algorithms (note that the surface water volume element is smaller than the soil volume element in this setup). As expected, a very small fraction of the mass of total mercury is in mammals and birds (i.e., less than 0.001 percent of the mass in the system). Most of the mercury in terrestrial wildlife is in the form of divalent and methylmercury (especially the former), with little mercury in elemental form.

Table 3-14
Distribution of Mass Across Compartments at the End of a Five-Year Simulation Period

Compartment	Elemental Hg	Divalent Hg	Methyl Hg
Total mass, g (not including sinks)	6.6 E+4	6.6E+8	1.3E+7
Abiotic compartments	99%	99%	99%
Biotic compartments	0.001%	0.052%	0.35%
Soil	98%	99%	99%
Air	0.76%	0%	0.018%

Surface water	0.023%	0%	0.001%
Sediment	0.34%	0.35%	0.35%
Fish	0%	0%	0.001%
Macrophyte	0%	0%	0.002%
Mammal	0%	0%	0%
Bird	0%	0%	0%
Plant	0%	0.052%	0.34%
Insect	0%	0%	0.001%
Worm	0.001%	0.001%	0.001%

Figure 3-8 presents concentrations of divalent and methylmercury in soil and key biotic compartments at the end of the five-year simulation period. The highest concentrations of divalent mercury in biota are predicted in the arthropod, shrew, racoon, and earthworm. The highest concentrations of methylmercury in biota are predicted in the kingfisher, arthropod, shrew, and mallard. The concentration of divalent mercury in soil is higher than the concentrations of divalent mercury in biota. However, the concentrations of methylmercury in the four biotic compartments noted above are higher than those in soil.

Figure 3-8
Mercury in Mammals and Birds After a Five-Year TRIM.FaTE Run

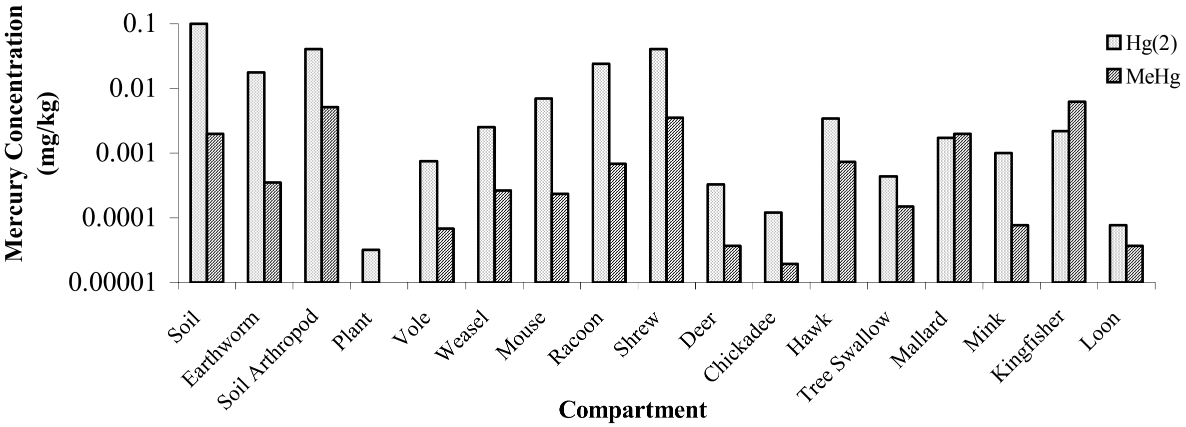


Figure 3-8 shows that the shrew has the highest concentration of total mercury of the vertebrates, which may be due to its high feeding rate, as well as its diet of earthworms and arthropods, both of which have high levels of mercury. In general, the final concentrations of mercury in the terrestrial wildlife compartments suggest that the input and output fluxes are reasonable for the wildlife species included.

Further evaluation of the mercury fluxes showed the primary route of exposure for terrestrial wildlife to be via the diet (including ingestion of soil), rather than via air, as expected (Gnamuš et al. 2000). For example, the flux of divalent mercury to white-tailed deer from the diet during the growing season was 4.1E-2 g/d, from water was 1.7E-2 g/d, and from air was 5.7E-7 g/d. (Deer also received 5.3E-5 g/d from inhalation of elemental mercury.) An unexpected observation of this evaluation was that the meadow voles ingested as much divalent mercury from consumption of soil (5.5E-3 g/d) as from consumption of plants (6.1E-3 g/d) during the growing season. Although this result was surprising, no evidence was readily available that contradicts this relationship.

Algorithms, including dietary links, are correct for the select wildlife species that were examined, with one exception. The wildlife were not linked to the leaf surface, which contains deposited particles that are a component of their diets. Version 1 of the model addressed this problem through a smart-linking feature that will automatically create basic links, including this one, during set-up of a modeling scenario.

Although TRIM.FaTE estimates whole-animal mercury concentrations, mercury concentration data for terrestrial mammals and birds generally are reported only for specific organs (e.g., liver) in the scientific literature. Thus, very limited empirical concentration data are available for comparison with the estimated biotic compartment mercury concentrations. Bull et al. (1977) and Talmage and Walton (1993) measure concentrations of mercury in mammalian organs only. The *Mercury Study Report to Congress*, Vol. VII (U.S. EPA 1997), emphasized risks to piscivorous wildlife, so data on body burdens in terrestrial wildlife were not compiled. It is reasonable to assume that piscivorous wildlife would have higher exposures to mercury than most terrestrial wildlife, and that is not evident in this model evaluation run; loons have among the lowest body burdens of mercury. However, concentrations of mercury in compartments in the aquatic food chain and those in the terrestrial chain in this simulation should not be compared for two reasons: (1) the fixed concentrations of mercury in soil and water may not have been consistent (e.g., the assumed background concentrations of mercury in soil may have been higher than mercury concentrations in most background soils and higher than would have been expected to be observed adjacent to water bodies containing 1E-6 mg/L Hg in water) and (2) fixing concentrations in abiotic compartments did not allow for exchange that may have changed the relative concentrations of mercury in the soil, water, air and sediment compartments. For example, if sediment is a long-term sink for mercury, that would not have been observed in this evaluation.

3.9.3 Conclusions

Based on this evaluation, a single model alteration was made to reflect the fact that herbivorous vertebrates eat particles on plant leaves along with the leaves themselves. Future versions of TRIM.FaTE could consider the addition of a change in biomass feature (e.g., incorporate growth, birth, death, migration) for terrestrial wildlife.

3.10 CONCENTRATIONS AND FLOWS THROUGH FISH

Two sets of algorithms for the uptake of mercury by fish are available in TRIM.FaTE:

(1) A bioenergetic model (i.e., all uptake occurs via the diet)[5]; and

(2) An equilibrium model (i.e., concentrations at one trophic level are assumed to be 3.5 times the concentration at the next lower level, when equilibrium is reached).

The equilibrium model is based on empirical data for mercury from Lindqvst et al. (1991). Thus, a comparison of the bioenergetic and equilibrium models is also a comparison of the bioenergetic model with empirical bioconcentration factors (BCFs) and bioaccumulation factors (BAFs).

At this time, trophic levels are designated as herbivore, omnivore, and carnivore. The current terminology may be confusing and potentially misleading to some users. For example, the term “omnivore” is currently applied to fish that eat only herbivores, and the term “carnivore” is applied to fish that eat only herbivorous fish. The current nomenclature is explained clearly in the TSD. In future versions of TRIM.FaTE, this nomenclature may be changed to trophic level X, X+1, and so on.

The evaluation of concentrations and flows through fish was designed to examine and compare the two sets of algorithms, with particular attention given to:

- Algorithm coding (e.g., whether all links are included, all units are correct, and the biomasses of different trophic levels are reasonable);
- Differences between dynamic and equilibrium results;
- The relationship between mercury concentrations in different trophic levels;
- The sensitivity of mercury concentrations in fish to biomass at each trophic level;
- Reasonableness of mercury concentrations in fish compared to surface water and sediment concentrations (at background concentrations, fixed abiotic concentrations, and concentrations representing chlor-alkali contamination); and
- Reasonableness of BCFs and BAFs relative to literature.

---

[5] Gill uptake of the chemical directly from water also is included in the bioenergetic model for use with nonionic organic chemicals and potentially other inorganic compounds. This is not included for mercury, as uptake of mercury directly from water via gills is considered negligible relative to dietary uptake.

3.10.1 Model Setup and Evaluation Methods

Compartment types included in this evaluation were surface water, sediment, three trophic levels of water column fish, two trophic levels of benthic feeding fish, benthic invertebrates, and loons. Algae were included as part of the surface water compartment (i.e., a phase). Air and surface soil were also included in runs but they are not the focus of this evaluation. The spatial configuration for this evaluation was similar to that shown in Figure 3-7.

Two scenarios were included in the evaluation, a background scenario and a contaminated scenario. Fixed abiotic concentrations of mercury in air, surface soil, and sediment were used in both scenarios; aquatic concentrations are presented in Tables 3-15 and 3-16. The background scenario was used for most evaluative runs. The contaminated scenario was generally used for comparisons with measured data, because some BAFs were derived using contaminated conditions and may not be valid under background conditions. However, because of the linear structure of the aquatic food chain in TRIM.FaTE, the model generated the same trophic-level specific BAFs (i.e., ratio of the chemical concentration in fish to the chemical concentration in water) regardless of the scenario used.

Table 3-15
Environmental Mercury Concentrations for the Background Scenario

Mercury Species	Fixed Concentration in Environmental Media		
	Surface Water (mg/L)	Sediment	
		(mg/L)	(mg/kg)
Elemental	1.0E-8	2.3E-5	1.0E-5
Divalent	9.0E-7	4.6E-1	2.0E-1
Methyl	1.0E-7	4.6E-3	2.0E-3

Table 3-16
Environmental Mercury Concentrations for the Contaminated Scenario

Mercury Species	Fixed Concentration in Environmental Media		
	Surface Water (mg/L)	Sediment	
		(mg/L)	(mg/kg)
Elemental	1.0E-7	2.3E-4	1.0E-4
Divalent	9.0E-6	4.6E+0	2.0E+0
Methyl	1.0E-6	4.6E-2	2.0E-2

Background concentrations of mercury species were obtained from the *Mercury Study Report to Congress* (U.S. EPA 1997). Ratios of species of mercury in the contaminated scenario were assumed to be the same as those in the background scenario. The 1E-5 mg/L (10 ng/L) concentration of total mercury in surface water in the contaminated scenario is typical of chlor-alkali-contaminated lakes in New York (Onondaga Lake) and Ontario (Clay Lake) (Wang and Driscoll 1995). The 2 mg/kg concentration of total mercury in sediment represents a high-end value (the maximum concentration reported by Gonzalez (1991) for lakes impacted by a chlor-alkali plant). In retrospect, 0.2 mg/kg would have been a better concentration to choose (a reasonable estimate in Gonzalez and the average of the sediment concentrations measured near the test case site), but because of the linear scaling of the model and the fact that BAF results were not affected, there was no need to rerun the model. Overall results after modifying the model confirmed biomagnification across trophic levels.

The ratio of methylmercury to divalent mercury (some of which is also taken up by algae, passed on to fish, and then converted to methylmercury) in surface water that was fixed in the model runs was realistic in comparison to literature values. For example, Watras et al. (1995) measured the median concentration of total mercury in Wisconsin lakes to be 0.96 ng/L, and methylmercury in Wisconsin lakes is 0.07 ng/L, giving a methylmercury to total mercury ratio of 7.3E-2. This ratio is close to the fixed ratio used in TRIM.FaTE of 9.9E-2 methylmercury to total mercury.

For most runs, the following biomasses of water column and benthic fish were used:

Water-Column Food Chain	Benthic Food Chain
Herbivore: 1.65E-3 kg/m^2	Mayfly/invertebrate: 3.73E-2 kg/m^2
Omnivore: 5.85E-4 kg/m^2	Omnivore: 1.89E-3 kg/m^2
Carnivore: 1.79E-4 kg/m^2	Carnivore: 2.14E-4 kg/m^2

As described in the next two sections, initial runs involved erroneous biomass values for water column herbivores and omnivores. Additionally, the biomasses of water column fish were altered for the evaluation described in Section 3.10.2.5. In all simulations, loons were assigned a biomass of 2.0E-7 kg/m^2, and an ingestion rate of 0.23 kg/kg body weight, with herbivores being their only food item.

3.10.2 Evaluations and Results

The discussion of evaluations and results includes basic relationships (Section 3.10.2.1), structural problems (Section 3.10.2.2), comparison of alternative models (Section 3.10.2.3), comparison of model outputs to measured concentrations (Section 3.10.2.4), sensitivity of the model to the biomass of higher trophic-level fish (Section 3.10.2.5), and options for addressing impact of fish biomass on fish mercury concentrations in the bioenergetic model (Section 3.10.2.6).

3.10.2.1 Basic Relationships

Initial results from the fish model were evaluated to confirm that two basic relationships were present. First, mercury speciation in fish was checked to ensure that methylmercury was the predominant species; this was found to be true. Second, model results were analyzed to determine if biomagnification of methylmercury occurs as it should in fish. Two situations were identified where biomagnification did not occur as expected:

- Methylmercury concentrations in water-column herbivores were higher than those in omnivores in the bioenergetic runs. This was rectified by correcting relative biomasses of trophic levels (see Section 3.10.2.2). The problem arose again due to an error in the ingestion rate equation.

- Methylmercury concentrations in benthic omnivores were higher than those in carnivores in the equilibrium model. This was rectified by correcting errors in the algorithms.

3.10.2.2 Structural Problems

The fish model evaluation revealed several structural problems with the model. The problems and their remedies are described below:

- Biomass input values for water column fish of different trophic levels did not reflect the reality that aquatic systems always have a lower biomass of fish at each higher trophic level. It was determined that some of the initial values had errors, and the biomass input values were modified based on the methodology described in Appendix I-B.

- There was no link in the model from the benthic invertebrate to the benthic omnivore in the bioenergetic scenario. The link was added.

- The elimination rate constant for methylmercury in fish in the bioenergetic model contained a term with incorrect units. The units were corrected.

- An exponent in the feeding rate equation was off by a factor of 10. In addition, the fish ingestion rate calculation did not include division by fish biomass. These algorithms were corrected.

- In initial equilibrium model runs, methylmercury concentrations in the benthic omnivore were higher than in the benthic carnivore. The concentration of methylmercury in the benthic carnivore was identical to that in the benthic invertebrate. A close inspection of the algorithm revealed that the equations for transfer between the omnivore and carnivore compartment types had been reversed. The partition coefficient was used in the transfer from carnivore to omnivore rather than in the opposite direction, which would have been correct and parallel to other transfers up the food chain. These algorithms were corrected.

In addition to checking and correcting algorithms, three additional tasks were carried out: (1) a comparison of results from the bioenergetic and equilibrium models; (2) a comparison of TRIM.FaTE outputs to measured values; and (3) a qualitative sensitivity analysis of changes in fish biomass. These tasks were initially completed when model algorithms contained errors but were updated to reflect the updated version of the TRIM.FaTE library.

3.10.2.3 Comparison of Alternative Models

Concentrations of methylmercury predicted in aquatic biota by the bioenergetic and equilibrium models were compared for both the background (Table 3-17) and contaminated (Table 3-18) scenarios. Except in the case of the benthic carnivore, methylmercury concentration differences between the two models were within a factor of three. While methylmercury concentrations in the water-column herbivore, water-column omnivore, and loon compartment types were slightly higher using the equilibrium model, concentrations in the water-column carnivore, benthic carnivore, and benthic omnivore were slightly lower. However, the concentration of mercury in benthic carnivores estimated by the bioenergetic model was 30 times the concentration estimated by the equilibrium model. It is not clear why this difference is this large. Future evaluations will consider this.

It is notable that the concentrations in fish in both models scale up perfectly with the concentrations in surface water or sediment. In the contaminated scenario, water-column and benthic fish concentrations were exactly 10 times those in the background scenario. These factors represent the change in surface water and sediment concentrations as well. Thus, to answer questions related to BAFs, only one of the two scenarios needs to be run.

Table 3-17
Comparison of Concentrations of Methylmercury (mg/kg) in Aquatic Organisms, As Calculated by Bioenergetic Model and Equilibrium Model (Five-Year Simulation) With Background Levels of Mercury in Water and Sediment

Aquatic Organism	Bioenergetic Model	Equilibrium Model	Bioenergetic/ Equilibrium Ratio
Water-column herbivore	2E-4	5E-4	4E-1
Water-column omnivore	6E-4	1E-3	5E-1
Water-column carnivore	1E-2	3E-3	3E+0
Benthic invertebrate	1E-2	1E-2	1E+0
Benthic omnivore	8E-2	3E-2	2E+0
Benthic carnivore	2E+0	7E-2	3E+1

Aquatic Organism	Bioenergetic Model	Equilibrium Model	Bioenergetic/ Equilibrium Ratio
Loon	4E-4[a]	9E-4[a]	4E-1

[a] total mercury

Table 3-18
Comparison of Concentrations of Methylmercury (mg/kg) in Aquatic Organisms, As Calculated by Bioenergetic Model and Equilibrium Model (Five-Year Simulation) with Fixed, Contaminated Levels of Mercury in Water and Sediment

Aquatic Organism	Bioenergetic Model	Equilibrium Model	Bioenergetic/ Equilibrium Ratio
Water-column herbivore	2E-3	5E-3	4E-1
Water-column omnivore	6E-3	1E-2	6E-1
Water-column carnivore	1E-1	3E-2	3E+0
Benthic invertebrate	1E-1	1E-1	1E+0
Benthic omnivore	8E-1	3E-1	2E+0
Benthic carnivore	2E+1	7E-1	3E+1
Loon	4E-3[a]	9E-3[a]	4E-1

[a] total mercury

3.10.2.4 Comparison of TRIM.FaTE Outputs to Measured Concentrations

To calculate BCFs and BAFs from TRIM.FaTE outputs to compare to the *Mercury Study Report to Congress* values, one must first calculate the dissolved concentration of methylmercury in surface water. The outputs from TRIM.FaTE for these runs indicate 98.7 percent of the mass of methylmercury in the surface water compartment was sorbed to suspended sediment, and 0.11 percent is in algae. By subtraction, 1.2 percent of the mass of methylmercury in the surface water compartment is in the dissolved phase. Multiplying 1.2 percent by the surface water concentrations yields 1.2E-9 mg/L as the appropriate denominator for calculating the BAF in the background runs and 1.2E-8 mg/L for the contaminated scenario runs. As is shown in Table 3-19, the BAFs derived from these TRIM.FaTE runs fall within the range reported in the *Mercury Study Report to Congress* (U.S. EPA 1997).

Table 3-19
Comparison of TRIM.FaTE Bioconcentration Factors (BCFs) and Bioaccumulation Factors (BAFs) to Related Factors from the *Mercury Study Report to Congress*

Factor	*Mercury Study Report to Congress*	TRIM.FaTE
Phytoplankton BCF	3,400 - 133,000	36,300
Trophic Level 3 Fish BAF	1.6E+6	Background and Contaminated Scenario Runs: – Herbivore: 1.47E+5 – Omnivore: 5.01E+5 Equilibrium Runs: – Herbivore: 4.11E+5 – Omnivore: 1.14E+5
Trophic Level 4 Fish BAF	6.8E+6	Background and Contaminated Scenario Runs: – Omnivore: 5.01E+5 – Carnivore: 1.19E+7 Equilibrium Runs: – Omnivore: 1.14E+5 – Carnivore: 2.12E+6
Foodchain Multipliers	Phytoplankton - Zooplankton: 6.3 Zooplankton - Forage Fish: 6.2 Forage Fish - Piscivores: 4.9	3.5
Biota/Sediment Accumulation Factors (BSAFs) (total Hg)	0.4 - 50	Bioenergetic Model – Benthic Omnivore: 1.9 – Benthic Carnivore: 45 Equilibrium Model – Benthic Omnivore: 0.78 – Benthic Carnivore: 1.6

The BCFs calculated for algae were compared to those in the *Mercury Study Report to Congress* (U.S. EPA 1997). BCFs for methylmercury in phytoplankton, which relate a concentration in algae (wet mass) to the dissolved concentration in water, have been calculated at 3,400 for Lake Michigan, 38,400 for East Fork Poplar Creek in Tennessee, 107,000 for Onondaga Lake in New York, 90,000 for a northern Wisconsin lake, and 133,000 for Little Rock Lake in Wisconsin (U.S. EPA 1997). The value calculated for all final test runs of TRIM.FaTE was 36,300, which is within this empirical range. Note that unlike other equilibrium relationships in TRIM.FaTE that have constant BAFs or BCFs, the BCF for phytoplankton is a calculated parameter, based on factors such as pH, chloride concentration in water, and algal radius.

The *Mercury Study Report to Congress* (U.S. EPA 1997) presents BAFs in L/kg (wet weight concentration divided by dissolved concentration) for fish at trophic levels 3 and 4, where trophic level 3 fish are forage fish feeding on zooplankton and trophic level 4 fish are piscivorous fish feeding on forage fish. It is difficult to equate these with the trophic levels currently used in TRIM.FaTE, but trophic level 3 fish are probably comparable to herbivores or omnivores in TRIM.FaTE, and trophic level 4 fish are probably comparable to omnivores or carnivores in TRIM.FaTE. As summarized in Table 3-19, the median BAF for level 3 fish is 1.6E+6 (5th percentile, 4.6E+5; 95th percentile, 5.4E+6), and for level 4 fish is 6.8E+6 (5th percentile, 3.3E+6; 95th percentile, 1.4E+7) (U.S. EPA 1997). These BAFs from the *Mercury Study Report to Congress* are based on measurements from field studies. In the background and contaminated scenario runs for TRIM.FaTE, BAFs for herbivorous, omnivorous, and carnivorous fish in the bioenergetic model were calculated to be 1.47E+5, 5.01E+5, and 1.19E+7, respectively. In equilibrium runs, the same BAFs were calculated to be 4.11E+5, 1.14E+6, and 2.12E+6, respectively for these three types of fish. These values are in line with the values in the *Mercury Study Report to Congress*.

The *Mercury Study Report to Congress* presents food-chain multipliers of 6.3, 6.2, and 4.9 for phytoplankton-to-zooplankton, zooplankton-to-forage fish, and forage fish-to-piscivore, respectively. These values are somewhat higher than the food chain multiplier of 3.5, which serves as the basis for the equilibrium model. However, 3.5 is well within the range of values from which the multipliers in the *Mercury Study Report to Congress* were derived. A separate evaluation will focus on the effect of consumers on concentrations of mercury in their prey, including effects on mercury accumulation across the food chains (e.g., on the resulting “food chain multipliers”).

Biota/sediment accumulation factors (BSAFs) for total mercury in aquatic biota (dry weight basis) range from 0.4 to about 50 (U.S. EPA 1997). Within a system, BSAFs usually increase with increasing trophic level (U.S. EPA 1997). In these TRIM.FaTE simulations, sediment is 20 percent pore space and has a density of 2.6E-3 kg/m^3; thus, given the density of water (1,000 kg/m^3), sediment is approximately 92 percent solids by weight, and wet weight concentrations may be multiplied by 1.08. Fish are assumed to be 80 percent water, on average, so wet weight concentrations may be multiplied by 5. Therefore, on a dry weight basis and under the scenarios with fixed abiotic concentrations, the bioenergetic model gives BSAFs of 1.9 for the benthic omnivore and 45 for the benthic carnivore. The equilibrium model gives BSAFs of 0.78 for the benthic omnivore and 1.6 for the benthic carnivore. These BSAFs are within the range of values in the *Mercury Study Report to Congress*.

Most measurements of concentrations of mercury in loon tissues are in feathers and blood; it is unclear how feather and blood concentrations relate to whole animal concentrations. However, EPA (1997a) cites two studies in which total mercury concentrations in breast muscle tissue were measured. These measurements should be more representative of concentrations in whole animals than the measurements taken in feathers or blood. In one of these studies (Wren et al. 1983), a single loon had a muscle tissue concentration of 1.5 mg/kg (total mercury, wet weight), which was higher than the total mercury concentration found in any fish in the study.

Concentrations of mercury in bluntnose minnow, rainbow smelt, smallmouth bass, northern pike, and lake charr ranged from 0.1 to 1 mg/kg. This small line of evidence suggests that TRIM.FaTE may be underestimating the mercury levels in the loon, because the modeled concentrations (for both models) of total mercury in the loon at five years of exposure (of an eight-year loon lifespan) are lower than those in the omnivore and carnivore. However, this measurement is only of a single loon. Also, the assumption was made in TRIM.FaTE that loons eat only herbivores, which may not be correct. The *Mercury Study Report to Congress* (U.S. EPA 1997) cites Barr (1996) in describing the diet of loons to be almost exclusively trophic level 3 (i.e., foraging fish). In addition, inhalation was not included as an exposure pathway in the fixed-abiotic concentration model runs.

3.10.2.5 Sensitivity of Models to Biomass of Higher Trophic-Level Fish

A comparison was performed of TRIM.FaTE runs using realistic biomass information (calculated from Kelso and Johnson 1991, Appendix I-B), which was also used in the analyses described above and artificial biomass values as shown in Table 3-20. This comparison was designed to determine the sensitivity of concentrations of methylmercury in fish at lower trophic levels to the biomass of fish in higher trophic levels for both the bioenergetic and the equilibrium models. The biomass values in upper trophic-level fish in the artificial scenario were lowered.

With the bioenergetic model, using a lower biomass of water-column omnivore and carnivore fish results in substantially higher methylmercury concentrations in all three water-column trophic levels (Table 3-21). The increase in methylmercury concentration in the carnivore was greater than an order of magnitude. With the equilibrium model, small differences were observed in methylmercury concentrations in fish between the two biomass scenarios (Table 3-22). Concentrations of total mercury in the loon were dependent on the fish biomass for both the bioenergetic and equilibrium runs. Thus, biomass of fish has an impact on the concentration of methylmercury in fish at lower trophic levels, as well as on piscivorous wildlife, and those impacts appear to be greater when the bioenergetic algorithm is used compared to the equilibrium model.

Table 3-20
Biomass of Water-Column Fish in Realistic and Altered Scenarios

Biotic Compartment	Realistic Biomass (kg/m^2)	Altered Biomass[a] (kg/m^2)
Water-Column Herbivore	1.7E-3	1.7E-3
Water-Column Omnivore	5.9E-4	1.7E-5
Water-Column Carnivore	1.8E-4	1.7E-7

[a] Altered to reduce potential impact of dietary uptake of higher trophic-level fish on lower trophic-level fish.

Table 3-21
Sensitivity of Methylmercury Concentrations to Biomass of Fish in Bioenergetic Model with Background Mercury Levels

Biotic Compartment	Concentration of Methyl Mercury (mg/kg)	
	Realistic Biomass Scenario	Altered Biomass Scenario
Water-Column Herbivore	1.8E-4	8.4E-4
Water-Column Omnivore	6.0E-4	1.6E-2
Water-Column Carnivore	1.4E-2	3.8E-1
Semi-aquatic Piscivore (Loon)	3.7E-4[a]	1.4E-3[a]

[a] total Hg

Table 3-22
Sensitivity of Methylmercury Concentrations to Biomass of Fish in Equilibrium Model with Background Mercury Levels

Biotic Compartment	Concentration of Methyl Mercury (kg/m^2)	
	Realistic Biomass Scenario	Altered Biomass Scenario
Water-Column Herbivore	4.9E-4	5.4E-4
Water-Column Omnivore	1.4E-3	1.8E-3
Water-Column Carnivore	2.6E-3	3.5E-3
Semi-aquatic Piscivore (Loon)	3.7E-4[a]	9.3E-4[a]

[a] total Hg

3.10.2.6 Options for Addressing Impact of Fish Biomass on Fish Mercury Concentrations in the Bioenergetic Model

An option for altering biomass of fish is to adjust the biomass of a compartment as a fish consumes the biomass of the compartment and the mercury contained in the biomass. However, consumption without replacement is probably not advisable, and concentrations in all fish should be diluted by growth, birth, death, and other natural processes.

The 1998 draft version of Aquatox (Park 1998 draft) includes a derivative of biomass ($g/m^3/d$) which equals the sum of:

- Load (usually from upstream)
- Consumption of food

- Migration
- Promotion (into size class or trophic level)

minus:

- Defecation
- Respiration
- Excretion
- Death
- Predation
- Gamete loss
- Washout downstream
- Migration
- Promotion (into next size class or trophic level)

The most important factors to include are likely consumption of food, predation, and death. Birth is apparently not included because it does not bring new biomass into the population. Migration is also not included, perhaps because biomass gains and losses may be balanced.

3.10.3 Conclusions and Summary

Based on this evaluation, the following model alterations have been implemented:

- Altered default biomasses of fish at different trophic levels;
- Corrected units of biomass in the elimination rate constant equation in the bioenergetic model;
- Added the link from benthic invertebrates to benthic omnivores in the bioenergetic equation;
- Corrected the algorithms for the bidirectional exchange between benthic omnivores and benthic carnivores in the equilibrium model;
- Corrected units in equation used to calculate mass fraction of algae in water;
- Corrected mass fraction of carbon in algae;
- Increased elimination rate constant for divalent mercury in fish;
- Corrected exponent in fish feeding rate equation; and
- Corrected fish ingestion rate to include division by the biomass of the fish consumer.

Future enhancements to TRIM.FaTE may consider dynamic modeling of fish biomass to simulate biomass losses and gains (e.g., via predation, etc.).

4. STRUCTURAL AND COMPLEXITY EVALUATION

This chapter presents the results of structural and complexity evaluations of TRIM.FaTE. The first section provides background on the types of analysis that are included in this evaluation and describes the general approach of the evaluation of TRIM.FaTE. The subsequent sections describe the specific evaluation activities that have been completed to date, including the analysis of air compartments only, evaluation of the effect of the biotic system on the overall mass balance, and analyses of how temporal and spatial characteristics affect TRIM.FaTE.

4.1 BACKGROUND AND APPROACH

This section provides an overview of the structural complexity evaluation for TRIM.FaTE. Section 4.4.1 is an introduction to model structural evaluation, and Section 4.1.2 explains the general structural evaluation approach for TRIM.FaTE.

4.1.1 Introduction

Structural evaluation activities focus on how changes in modeling complexity affect model performance. These activities seek to determine how the model will respond when modeling scenarios are changed for different applications.

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

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

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

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

4.1.2 General Structural Evaluation Approach for TRIM.FaTE

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

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

- **Response to changes in the size, shape, and location of parcels.** Using the mercury case study data set, EPA examined the effect of varying spatial configurations on TRIM.FaTE results. This included changing the size of parcels in multiple dimensions to determine the most appropriate way to set up the model layout, as well as adding parcels at the edges of the model region to examine the boundary effects around the model system (i.e., flux of chemical mass into or out of the system).

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

- **Response to temporal scales of analysis and to aggregate inputs.** Detailed meteorological data (and in some cases other time-varying input data, such as emission rates) are available and have been used in a simplified scenario to test the model's response to aggregation of input data over various time periods. By running the model with varying degrees of input aggregation, (e.g., hourly vs. daily vs. seasonal average wind or temperature data), the level of input detail required to achieve a specified level of detail in the output can be determined.

4.2 AIR COMPARTMENT EVALUATION

All aspects of TRIM.FaTE, including the air transport module, comprise a mass-balanced grid model. For the air module, advection and diffusion are the processes currently included to transport chemical mass between different air parcels. Although TRIM.FaTE is not designed to replace currently existing air transport or dispersion models for inhalation exposure and risk assessments, the air module serves as the key link in transporting mass from an emission source to other media (e.g., soil, water, sediment) and biota compartments.

Four separate initial structural and complexity evaluations of the TRIM.FaTE air module[6] have focused on evaluating the effect of parcel size and shape, grid layout, and grid orientation on air concentration results:

- **Regular grid with controlled variation in meteorology.** A regular grid (i.e., a "checkerboard" with square parcels) was used with "controlled" meteorology input data constructed to test particular aspects of TRIM.FaTE;

- **Variation of parcel sizes.** Actual hourly meteorological data for a location in the northeastern United States was used with a series of regular grids with parcels of various sizes;

- **Variation of overall grid area.** Actual hourly meteorological data for a location in the northeastern United States was used with a series of regular grids covering different total grid areas; and

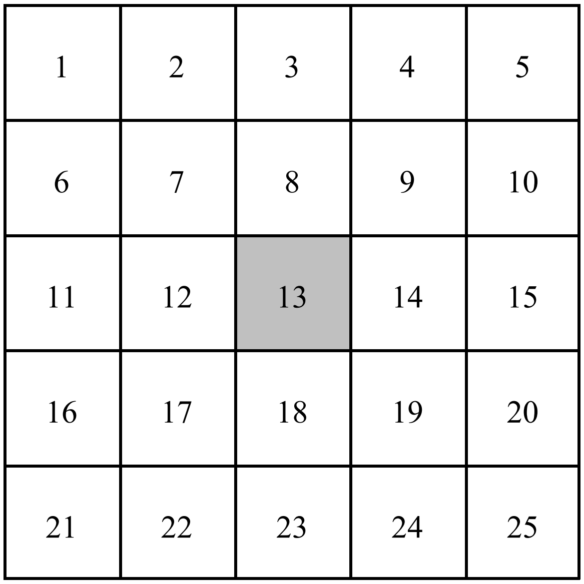
- **Variation of parcel shape.** Actual hourly meteorological data for a location in the northeastern United States was used with an "approximated polar" grid (parcels were regularly shaped, non-square polygons).

The orientations of these layouts are presented in Figures 4-1 and 4-2. For each of these analyses, TRIM.FaTE was set up with air compartments only (i.e., no other media were included in these runs). The model setup, inputs, and results and observations for each analysis are described in the subsequent sections.

---

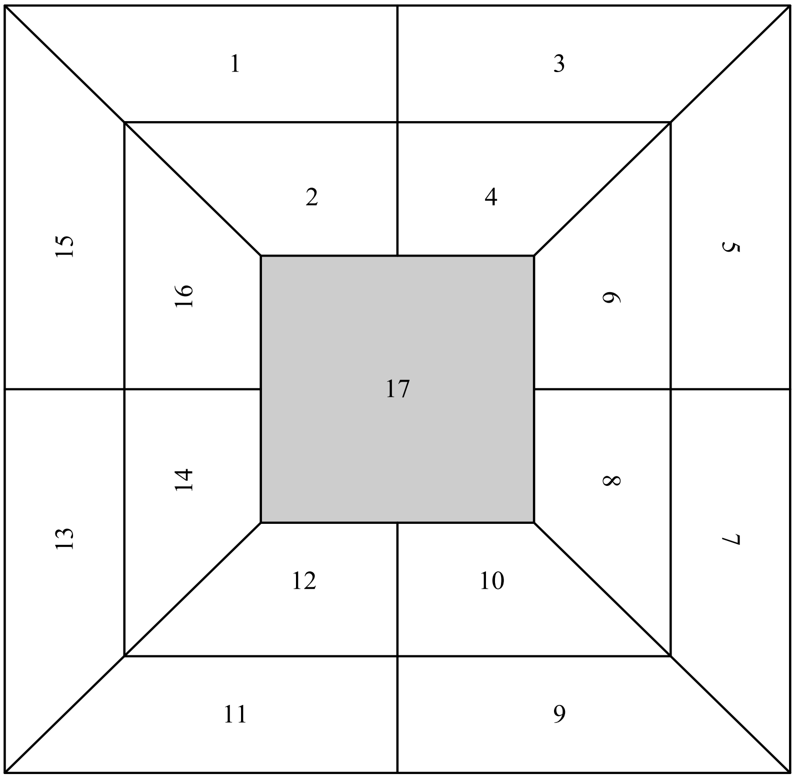
[6] Only the air module has been tested separately as part of the structural and complexity evaluation; other modules of TRIM.FaTE have been evaluated collectively as part of the biotic, temporal, and spatial complexity analyses described in subsequent sections of this chapter.

Figure 4-1
Example of Regular Grid Layout
(the shaded parcel is the source location)



1	2	3	4	5
6	7	8	9	10
11	12	13	14	15
16	17	18	19	20
21	22	23	24	25

Figure 4-2
Example of Approximated Polar Grid Layout
(the shaded parcel is the source location)



4.2.1 Regular Grid with Controlled Variation in Meteorology

For this evaluation, TRIM.FaTE was run under controlled meteorological conditions to evaluate the impact of using a regular grid parcel layout on mass transfer in the air transport component of TRIM.FaTE.

4.2.1.1 Model Inputs and Grid Layout

Two regular grids comprised of a single layer of square parcels centered on a single source were tested:

- 5 x 5 parcel grid (770.6 km^2 total area, 5.55 km x 5.55 km parcels)
- 13 x 13 parcel grid (770.6 km^2 total area, 2.14 km x 2.14 km parcels)

The simulation was run for 30 days with background concentrations set to zero and constant source emissions. The output concentrations (i.e., average air concentrations for each parcel) were obtained at hourly intervals. In order to focus on the effects of a regular grid layout, a controlled meteorological data set was used consisting of the following values:

- Constant height of air compartment: 30 m.

- Constant wind speed: 3 m/s.

- Constant vertical wind velocity: 0 m/s.

- Constant stability class: 4 (unitless).

- Uniformly changing wind direction: an initial southerly wind was used (in the meteorological sense, hence, blowing toward due north); the value of the wind direction was changed 0.5 degree/hour in the clockwise direction (i.e., one clockwise sweep of the compass over a 30-day period).

4.2.1.2 Results and Observations

For a single time step (i.e., one hour), mass emitted by the source is always transported from the source compartment into one quadrant only, where a quadrant is defined as the area between the axes of the four compass directions (i.e., due north, south, east, and west). These results were observed for both sizes included in this analysis. The following related results were also observed:

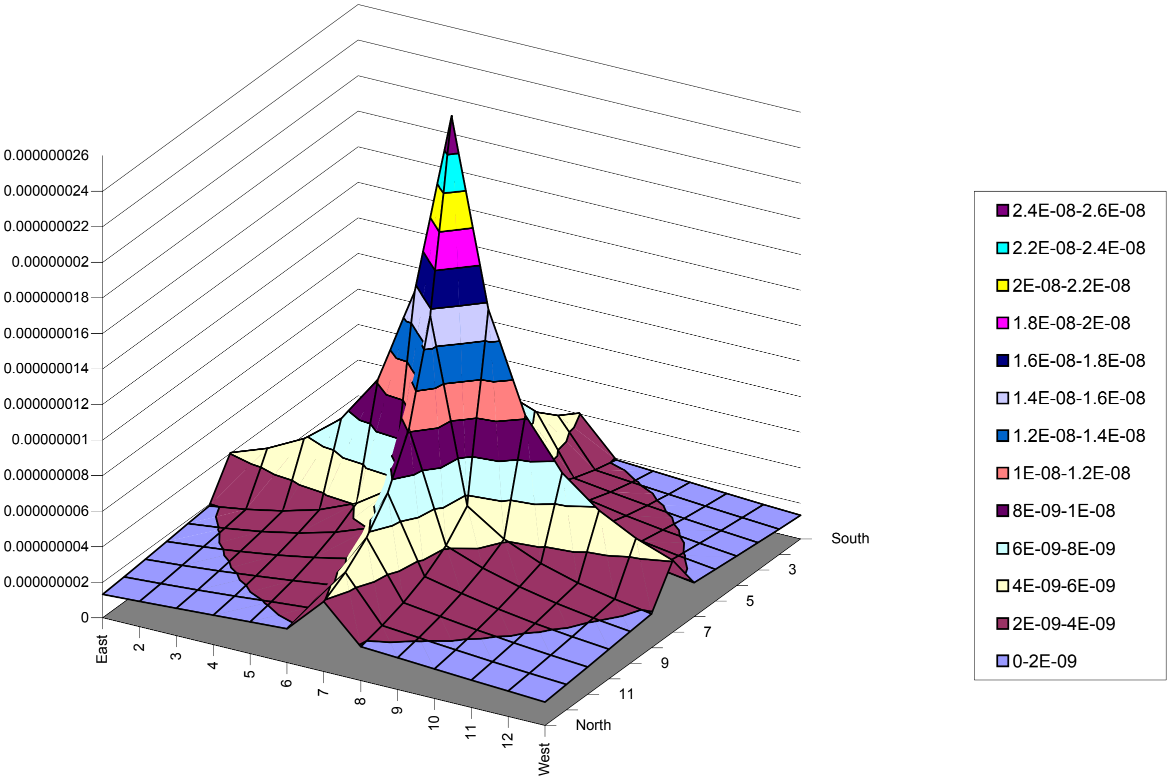
- For wind directions directly along the axis lines (e.g., due east or 90°), mass was transported into volume elements along the axis only.

- For wind directions (angles) close to the axis lines defining the quadrants, mass transport was biased toward the axis lines, with no crossing of the boundary to the adjacent quadrant. For wind directions more centrally located between axes (e.g., 45°, or northeast), mass was transported to a greater number of volume elements, resulting in greater distribution of mass.

As a result, greater mass occurred in parcels along the four axes than in other parcels in this grid layout over the 30-day period. Increasing the square grid resolution for the fixed total area (i.e., from 5 x 5 to 13 x 13) resulted in larger variation in results across parcels within the quadrants. In both layouts, somewhat higher average concentrations were observed along the axes.

Monthly average air concentrations for the 13 x 13 grid are shown in Figure 4-3. Each linear intersection on this plot represents an average concentration for an individual volume element (i.e., parcels would actually be centered on the intersections of the x-y grid in this chart). For this figure, the concentrations for each volume element were used to derive a three-dimensional surface with contour lines. The different shades on this plot represent ranges of concentrations (contour interval = 2E-9). Note that the large peak in the center of the plot represents the concentration in the source parcel.

Figure 4-3
Monthly Air Concentrations (g/m^3), Controlled Meteorology Data



In a separate analysis (results not shown), wind direction was varied by 15 degrees per hour (i.e., one clockwise sweep of the compass each day). The overall monthly average concentrations for parcels were comparable to the results (shown here) obtained when varying the wind direction by only 0.5 degree/hour.

Two additional observations were noted. First, the amount of mass and the resulting air concentrations in the source parcel changed with wind direction in relationship to grid orientation. Concentrations were higher when the wind blew along the axes than when the wind blew between the axes, with the greatest difference being about 30 percent (for 13 x 13 grid). Secondly, total mass in the modeling domain also changed with wind direction. The total mass and resulting average air concentration in the modeling domain was lower when the wind blew along the axes than when it blew at angles to the axes, with the greatest difference being less than 15 percent (for 13 x 13 grid). These effects appear to result from changes in cross-section area (i.e., the area perpendicular to the wind direction) of the source parcel or the whole grid as the wind changes direction.

Because wind direction was the only varying parameter for all runs performed in this analysis, the effects noted here (i.e., bias along the axes and the fluctuating source parcel and overall concentration patterns) are concluded to result from the geometric relationship between wind direction and source-parcel orientation (e.g., the trigonometric resolution of wind vectors relative to the volume element surfaces). The significance of these air compartment design findings will need to be considered in the context of other uncertainties in the simulation and their impact on the prediction of mass distribution and concentrations in non-air media. Investigation of this effect on the alternate parcel layout design is presented in Section 4.2.4.

4.2.2 Variation of Parcel Sizes

This evaluation was focused on the effect of grid resolution on mass transfer in the air component of TRIM.FaTE. In particular, this evaluation examined the impact of dividing a given modeling area into different-sized square parcels.

4.2.2.1 Model Inputs and Grid Layout

This analysis used five regular grids comprised of square parcels centered on a single source:

- One-parcel grid (770.6 km^2 total area, 27.76 km x 27.76 km parcel)
- 3 x 3 parcel grid (770.6 km^2 total area, 9.25 km x 9.25 km parcels)
- 5 x 5 parcel grid (770.6 km^2 total area, 5.55 km x 5.55 km parcels)
- 9 x 9 parcel grid (770.6 km^2 total area, 3.08 km x 3.08 km parcels)
- 13 x 13 parcel grid (770.6 km^2 total area, 2.14 km x 2.14 km parcels)

A single source with constant emissions of elemental mercury only was located in the center of the grid. A simulation period of one month (744 hours) was used, and hourly results were obtained and averaged to calculate an overall monthly average. Actual hourly meteorological data from January 1990 for a location in the northeastern U.S. were used for the runs. One vertical layer was defined with the height equal to the mixing height. Vertical wind velocity data were not relevant for this evaluation because only one vertical layer was used. Note that the conclusions from this analysis are dependent upon the ratio of advection to dispersion for the location and season. Analyses for sites where mean wind speeds are low but considerable direction changes occur (e.g., wintertime in the San Joaquin Valley of California) may be significantly different.

4.2.2.2 Results and Observations

As expected, the highest average monthly concentration for each of the scenarios occurred in the air parcel containing the source. For the most part, the results for all of the scenarios seemed qualitatively consistent with each other and the modeled meteorological data (i.e., the higher concentrations occurred in the directions the wind blew most frequently).

Monthly average concentrations for the entire grid were very consistent across scenarios (average concentration of 6.2E-10 g/m^3, standard deviation of 3.6E-11), especially when the one-parcel scenario was omitted (see Table 4-1). Thus, the amount of grid resolution did not have significant effects on the total mass in the system (if the one-parcel grid is ignored). It did, however, have an impact on the spatial distribution of mass in the system. For example, the effect of the regular grid (described in Section 4.2.3) of producing somewhat higher concentrations along the axes than between the axes is also observed here, although it is less pronounced here than with the constant meteorological data scenarios described in Section 4.2.3. Additionally, this effect seems to be lessened further with increased spatial resolution.

Table 4-1
Average Monthly Concentrations Across Modeled Area

Regular Grid Scenarios	Average Concentration Over Regular Grid Area (g/m^3)
One-parcel grid	6.8E-10
3 x 3 parcel grid	6.1E-10
5 x 5 parcel grid	6.0E-10
9 x 9 parcel grid	6.0E-10
13 x 13 parcel grid	6.0E-10
Average	6.2E-10
Standard Deviation	3.6E-11
Average (without one-parcel grid)	6.0E-10
Standard Deviation (without one-parcel grid)	4.3E-12

As expected, additional grid resolution provided greater spatial variation in the results. For example, the ratios of maximum:minimum values, going from the 3 x 3 grid to the 13 x 13 grid, are 42, 96, 236, and 414. To compare the concentration patterns between scenarios, the results were processed in two ways:

- First, the results of the 9 x 9 Regular Grid were projected into the grid layout of the 3 x 3 Regular Grid. Based on these results, it appears that increased grid resolution results in higher concentration estimates in the grid corners, especially in the predominant wind direction. It appears that as the grid resolution increases, the movement of mass is less biased to the north-south and east-west axes and thus more mass is able to reach the corners before exiting the system to the sinks. It also appears that added resolution around the source parcel and/or decreased source parcel size will result in higher concentrations in the source parcel but lower overall concentrations in the area surrounding the source. These differences were less than 20 percent for the two grids evaluated.

- Second, the concentration estimates for the 3 x 3, 5 x 5, 9 x 9, and 13 x 13 Regular Grid scenarios were averaged into quadrants. This was done by dividing the modeling region of each scenario into four pieces, defined by axes running through the middle of the source parcel in the north-south and east-west directions. For parcels that were divided between two quadrants (i.e., those along the axes), their concentrations were weighted half as much as those that fit completely into the quadrant. Furthermore, the source parcel was divided equally between the quadrants and its concentration was weighted one-fourth as much as the parcels contained completely within the quadrant. The results are presented in Table 4-2.

  The estimated quadrant concentrations decrease with increased resolution in the NW, NE, and SW quadrants, while increasing with increased resolution in the SE quadrant. It also should be noted that the SE quadrant had the highest average concentration among the quadrants. In general, it appears that increased resolution will result in lower concentrations upwind and higher concentrations downwind. This may be attributable to the lessening of "artificial" dispersion[7] with increased resolution. The concentration difference from the grid layout with the least resolution (3 x 3) to that with the greatest resolution (13 x 13) was less than a factor of two.

Table 4-2
Quadrant Average Concentrations (g/m^3) for Grids in the Parcel Size Evaluation

Grid Layout	NW	SW	NE	SE	Average
3 x 3 Regular Grid	4.1E-10	5.5E-10	6.4E-10	8.4E-10	6.1E-10
5 x 5 Regular Grid	3.3E-10	5.1E-10	6.2E-10	9.4E-10	6.0E-10
9 x 9 Regular Grid	2.7E-10	4.7E-10	6.0E-10	1.1E-09	6.0E-10
13 x 13 Regular Grid	2.4E-10	4.4E-10	5.9E-10	1.1E-09	6.0E-10

---

[7] "Artificial" dispersion refers to instantaneous dispersion of chemical mass throughout a given air compartment, regardless of size or shape. A larger compartment will spread chemical mass evenly throughout a larger volume in the same time period relative to a smaller compartment.

4.2.3 Variation of Overall Grid Area

This evaluation considered the effect of varying total grid area on mass transfer in the air component of TRIM.FaTE. In particular, this evaluation looked at the impact of changing the modeled area for different grid resolutions.

4.2.3.1 Model Inputs and Grid Layout

For this evaluation, the total grid area (i.e., the modeling domain) was changed by either adding or subtracting parcels around the edge of a regular, square grid. Two scenarios were designed to test this effect:

- **Increased area scenario.** An additional ring of square parcels was added to the 5 x 5, 9 x 9, and 13 x 13 Regular Grid layouts described in Section 4.2.1.2, thus creating three new scenarios (7 x 7, 11 x 11, and 15 x 15) comprised of identical square parcels and larger total areas than the Regular Grid scenarios from which they were derived. The new scenarios consisted of the following grids:
    - 7 x 7 parcel grid (1510.4 km^2 total area, 5.55 km x 5.55 km parcels)
    - 11 x 11 parcel grid (1151.2 km^2 total area, 3.08 km x 3.08 km parcels)
    - 15 x 15 parcel grid (1026 km^2 total area, 2.14 km x 2.14 km parcels)

- **Decreased area scenario.** The outer ring of square parcels was removed from the 5 x 5 Regular Grid scenario to create a 3 x 3 grid with a smaller total area. (277.4 km^2 total area, 5.55 km x 5.55 km parcels)

A single source with constant emissions of elemental mercury only was located in the center of the grid. A simulation period of one month (744 hours) was used, and hourly results were obtained and averaged to derive an overall monthly average. Actual hourly meteorological data for a location in the northeastern U.S. were used for the runs. One vertical layer was defined with the height set equivalent to the mixing height. Vertical wind velocity data were not relevant for this evaluation because only one vertical layer was used.

4.2.3.2 Results and Observations

Overall, the trends in the results for the Increased Area scenarios were relatively consistent with those from the Regular Grid scenarios described in Section 4.2.2 (i.e., the highest average monthly concentration for each of the scenarios occurred in the parcel containing the source and the results for all of the scenarios seemed consistent with the wind direction data).

To assess the impact of increasing the modeled area, the estimated concentrations in the common parcels between the original grids (i.e., 5 x 5, 9 x 9, and 11 x 11 Regular Grids) and the corresponding grids with increased area (i.e., 7 x 7, 11 x 11, and 15 x 15 Grids) were compared. The results for the 7 x 7 and 11 x 11 grids are presented in Figures 4-4 and 4-5. The estimated concentrations from the Increased Area scenarios were higher than the estimates for the corresponding Regular Grid parcels across the entire grid. In general, the differences were larger farther from the source parcel (i.e., nearer the edges). The differences were smaller when grid resolution was increased. However, in both comparisons, the difference was less than 25 percent. This effect could be minimized in future model applications by increasing the distance of the boundary of the modeling domain from the area of interest.

Figure 4-4
Percentage Difference in Common Parcels Between
7 X 7 Increased Area Grid and 5 X 5 Regular Grid

21%	16%	6.1%	11%	15%
15%	12%	3.2%	6.4%	9.2%
6.3%	3.6%	0.41%	1.6%	3.4%
9.7%	5.3%	1.2%	2.7%	5.2%
13.%	7.3%	2.3%	4.6%	8.2%

N
↑

The value in each cell represents (7x7-5x5)/5x5.
Note that the source parcel is shaded.

Figure 4-5
Percentage Difference in Common Parcels Between
11 X 11 Increased Area Grid and 9 X 9 Regular Grid

12%	11%	9.8%	8.5%	3.2%	5.4%	7.4%	9.6%	11%
11%	9.8%	8.9%	7.7%	2.6%	4.6%	6.4%	8.1%	9.4%
9.0%	7.9%	7.0%	6.0%	1.7%	3.2%	4.4%	5.6%	6.6%
6.9%	5.9%	5.0%	4.2%	0.99%	2.0%	2.9%	4.0%	4.9%
4.1%	2.9%	2.0%	1.2%	0.11%	0.46%	0.90%	1.6%	2.3%
7.0%	4.5%	2.8%	1.8%	0.31%	0.65%	1.2%	2.0%	3.0%
8.1%	5.1%	3.2%	2.1%	0.48%	0.85%	1.4%	2.5%	3.7%
10%	6.8%	4.3%	2.9%	0.88%	1.4%	2.2%	3.6%	5.3%
13%	9.2%	6.2%	4.3%	1.7%	2.3%	3.4%	5.2%	7.4%

N
↑

The value in each cell represents (11x11 - 9x9)/9x9.
Note that the source parcel is shaded.

Monthly average concentrations across the entire Regular Grid area region of the Increased Area scenarios were very similar. That is, the average of the interior 5 x 5, 9 x 9, and 13 x 13 areas of the 7 x 7, 11 x 11, and 15 x 15 grids, respectively, was 6.2E-10 g/m^3, with a standard deviation of 6.7E-12. However, across the three Increased Area scenarios, the average concentration for the Regular Grid regions decreased slightly as the grid resolution increased (e.g., the average concentration of the regular grid area for the 7 x 7 scenario is greater than the 11 x 11 average concentration). This result (shown in Table 4-3) was expected, considering that the lower resolution scenarios had larger total grid areas providing more area over which the mass could distribute prior to irretrievably reaching the sinks.

Table 4-3
Average Monthly Concentrations in the Increased Area Scenarios

Increased Area Scenarios	Average Concentration Over Regular Grid Area* (g/m^3)
7 x 7 grid	6.2E-10
11 x 11 grid	6.1E-10
15 x 15 grid	6.1E-10
Average	6.2E-10
Standard Deviation	6.7E-10

* Regular grid scenarios (5 x 5, 9 x 9, and 13 x 13) averaged 6.0E-10 g/m^3

To further examine the impact of changing the number of identically sized parcels on concentration estimates, the common parcels between the 3 x 3 Decreased Area Grid, the 5 x 5 Regular Grid, and the 7 x 7 Increased Area Grid were compared. These results are presented in Table 4-4. As the number of parcels (and thus the modeled area) increases, the concentrations in all of the common parcels increases. This increase is greatest in the directions of the predominant winds (i.e., NE, E, and SE). The largest increase was on the order of 20 percent. These differences are likely a result of increasing the area of the modeled system, thus preventing mass from leaving the system via the sinks as quickly.

Table 4-4
Comparison of Common Parcels Between
3 X 3 Decreased Area Grid, 5 X 5 Regular Grid, and 7 X 7 Increased Grid

Scenario	Concentrations in Air Parcels (g/m^3)									
	Source	N	NE	E	SE	S	SW	W	NW	Average
3 x 3	4.2E-09	5.5E-10	3.5E-10	1.4E-09	8.0E-10	1.4E-09	2.2E-10	3.2E-10	9.1E-11	6.1E-10
5 x 5	4.3E-09	5.9E-10	3.9E-10	1.5E-09	8.5E-10	1.5E-09	2.4E-10	3.4E-10	1.1E-10	9.7E-09
7 x 7	4.3E-09	6.1E-10	4.2E-10	1.5E-09	8.8E-10	1.5E-09	2.5E-10	3.6E-10	1.2E-10	9.9E-09

4.2.4 Variation of Parcel Shape for a Constant Grid Area

This evaluation considered the effect of varying grid resolution and parcel shape on mass transfer in the air component of TRIM.FaTE. In particular, this evaluation looks at the impact of dividing a given area into different sized polygons.

4.2.4.1 Model Inputs and Grid Layout

For this evaluation, three grid layouts were designed in an attempt to replicate a radial grid using polygons. The resulting grids subdivided the total grid area referenced in Sections 4.2.1. and 4.2.2 (770.6 km^2) into four-sided parcels centered on a square-shaped source (see Figure 4-2 for the layout of the 17-parcel grid as an example). The source parcel is the shaded square parcel in the center of the grid.

- 17-parcel grid (770.6 km^2 total area, same source size and shape as 5 x 5 Regular Grid)
- 33-parcel grid (770.6 km^2 total area, same source size and shape as 9 x 9 Regular Grid)
- 49-parcel grid (770.6 km^2 total area, same source size and shape as 13 x 13 Regular Grid)

As in the analyses described previously, a single source with constant emissions of elemental mercury only was located in the center of the grid. A simulation period of one-month (744 hours) was used; hourly results were obtained and averaged to derive an overall monthly average. Actual hourly meteorological data for a location in the northeastern United States were used for the runs. Vertical wind speeds were derived from these actual data using a simplified method based on stability class and horizontal wind speed. One vertical layer was defined with the height set equivalent to the mixing height.

4.2.4.2 Results and Observations

The general trend in the estimated monthly average concentrations was that the larger the number of parcels, the higher the average concentration across the full grid area. This was the opposite of the trend observed with the Regular Grid scenarios, where increasing the number of parcels resulted in lower average concentrations across the full grid area. As with the Regular Grid findings (Section 4.2.1), this difference is small (e.g., less than a factor of 2). Furthermore, the estimated concentrations from the Irregular Grid scenarios (area-weighted average concentration of 5.6E-10 g/m^3, standard deviation of 1.1E-11; full results presented in Table 4-5) varied slightly less than the results from the Regular Grid and generally predicted lower overall concentrations. Variation was greater when the one-parcel Regular Grid scenario was omitted.

Table 4-5
Area-weighted Average Monthly Concentrations Across Modeled Area

Irregular Scenarios	Average Concentration (g/m^3)
17 Parcel Grid	5.5E-10
33 Parcel Grid	5.6E-10
49 Parcel Grid	5.7E-10
Average	5.6E-10
Standard Deviation	1.1E-11

The estimated concentration patterns for the Irregular Grid scenarios were compared by averaging the concentrations into quadrants. To account for the varying parcel sizes within the scenarios, the concentrations were weighted based on the area of the parcels. Overall, the concentrations (presented in Table 4-6) in the Irregular Grid scenarios decreased with increased numbers of parcels in the upwind quadrants (i.e., NW and SW quadrants) and increased with increased numbers of parcels in the downwind quadrants (NE and SE).

The area-weighted quadrant concentrations from the Irregular Grid scenarios were also compared to the estimated quadrants concentrations from the Regular Grid scenarios. Overall, the Irregular Grid scenarios seem to estimate similar concentrations to the Regular Grid scenarios, but with fewer modeled parcels (i.e., the results for the 49-Parcel Irregular Grid are similar to the results for the 13 x 13 Regular Grid and the results from the 33-Parcel Irregular Grid are similar to the results from the 9 x 9 Regular Grid). Furthermore, the concentrations in both the Regular and Irregular scenarios decreased with increased numbers of parcels in the upwind quadrants (i.e., NW and SW quadrants) and increased with increased numbers of parcels in the SE quadrant. However, whereas concentrations in the NE quadrant decreased with increased numbers of parcels in the Regular Grid scenarios, concentrations in this quadrant of the Irregular Grid increased as the grid resolution increased. In addition, the concentrations in the downwind directions (i.e., NE and SE) were generally lower in the Irregular Grid scenarios, possibly indicating that this grid layout causes mass to leave the system via the downwind sinks more rapidly than the Regular Grid layouts.

Table 4-6
Quadrant Average Concentrations (g/m^3)

Scenario	NW	SW	NE	SE	Overall Average
3x3 Regular Grid	4.1E-10	5.5E-10	6.4E-10	8.4E-10	6.1E-10
5x5 Regular Grid	3.3E-10	5.1E-10	6.2E-10	9.4E-10	6.0E-10
9x9 Regular Grid	2.7E-10	4.7E-10	6.0E-10	1.1E-09	6.0E-10
13x13 Regular Grid	2.4E-10	4.4E-10	5.9E-10	1.1E-09	6.0E-10
17-Parcel Grid	3.7E-10	4.7E-10	5.6E-10	8.4E-10	5.5E-10
33-Parcel Grid	2.7E-10	4.5E-10	5.7E-10	9.5E-10	5.6E-10
49-Parcel Grid	2.5E-10	4.4E-10	5.7E-10	1.0E-09	5.7E-10

As opposed to the square parcel layouts, the Irregular Grid layouts did not seem to produce the finding noted in Section 4.2.1 for the Regular Grid of somewhat higher concentrations along the axes. The geometry of these layouts allowed mass emitted from the source to be transported over half of the full grid area (180 degrees) for a given wind direction unless the wind blew directly in either the north, south, east, or west direction, in which case mass would be transported over one-quarter of the full grid area (90 degrees). However, this feature seemed to allow transport of some mass in directions that did not seem reasonable (e.g., a wind blowing one degree east of north would result in a small amount of mass in the southeast corner of the grid).

In general, the concentration estimates for all three Irregular Grid scenarios were more evenly spread over the full grid area than were the Regular Grid scenarios. This is likely due to differences in the range of directions mass can be transported and increased “artificial dispersion” caused by the shape of the parcels.

Several advantages of the Irregular Grid layout versus the Regular Grid layout were noted. Specifically, implementing the Irregular Grid layout used in these evaluations:

- Avoided or minimized the occurrence of somewhat higher concentrations along the north-south and east-west axes than between the axes;
- Produced similar results to the Regular Grid with far fewer parcels, thus reducing computational burden;
- Provided more grid resolution near the source (where concentrations are typically higher) and less resolution farther from the source (where concentrations are typically lower); and
- Appeared to be potentially less sensitive to small fluctuations in wind direction.

The following disadvantages of the Irregular Grid layout versus the Regular Grid layout were also observed:

- Some, albeit relatively small, mass can be transported in directions that do not seem reasonable for certain wind directions; and
- Mass seems to exit the system via the sinks more quickly in the downwind direction.

4.3 BIOTIC COMPLEXITY EVALUATION

This section of the complexity evaluation examines how biotic compartments (including terrestrial and aquatic plant and animal compartments) affect the mass balance of modeled compounds. It has typically been assumed that the chemical mass in biota is small compared to the chemical mass in abiotic compartments and is not large enough to influence the overall chemical mass balance. The biotic complexity analysis tests this assumption by successively adding biotic compartments in a series of simulations. Comparison of the results for the simulations helps to identify TRIM.FaTE's response to biota and to determine which biotic compartments need to be included to effectively model chemical concentration in the compartments of concern. The results of this evaluation have been used to select biotic compartments to include in further complexity evaluations reported in Sections 4.4 and 4.5.

Biotic complexity evaluations were performed using benzo(a)pyrene and mercury in order to compare the effects of biotic systems for both organic and inorganic pollutants. Section 4.3.1 and Section 4.3.2 present the biotic complexity evaluations using benzo(a)pyrene and mercury, respectively.

4.3.1 Benzo(a)pyrene

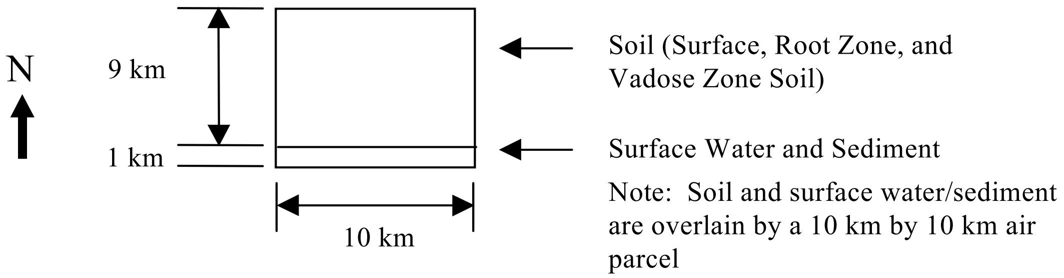
Section 4.3.1.1 presents the modeling scenarios for the biotic complexity evaluation using benzo(a)pyrene. Results of the evaluation are presented in Section 4.3.1.2.

4.3.1.1 Modeling Scenarios for Benzo(a)pyrene

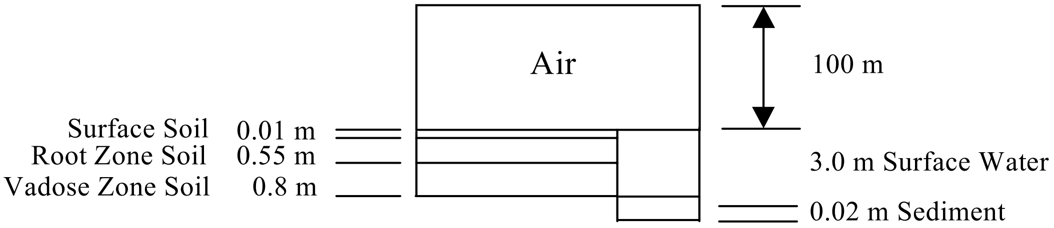
The biotic complexity evaluation for benzo(a)pyrene included simulations with four scenarios. Figure 4-6 shows the configuration of abiotic compartments used in the four scenarios. This modeling configuration included a single air parcel above adjacent surface soil and surface water parcels. Root zone and vadose zone soil parcels were included beneath the surface soil parcel, and a sediment parcel was included beneath the surface water parcel. The horizontal and vertical dimensions of all parcels are shown in Figure 4-6.

Figure 4-6
Modeling Configuration for the Biotic Complexity Analysis with Benzo(a)pyrene

Horizontal Dimensions



Vertical Dimensions



Note: Not to scale

Biotic compartments included in the four scenarios are shown in Table 4-7. Scenario 1 included only abiotic compartments.[8] Scenario 2 included abiotic compartments plus herb/grassland terrestrial vegetation compartments. Scenario 3 included abiotic compartments, terrestrial vegetation compartments, and terrestrial and semi-aquatic animal compartments. Scenario 4 equaled Scenario 3 with the addition of aquatic plant and animal compartments.

---

[8] As algae are represented as a phase in surface water, they are included in all scenarios with inclusion of the surface water compartment.

Table 4-7
Biotic Compartments Included in the Biotic Complexity Evaluation with Benzo(a)pyrene

Compartment Type (Trophic Functional Group)[a]	Representative Population or Subgroup	Scenario			
		1	2	3	4
Algae	Generalized algal species	✓	✓	✓	✓
Aquatic macrophyte	User input				✓
Water column herbivore	NA[b]				✓
Water column omnivore	NA[b]				✓
Water column carnivore	NA[b]				✓
Benthic invertebrate (herbivore)	Mayfly				✓
Benthic omnivore	NA[b]				✓
Benthic carnivore	NA[b]				✓
Terrestrial omnivore	White-footed mouse			✓	✓
Semi-aquatic piscivore	Common loon; mink; belted kingfisher			✓	✓
Semi-aquatic predator/scavenger	Bald eagle			✓	✓
Terrestrial insectivore	Black-capped chickadee			✓	✓
Semi-aquatic herbivore	Mallard duck			✓	✓
Terrestrial predator/scavenger	Red-tailed hawk; long-tailed weasel			✓	✓
Semi-aquatic insectivore	Tree swallow			✓	✓
Terrestrial herbivore	White-tailed deer; mule deer; black-tailed deer; meadow vole; long-tailed vole			✓	✓
Semi-aquatic omnivore	Raccoon			✓	✓
Terrestrial ground-invertebrate feeder	Short-tailed shrew; Trowbridge shrew			✓	✓
Flying insect	Mayfly			✓	✓
Soil detritivore	Earthworm; soil arthropod			✓	✓
Plant-leaf	Leaf (herb/grassland)		✓	✓	✓
Plant-particle on leaf	Particle on leaf (herb/grassland)		✓	✓	✓
Plant-stem	Stem (herb/grassland)		✓	✓	✓
Plant-root	Root (herb/grassland)		✓	✓	✓

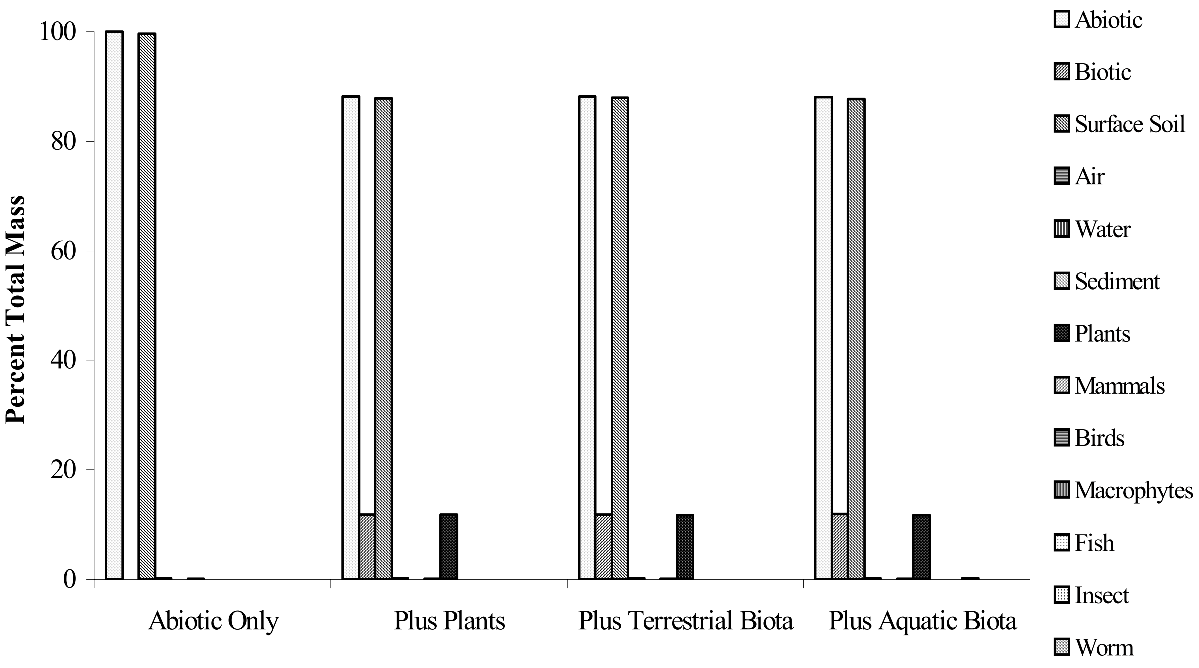
[a] Plant parts constitute different compartment types even though they are not different trophic groups.
[b] This compartment represents a mixed population of species fitting this trophic functional group.

All four scenarios were run with constant meteorological inputs, including a wind of 4 m/sec from due north and rainfall of 1.0E-3 m/d. In all scenarios, boundary conditions and initial benzo(a)pyrene concentrations were set equal to zero, and the benzo(a)pyrene source emitted a constant 100 g/d (1.2E-3 g/s) into the air compartment. The simulation period was ten years. The evaluation does not address how biotic complexity affects mass balance over time.

4.3.1.2 Results for Benzo(a)pyrene

As shown in Figure 4-7, the largest effect of the biotic compartment additions on distribution of mass in the modeling system appears to be on the surface soil compartment. The addition of plant compartments with Scenario 2 decreased the final concentration and mass of benzo(a)pyrene in surface soil by about six percent (from approximately 880 g to 830 g). This reduction may occur because a portion of the chemical mass is now contained in the plants and thus is unavailable to the surface soil compartment. When present, the plant leaf compartment accounted for just over ten percent of the total mass in the system. The macrophytes accumulated the most mass among the aquatic biota compartments, although this represented less than one percent of the total system mass in the simulation.

Figure 4-7
Benzo(a)pyrene Mass in Biotic and Abiotic Compartments



Because inclusion of terrestrial vertebrates and invertebrates and aquatic biota did not appear to significantly affect the masses and concentrations in the plants or abiotic media for benzo(a)pyrene (see Table 4-8), they were not included in other complexity evaluations for benzo(a)pyrene. Thus, only abiotic media and plants are included in other further complexity evaluations for benzo(a)pyrene. The response of the modeling system to addition of biotic compartments may vary for other chemicals.

Table 4-8
Benzo(a)pyrene Concentrations in Biotic and Abiotic Compartments

Compartment	Abiotic Only	Plus Plants	Plus Terrestrial Biota	Plus Aquatic Biota
Air (g/m^3)	2.1E-10	2.1E-10	2.1E-10	2.1E-10
Water (mg/L)	2.4E-09	2.4E-09	2.4E-09	2.4E-09
Sediment (g/m^3)	5.8E-06	5.8E-06	5.8E-06	5.8E-06
Surface Soil (g/m^3)	9.7E-04	9.7E-04	9.7E-04	9.7E-04
Leaf (g/kg)	--	1.8E-06	1.8E-06	1.8E-06
Weasel (g/kg)	--	--	6.3E-09	6.3E-09
Loon (g/kg)	--	--	3.8E-10	1.6E-08
Eagle (g/kg)	--	--	1.1E-09	5.6E-09

4.3.2 Mercury

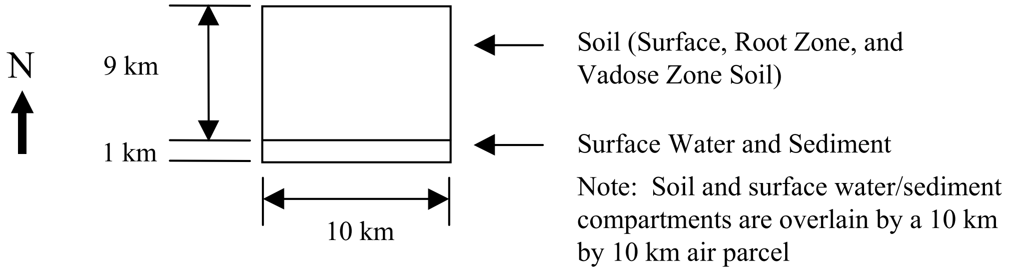
The objectives of the biotic complexity evaluation with mercury were (1) to determine the most important biotic compartment types to include in mercury fate and transport assessments (where fish are a major focus), and (2) to determine which biotic compartment types need to be included to effectively model chemical concentrations in the compartment types of concern. In addition, the biotic complexity evaluation with mercury focused specifically on whether terrestrial animal compartments affect the contaminant mass in fish. This latter objective is intended to inform TRIM users about the importance of including terrestrial animals in simulations focused on mercury accumulation in fish.

4.3.2.1 Modeling Scenarios for Mercury

Five modeling scenarios were developed for the biotic complexity analysis with mercury. The configuration of abiotic compartments used in all five scenarios is shown in Figure 4-8. This configuration is similar to the configuration of abiotic compartments used for the benzo(a)pyrene biotic complexity evaluation.

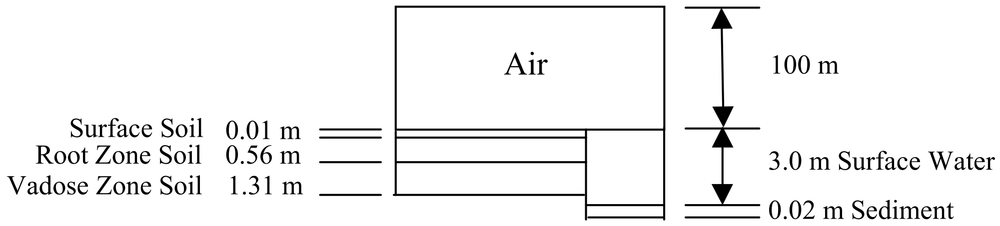
Figure 4-8
Modeling Configuration for the Biotic Complexity Evaluation With Mercury

Horizontal Dimensions



Note: Soil and surface water/sediment compartments are overlain by a 10 km by 10 km air parcel

Vertical Dimensions



Note: Not to scale

The biotic compartments included in the five scenarios are presented in Table 4-9. All scenarios included the minimum set of aquatic and semi-aquatic animals identified for Scenario 1. Scenario 1 includes all abiotic compartments, all fish compartments, and the benthic invertebrate and loon compartments, as well as the short-tailed shrew and earthworm, both of which are expected to accumulate mercury from the soil.

In Scenario 2, aquatic macrophytes were added to the baseline biotic compartments of Scenario 1. The results for Scenarios 1 and 2 were compared to determine whether aquatic macrophytes affect mercury concentration in fish. The addition of aquatic macrophytes in Scenario 2 may decrease mercury concentration in fish if the plants absorb a significant mass of mercury from the surface water compartment.

Table 4-9
Biotic Compartments Included in the Biotic Complexity Evaluation with Mercury

Compartment Type (Trophic Functional Group)[a]	Representative Population or Subgroup	Scenario				
		1	2	3	4	5
Algae	Generalized algal species	✓	✓	✓	✓	✓
Aquatic Macrophyte	User input		✓	✓	✓	✓
Water column herbivore	NA[b]	✓	✓	✓	✓	✓
Water column omnivore	NA[b]	✓	✓	✓	✓	✓
Water column carnivore	NA[b]	✓	✓	✓	✓	✓
Benthic invertebrate (herbivore)	Mayfly	✓	✓	✓	✓	✓
Benthic omnivore	NA[b]	✓	✓	✓	✓	✓
Benthic carnivore	NA[b]	✓	✓	✓	✓	✓
Terrestrial omnivore	White-footed mouse					✓
Semi-aquatic piscivore	Common loon	✓	✓	✓	✓	✓
	Mink				✓	✓
	Belted kingfisher					✓
Semi-aquatic predator/scavenger	Bald eagle					✓
Terrestrial insectivore	Black-capped chickadee					✓
Semi-aquatic herbivore	Mallard duck					✓
Terrestrial predator/scavenger	Red-tailed hawk; long-tailed weasel					✓
Semi-aquatic insectivore	Tree swallow					✓
Terrestrial herbivore	White-tailed deer; mule deer; black-tailed deer; meadow vole; long-tailed vole					✓
Semi-aquatic omnivore	Raccoon				✓	✓
Terrestrial ground-invertebrate feeder	Short-tailed shrew; Trowbridge shrew	✓	✓	✓	✓	✓
Flying insect	Mayfly	✓	✓	✓	✓	✓
Soil detritivore	Earthworm; soil arthropod	✓	✓	✓	✓	✓
Plant-leaf	Leaf (herb/grassland)			✓	✓	✓
Plant-particle on leaf	Particle on leaf (herb/grassland)			✓	✓	✓
Plant-stem	Stem (herb/grassland)			✓	✓	✓
Plant-root	Root (herb/grassland)			✓	✓	✓

[a] Plant parts constitute different compartment types even though they are not different trophic groups.
[b] This compartment represents a mixed population of species fitting this trophic functional group.

Scenario 3 was equal to Scenario 2 with the addition of terrestrial plant compartments. In Scenario 4, a semi-aquatic piscivore (mink) and a semi-aquatic omnivore (raccoon) were added to the biotic compartments included in Scenario 3. This scenario was developed to evaluate how these semi-aquatic fish-eaters influence the mercury concentrations in fish. Because TRIM.FaTE uses a fixed fish population (i.e., fish biomass in a surface water compartment stays constant over time) rather than modeling population dynamics, fish predation by raccoons and mink acts to remove mercury mass from the fish compartments.

Scenario 5 included everything in Scenario 4 plus all other terrestrial biota that were being considered for the mercury test case (i.e., black-capped chickadee, kingfisher, bald eagle, mallard, red-tailed hawk, tree swallow, meadow vole, long-tailed vole, long-tailed weasel, white-footed mouse, white-tailed deer, black-tailed deer, mule deer).

The simulation period for all five scenarios was five years. Meteorological inputs were annually averaged data of a controlled dataset. These data included a constant precipitation rate of 3.088E-3 m/d and a wind of 4.862 m/sec from 112 degrees. The mercury emission rate into the compartment was 1,308 g/d. Mercury emissions speciation was 95 percent elemental and 5 percent divalent. Boundary conditions and initial mercury concentrations were set to zero in all compartments.

4.3.2.2 Results for Mercury

The presentation of results for the biotic complexity evaluation with mercury focuses on selected biotic and abiotic compartments. All results presented are the concentrations predicted in the selected compartments at the end of the five-year simulation period. Figures 4-9, 4-10, and 4-11 present concentrations of elemental, divalent, and methylmercury, respectively, in surface soil, a terrestrial ground-invertebrate feeder (i.e., short-tailed shrew), surface water, and a semi-aquatic piscivore (i.e., common loon). Figure 4-11 also presents concentrations of methylmercury in the water column carnivore compartment. Concentrations of elemental and divalent mercury in the water column carnivore compartment were predicted to be zero in all scenarios and are not included in the figures. Results presented in Figures 4-9 to 4-11 are also presented in tabular form in Tables 4-10 to 4-12.

Figure 4-9
Elemental Mercury Concentrations in Selected Compartments After Five Years

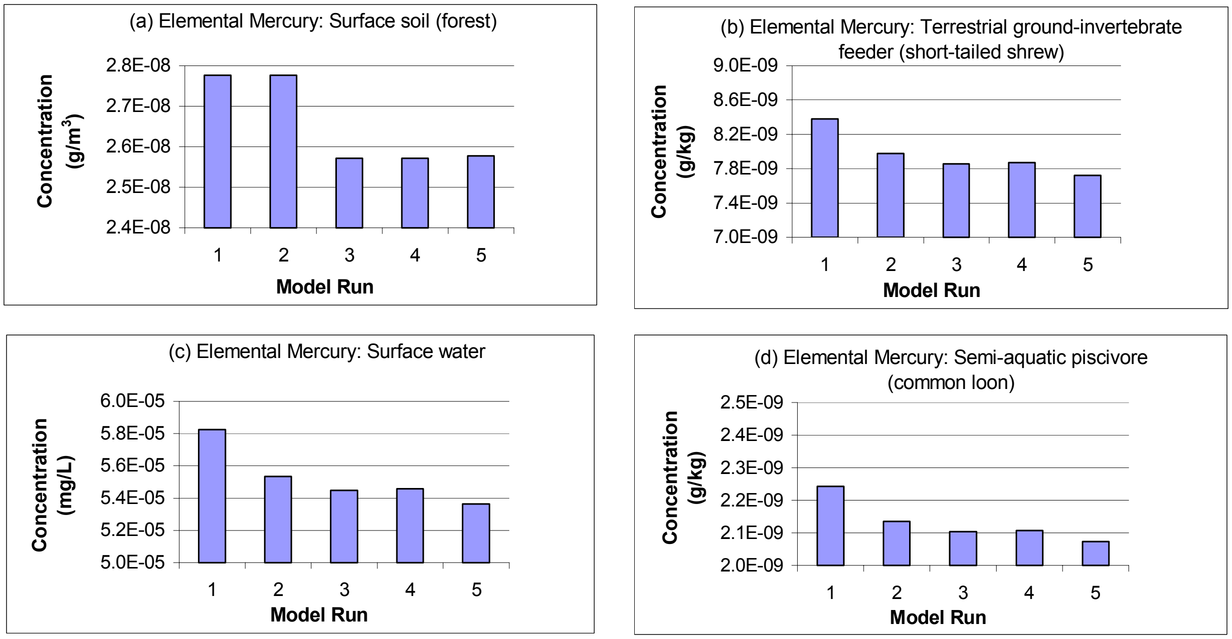


Figure 4-10
Divalent Mercury Concentrations in Selected Compartments After Five Years

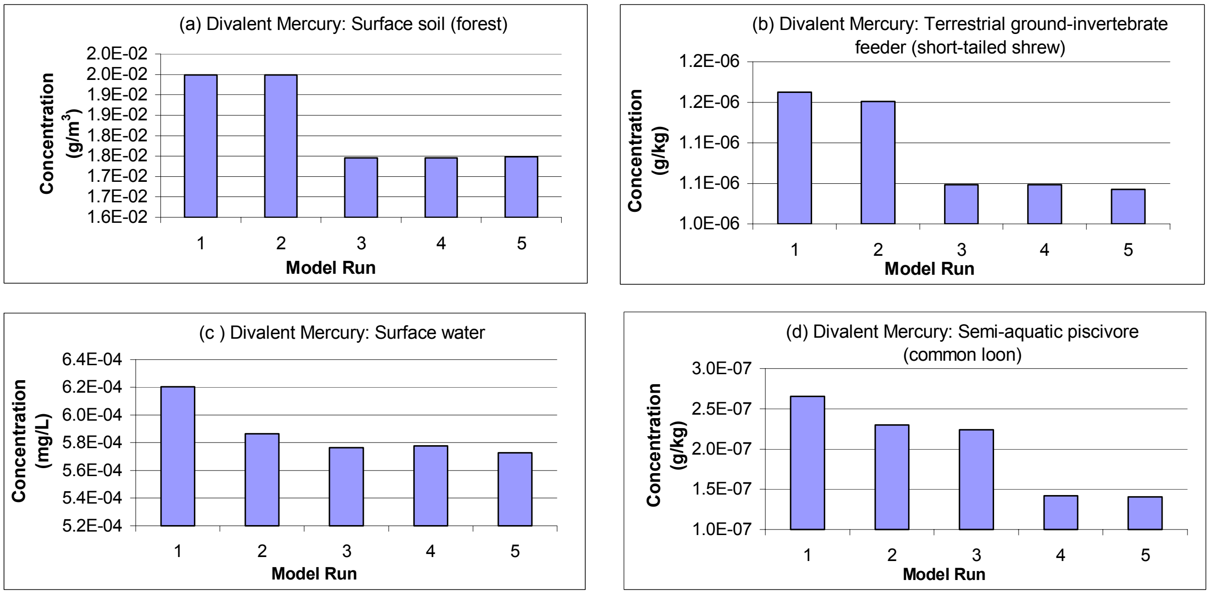


Figure 4-11
Methylmercury Concentrations in Selected Compartments After Five Years

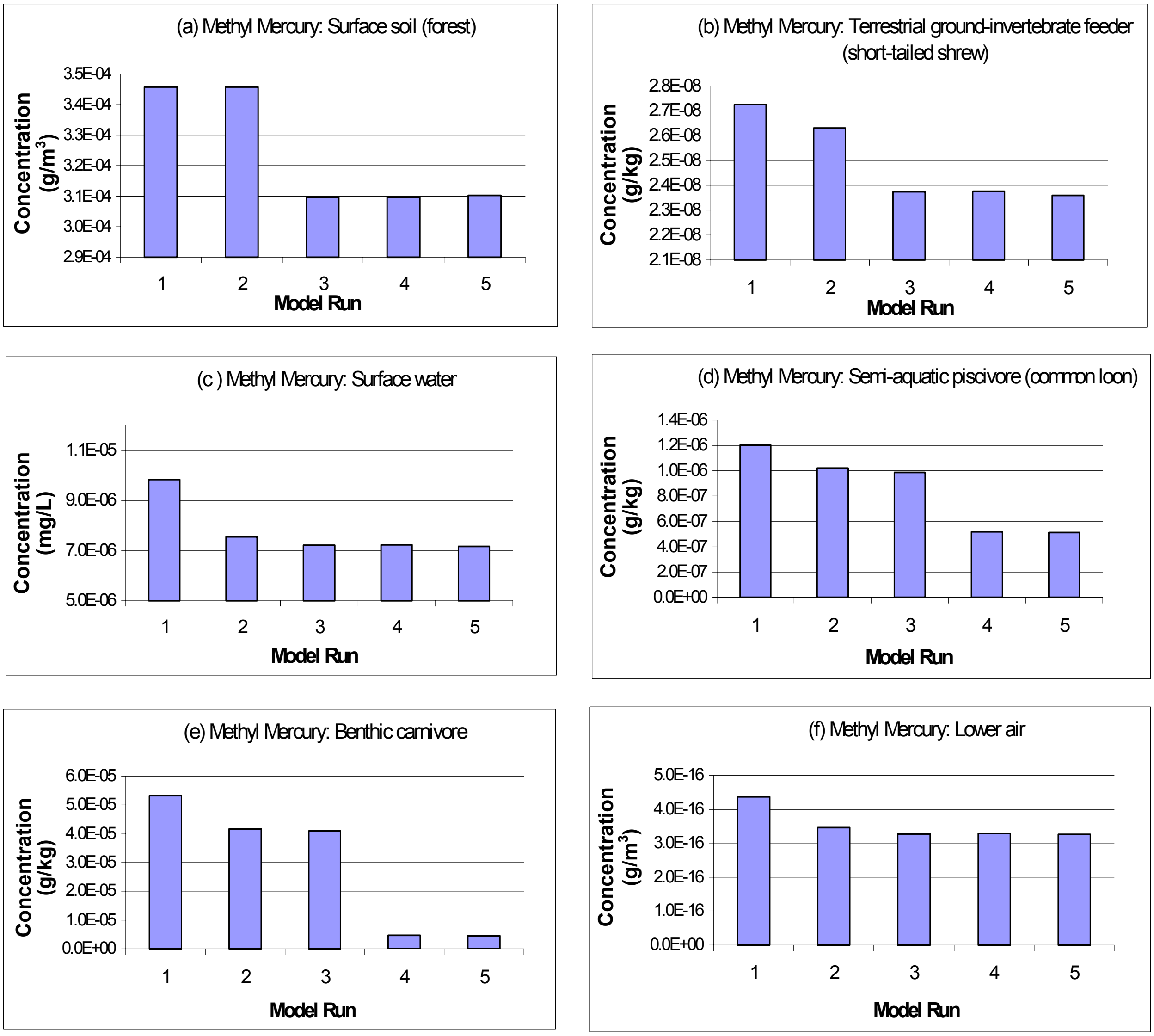


Table 4-10
Concentrations of Elemental Mercury After Five Years

Compartment	Scenario				
	1	2	3	4	5
Surface Water (mg/L)	5.8E-05	5.5E-05	5.5E-05	5.5E-05	5.4E-05
Water Column Carnivore (g/kg)	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
Common Loon (g/kg)	2.2E-09	2.1E-09	2.1E-09	2.1E-09	2.1E-09
Surface Soil (g/m^3)	2.8E-08	2.8E-08	2.6E-08	2.6E-08	2.6E-08
Short-tailed Shrew (g/kg)	8.4E-09	8.0E-09	7.9E-09	7.9E-09	7.7E-09
Air (g/m^3)	4.0E-10	4.0E-10	4.0E-10	4.0E-10	4.0E-10

Table 4-11
Concentrations of Divalent Mercury After Five Years

Compartment	Scenario				
	1	2	3	4	5
Surface Water (mg/L)	6.2E-04	5.9E-04	5.8E-04	5.8E-04	5.72E-04
Water Column Carnivore (g/kg)	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
Common Loon (g/kg)	2.7E-07	2.3E-07	2.2E-07	1.4E-07	1.4E-07
Surface Soil (g/m^3)	2.0E-02	2.0E-02	1.8E-02	1.8E-02	1.8E-02
Short-tailed Shrew (g/kg)	1.2E-06	1.2E-06	1.1E-06	1.1E-06	1.0E-06
Air (g/m^3)	1.7E-11	1.7E-11	1.8E-11	1.8E-11	1.8E-11

Table 4-12
Concentrations of Methylmercury After Five Years

Compartment	Scenario				
	1	2	3	4	5
Surface Water (mg/L)	9.8E-06	7.6E-06	7.2E-06	7.2E-06	7.1E-06
Water Column Carnivore (g/kg)	5.3E-05	4.2E-05	4.1E-05	4.7E-06	4.5E-06
Common Loon (g/kg)	1.2E-06	1.0E-06	9.9E-07	5.2E-07	5.1E-07
Surface Soil (g/m^3)	3.5E-04	3.5E-04	3.1E-04	3.1E-04	3.1E-04
Short-tailed Shrew (g/kg)	2.7E-08	2.6E-08	2.4E-08	2.4E-08	2.4E-08
Air (g/m^3)	4.4E-16	3.5E-16	3.3E-16	3.3E-16	3.3E-16

In Scenario 2, aquatic macrophytes were added to the baseline biotic compartments of Scenario 1 to determine whether aquatic macrophytes affect mercury concentrations in other compartments, particularly the surface water and aquatic carnivore compartments. As shown by Figure 4-11(c), the inclusion of aquatic macrophytes in Scenario 2 reduced the concentration of methylmercury in the surface water by approximately 21 percent and, apparently consequently, resulted in a 21 percent reduction in the concentration of methylmercury in the water column carnivore compartment, as seen in Figure 4-11(e).

The addition of aquatic macrophytes affected the mass balances of elemental and divalent mercury less than it affected the mass balance of methylmercury. As shown in Figure 4-9(c) and Figure 4-10(c), concentrations of elemental and divalent mercury in surface water with aquatic macrophytes (i.e., Scenario 2) were about five percent less than the concentrations of elemental and divalent mercury in surface water without aquatic macrophytes (i.e., Scenario 1). The addition of aquatic macrophytes did not affect concentrations of elemental and divalent mercury in the air aquatic carnivore compartments.

Scenario 3 included all compartments included in Scenario 2, plus the terrestrial plant compartments. Comparison of the results for Scenarios 2 and 3 in Figures 4-9(a), 4-10(a), and 4-11(a) shows that the addition of terrestrial plant compartments to the modeling scenario reduced the concentrations of all three mercury species in surface soil by approximately 7 to 11 percent. This result is possibly due to the interception of atmospheric mercury deposition by the terrestrial plants and is comparable to findings presented for benzo(a)pyrene (see Section 4.3.1). Further, the addition of the terrestrial plant compartments decreased the concentrations of divalent and methylmercury in the terrestrial ground-invertebrate feeder (i.e., short-tailed shrew) by approximately 8 percent, as shown by Figures 4-10(b) and 4-11(b). This effect is likely due to the fact that the shrew diet is comprised of soil-residing biota.

The addition of a semi-aquatic piscivore (mink) and a semi-aquatic omnivore (raccoon) in Scenario 4 significantly affected methylmercury concentrations in fish. Specifically, inclusion of these fish-eaters in Scenario 4 reduced methylmercury concentration in the water column carnivore compartment by approximately 88 percent. This result can be seen by comparing methylmercury concentrations for Scenarios 3 and 4 in Figures 4-11(e). Because TRIM.FaTE uses a fixed population for the aquatic carnivore compartment rather than a dynamic population model, predation of largemouth bass by mink and raccoon removes mercury mass from the aquatic carnivore compartment without reducing the population size (i.e., the biomass). Thus, the predicted average mercury concentration in the aquatic carnivores is reduced.

Figure 4-11(d) also shows that Scenario 4 reduced mercury concentrations in the semi-aquatic piscivore (i.e., common loon) by about 48 percent. The decrease in the concentration of mercury in the common loon in Scenario 4 is likely to have resulted from the greatly decreased mercury concentrations in the fish compartment eaten by loons (e.g., herbivore). As expected, Scenario 4 did not significantly affect mercury concentrations in surface soil, the terrestrial ground-invertebrate feeder (i.e., short-tailed shrew), surface water, or air.

Scenario 5 included all remaining terrestrial biota not included in Scenario 4. The inclusion of all other terrestrial biota compartments did not greatly affect mercury concentrations (i.e., less than five percent change) in most compartments for any of the mercury species, as shown by comparing Scenarios 4 and 5 in Figures 4-9 through 4-11.

In summary, it appears that the following biotic compartments should be included in further complexity evaluations with mercury to enable effective prediction of contaminant mass distribution among the abiotic compartments of interest:

- Aquatic macrophytes (*Elodea densa*);
- Water column herbivore;
- Water column omnivore;
- Water column carnivore;
- Benthic invertebrate (mayfly);
- Benthic omnivore;
- Benthic carnivore;
- Semi aquatic piscivore (common loon);
- Semi-aquatic predator/scavenger (bald eagle);
- Semi-aquatic carnivore (raccoon)
- Terrestrial ground-invertebrate feeder (short-tailed shrew);
- Soil detritovore (soil arthropods); and
- Terrestrial plants.

These biota include those whose inclusion in the scenario significantly affected mercury fate in the system, as well as in compartments of particular interest (e.g., fish).

4.4 TEMPORAL COMPLEXITY EVALUATION

The temporal complexity evaluation examines how predicted pollutant concentrations are affected by changes in the simulation time step. In particular, the evaluation examines the effects of aggregating meteorological data (and in some cases other time-varying input data, such as emission rates) over various time periods. By comparing the results of simulations with varying time steps, the level of input parameter detail required to achieve a specified level of detail in the output can be evaluated. For example, longer input data averaging times (e.g., seasonal meteorological data) may be useful and sufficient for some analyses.

Temporal complexity evaluations were performed with benzo(a)pyrene and mercury. Chemical transformation was not included in runs for benzo(a)pyrene.

4.4.1 Benzo(a)pyrene

This section presents the temporal complexity evaluation for benzo(a)pyrene.

4.4.1.1 Modeling Scenarios for Benzo(a)pyrene

The temporal complexity evaluation for benzo(a)pyrene was performed with a series of scenarios based on two modeling configurations. Modeling configuration A is the spatial configuration of abiotic parcels developed for the biotic complexity analysis with benzo(a)pyrene (see Section 4.3.1). Modeling configuration B is slightly more complex than modeling configuration A. The scenarios for each modeling configuration are described further below.

Scenarios for Modeling Configuration A

The spatial configuration of abiotic parcels for modeling configuration A was described in Section 4.3.1 of the biotic complexity evaluation and is shown in Figure 4-6. The modeling configuration includes an air parcel above adjacent surface soil and surface water parcels. Root zone and vadose zone soil parcels are beneath the surface soil parcel, and a sediment parcel is beneath the surface water parcel. All scenarios for modeling configuration A include all terrestrial plant compartments, but no other biotic compartments.

No source term was included. Instead, all benzo(a)pyrene was introduced as constant boundary condition levels in air blowing into the system. This approach facilitated analysis of the effect of rain patterns. Because the input of chemical was constant, temporal variation in deposition was associated with precipitation events. Meteorological inputs were the meteorological data described previously (e.g., Section 4.2.2). The key meteorological conditions that varied in these data were wind direction, wind speed, rainfall, and temperature.

The temporal complexity runs performed with modeling configuration A featured various combinations of input data averaging time (i.e., aggregation period for meteorological data), simulation period, and reporting time step. The modeling runs are summarized in Table 4-13.

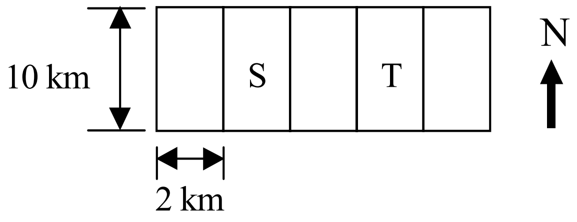
Table 4-13
Temporal Complexity Runs for Modeling Configuration A

Simulation Period	Input Data Averaging Time	Reporting Time Step
One year	Hourly	Every six hours
One year	Day/Night	Every six hours
One year	Daily	Every six hours

Scenarios for Modeling Configuration B

Modeling configuration B is shown in Figure 4-12. The modeling configuration consisted of five adjacent air and surface soil parcels each measuring 2 km wide by 10 km long. Root zone soil, vadose zone soil, and groundwater parcels are under each surface soil parcel, and all terrestrial plant compartments were included. The vertical dimensions of the abiotic parcels are the same as the vertical dimensions of the abiotic parcels in modeling configuration A (see Figure 4-6).

Figure 4-12
Modeling Configuration B



A source of benzo(a)pyrene was emitted directly into the air parcel labeled with an "S" in Figure 4-12, and media concentrations were evaluated for the target parcel marked with a "T." For these scenarios, the initial concentration of benzo(a)pyrene was set equal to zero in all parcels, and boundary conditions were set to zero. The source emitted a constant 1 g/s. The meteorological data, which were used in scenarios for modeling configuration A, also were used in scenarios for modeling configuration B. Simulations with modeling configuration B were run using hourly, daily, and monthly input averaging times.

4.4.1.2 Results for Benzo(a)pyrene

Modeling Configuration A

Average concentrations over a one-year run in the air and surface water compartments were obtained using meteorology inputs at all input averaging and reporting time steps shown in Table 4-13. The overall average concentrations for the first year of the modeling run are presented in Table 4-14. The averages for the entire year are compared (rather than results at a particular time step) because the individual concentration values for these compartments fluctuated widely throughout the year. For other compartments, the mass may be compared over time because the fluctuations were not as great. The average benzo(a)pyrene mass over the first year of each run is presented in Table 4-15. As Table 4-15 shows, lengthening the input averaging time interval had only a small effect on average benzo(a)pyrene mass in the air compartment for a one-year run. However, lengthened input averaging time tended to increase the average benzo(a)pyrene mass in surface water and surface soil for one-year runs. For example, the average mass in surface soil estimated with monthly input averaging and reporting time steps is about 30 percent larger than the average mass estimated with hourly input averaging time.

Cumulative estimates of benzo(a)pyrene mass in the surface soil compartment for hourly, daily, and monthly input averaging times are shown in Figure 4-13. As can be seen in this figure, mass accumulated over time in all scenarios, although scenarios with shorter input averaging times exhibited greater fluctuations in mass. Concentration and mass were proportional because concentration is equal to mass divided by volume, which is constant.

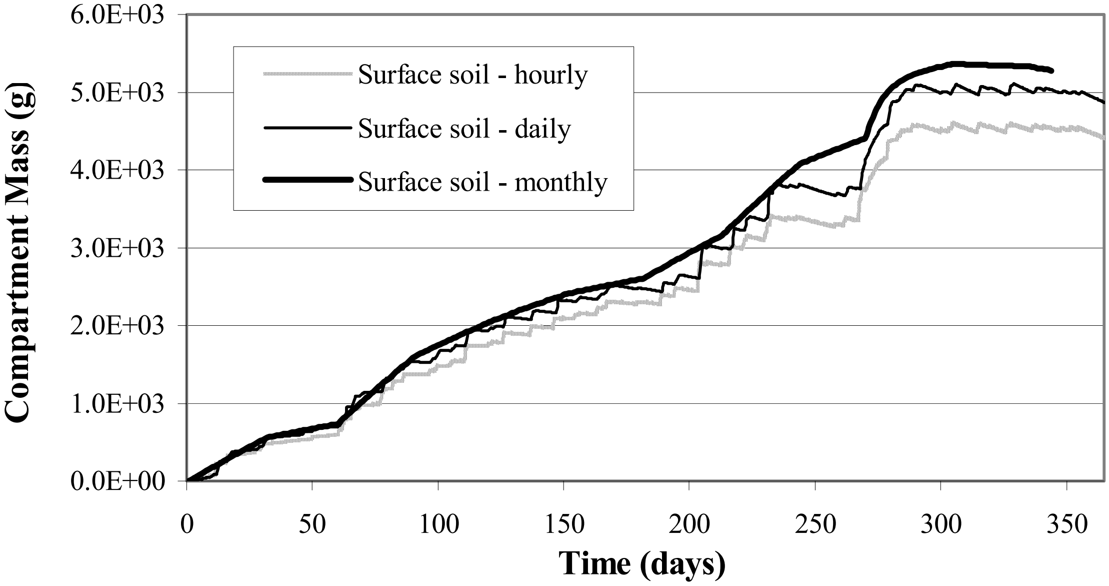
Table 4-14
Average Benzo(a)pyrene Concentrations over One Year in Air and Surface Water for Various Input Averaging Times

Compartment	Length of Meteorological Data Averaging				
	Hourly	Day/Night	Daily	Monthly	Yearly
Air (g/m^3)	1.2E-09	7.6E-10	8.3E-10	8.1E-10	8.2E-10
Surface Water (mg/L)	1.8E-08	2.0E-08	2.0E-08	2.2E-08	2.2E-08

Table 4-15
Average Benzo(a)pyrene Mass (g) over One Year in Air, Surface Water, and Surface Soil for Various Time Steps

Input Data Averaging Time	Reporting Times	Air	Surface Water	Surface Soil
Hourly	Every six hours	4.5E+1	5.3E-1	2.5E+3
Day/Night	Every six hours	4.5E+1	5.9E-1	2.7E+3
Daily	Every six hours	4.6E+1	6.1E-1	2.8E+3
Daily	Daily	4.6E+1	6.1E-1	2.8E+3
Monthly	Daily	4.6E+1	6.5E-1	3.0E+3
Monthly	Monthly	4.5E+1	6.8E-1	3.2E+3
Annual	Monthly	4.6E+1	6.6E-1	3.2E+3

Figure 4-13
Benzo(a)pyrene Mass in Surface Soil Compartment for Various Input Averaging Times



Modeling Configuration B

Figure 4-14 shows how increasing input averaging times affected benzo(a)pyrene mass in the surface soil compartment of the target parcel in modeling configuration B. Benzo(a)pyrene mass estimates for surface soil were more affected by input averaging times with the five-parcel modeling configuration B than with the simple, one-parcel modeling configuration A. This difference between the results for the two modeling configurations can be explained by wind direction considerations that apply to modeling configuration B, but not modeling configuration A. In particular, wind had negligible effect on the results of modeling configuration A, and all air changes were due to precipitation only.

The combined influence of spatial and temporal complexity is further illustrated in Figures 4-15 and 4-16, which show the benzo(a)pyrene concentrations in surface soil in the source and target parcels, respectively, of modeling configuration B. Concentration estimates are plotted for both the daily- and monthly-average input averaging times.

Figure 4-15 shows that benzo(a)pyrene concentrations in surface soil near the source were much higher using the daily averaging times than the monthly averaging times. Figure 4-16 shows that the opposite was true in the target parcel (i.e., benzo(a)pyrene concentrations were higher using the monthly averaging times than the daily averaging times). This difference may result primarily from the effects of rain events. In the source parcel, large rain events, which are shown with arrows in Figure 4-15, are generally associated with increases in the concentration in the soil, regardless of the wind direction. The deposition due to distinct rain events is greater than the deposition due to a steady rain in this parcel; thus, the concentration with daily averaging time is greater than for monthly averaging time.

In contrast, large deposition of benzo(a)pyrene to the soil further from the source (i.e., in the target parcel) seems to require that the wind blow in that direction while it is raining. In Figure 4-16, the arrows point to times when there were both strong winds blowing from the source to the target parcel and a strong rain, conditions which increased the deposition rate to soil. Because rain events typically do not continue over extended time periods, using monthly averaged meteorological data can impact where deposition occurs. In this case, benzo(a)pyrene concentrations in the target parcel were higher using monthly averaged meteorological data rather than daily averaged data because the wind direction changed less frequently, causing deposition to occur only in the average monthly wind direction. If the daily averaging times are used, the wind is often blowing a different direction during the distinct rain events resulting in fewer large-deposition events.

This evaluation showed that the interaction of wind direction and rain events is important for determining the benzo(a)pyrene concentration in the soil downwind from the site. These results imply that it may be important to consider increased temporal resolution with increased spatial resolution. However, it may be appropriate to aggregate input data if long-term, average exposures are of interest for a simple, non-transforming (in this analysis) chemical such as benzo(a)pyrene in a modeling configuration with limited spatial resolution.

These results (which suggest variation in soil concentration values on the order of 20 percent for parcels not adjacent to the source) should be compared to the variance resulting from parameter uncertainty. It has not been determined whether differences due to time fluctuations are greater or less than those derived from parameter uncertainty. If the differences are less, there should be a focus on gathering more information on the other parameter values prior to additional attention to details regarding increased temporal resolution.

Figure 4-14
Benzo(a)pyrene Mass in Target Surface Soil Parcel, Modeling Configuration B

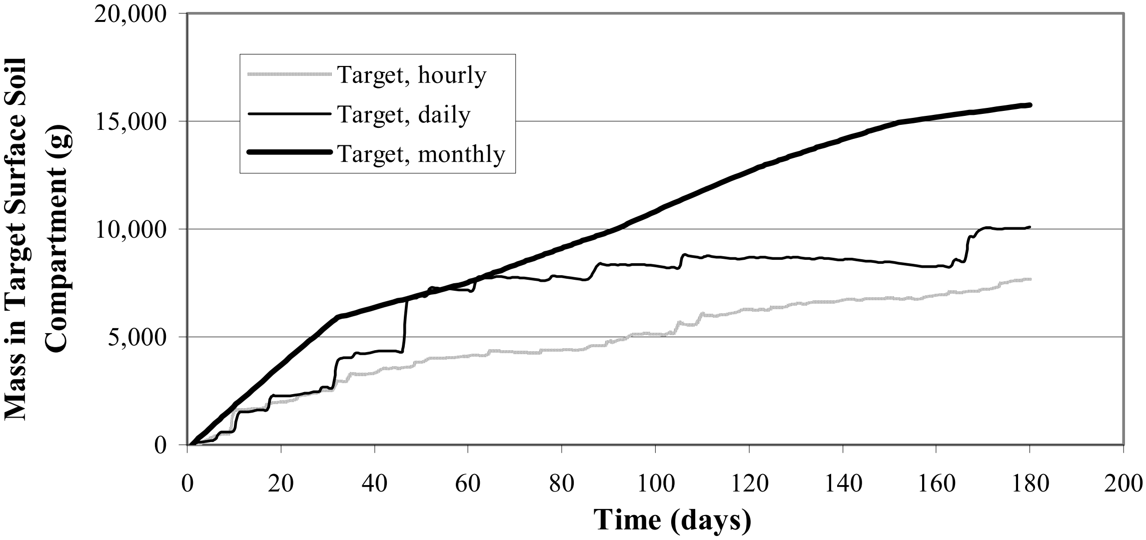


Figure 4-15
Benzo(a)pyrene Surface Soil Concentrations for Modeling Configuration B-Source Location

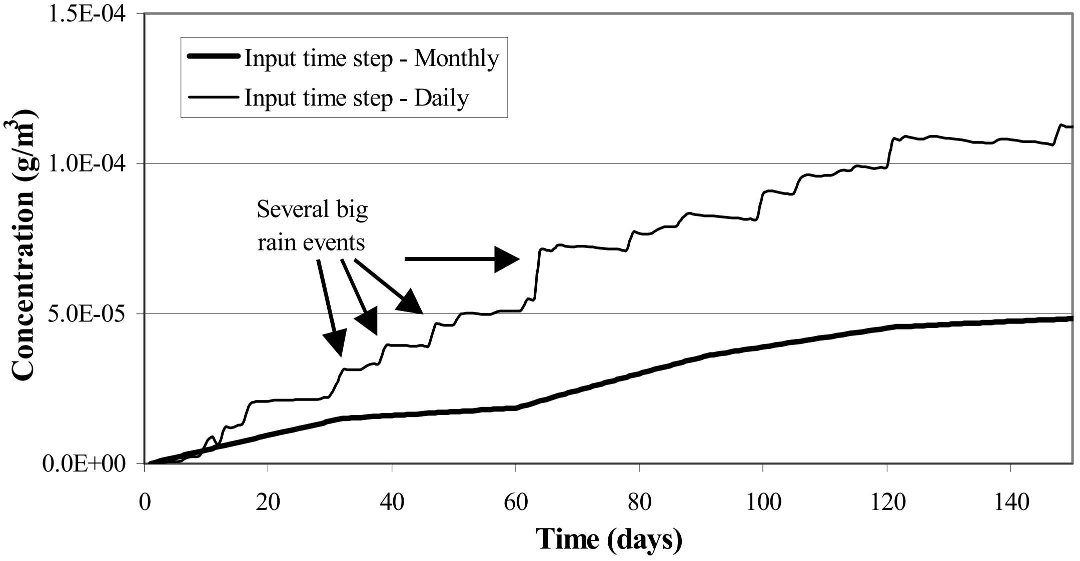
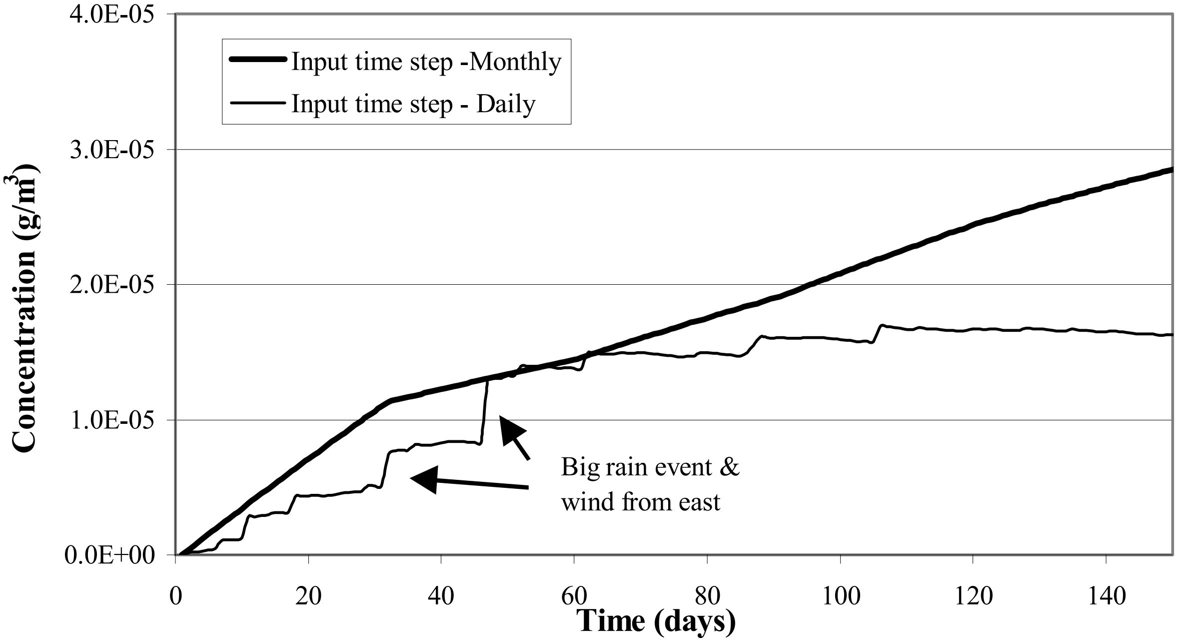


Figure 4-16
Benzo(a)pyrene Surface Soil Concentrations for Modeling Configuration C-Target Location



4.4.2 Mercury

This section presents the temporal complexity evaluation for mercury.

4.4.2.1 Model Setup for Mercury

The temporal complexity evaluation with mercury focused on methylmercury in surface water and aquatic biota. The temporal evaluation for mercury used the same modeling configuration used for the biotic complexity evaluation for mercury, which is shown in Figure 4-8. Biotic compartments in the model setup included:

- Terrestrial plants (leaves, particles on leaves, roots, and stems for grasses/herbs);
- Terrestrial ground-invertebrate feeder (shrew);
- Water column herbivore;
- Water column omnivore;
- Water column carnivore;
- Benthic invertebrate (mayfly);
- Benthic omnivore;
- Benthic carnivore;
- Semi-aquatic omnivore (raccoon); and
- Semi-aquatic piscivore (mink).

The model setup also included a constant source term of 1,300 g/day of 95 percent elemental and 5 percent divalent mercury. All initial mercury concentrations and boundary conditions were set equal to zero. Five-year simulations were run with a controlled meteorological data set. In separate runs, meteorological data were averaged for daily, monthly, and annual input averaging time steps.

4.4.2.2 Results

Results presented for this evaluation focus on surface water and fish, because exposure to methylmercury through fish ingestion is a primary focus for mercury human health risk assessment. Average mercury concentrations in the surface water compartment are presented in Table 4-16 and average methylmercury concentrations in fish are shown in Figure 4-17. Table 4-16 shows that, for this simple spatial configuration, the average concentrations of all mercury species in surface water increased slightly with increasing resolution of input averaging time steps. This relationship between input averaging time and surface water mercury concentrations appears to be magnified in the water column fish compartments, particularly in the water column carnivore compartment. Average mercury concentrations in the water column herbivore and carnivore fish compartments are presented in Table 4-17. Figures 4-17, 4-18, and 4-19 illustrate this relationship further. Figure 4-17 presents the concentrations of elemental and divalent mercury in surface water with daily, monthly and yearly input averaging times, and mercury concentrations in fish are presented in Figures 4-18 and 4-19, respectively. These results indicate that for a single air compartment, the mercury concentrations in underlying surface water did not vary greatly as the input averaging time was changed. However, input averaging time more significantly affected mercury concentrations in some fish compartments. In addition, as suggested in the multi-parcel temporal complexity analysis with benzo(a)pyrene (Section

4.4.1.2), changes in averaging time for input data may have had a greater impact if the modeling configuration was more spatially complex and/or a source compartment was included in the evaluation.

Table 4-16
Average Mercury Concentrations in Surface Water[a]

Input Averaging Time Step	Mercury Concentration (g/L)		
	Elemental Mercury	Divalent Mercury	Methylmercury
Daily	6.4E-05	5.7E-04	7.0E-06
Monthly	5.8E-05	5.7E-04	6.8E-06
Annual	5.2E-05	5.5E-04	6.6E-06

[a] Average concentrations are presented for the fifth year of the five-year simulation period.

Table 4-17
Average Methylmercury Concentrations in Water Column Fish[a]

Input Averaging Time Step	Methylmercury Concentration (g/kg)	
	Water Column Herbivore	Water Column Carnivore
Daily	3.9E-06	6.8E-06
Monthly	3.8E-06	6.4E-06
Annual	3.7E-06	4.1E-06

[a] Average concentrations are presented for the fifth year of the five-year simulation period.

Figure 4-17
Mercury Concentrations in Surface Water

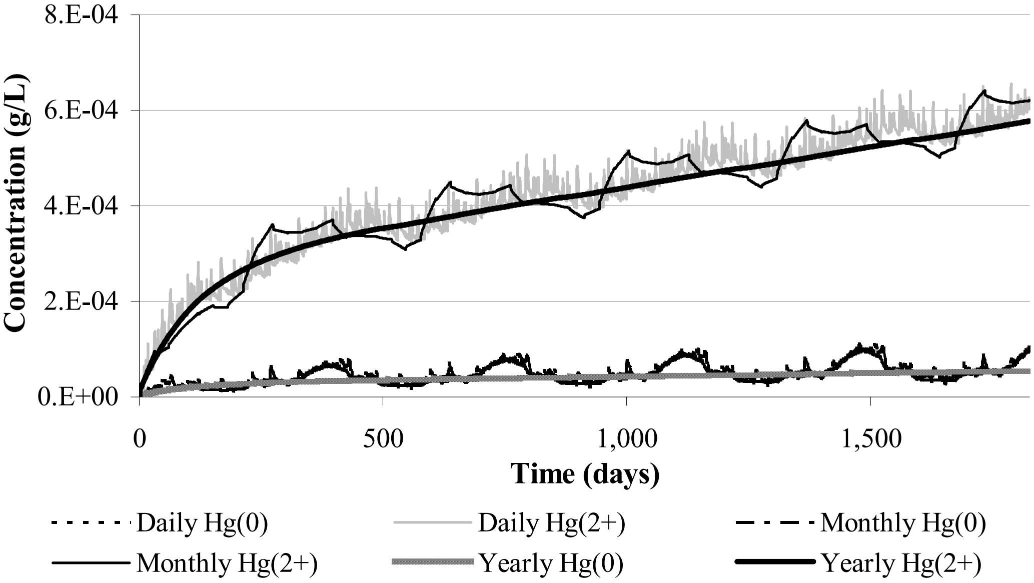


Figure 4-18
Divalent Mercury Concentrations in the Water Column Herbivore Compartment

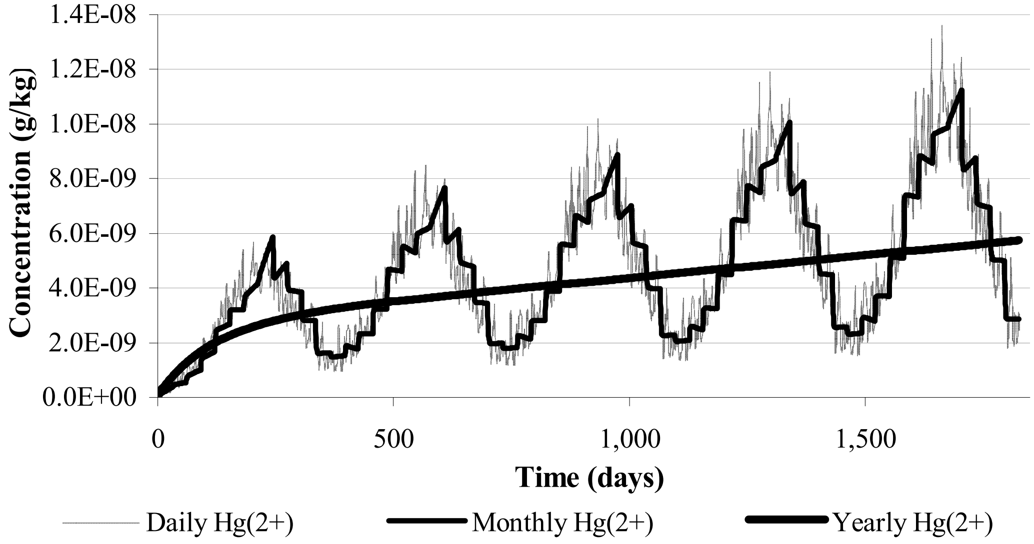
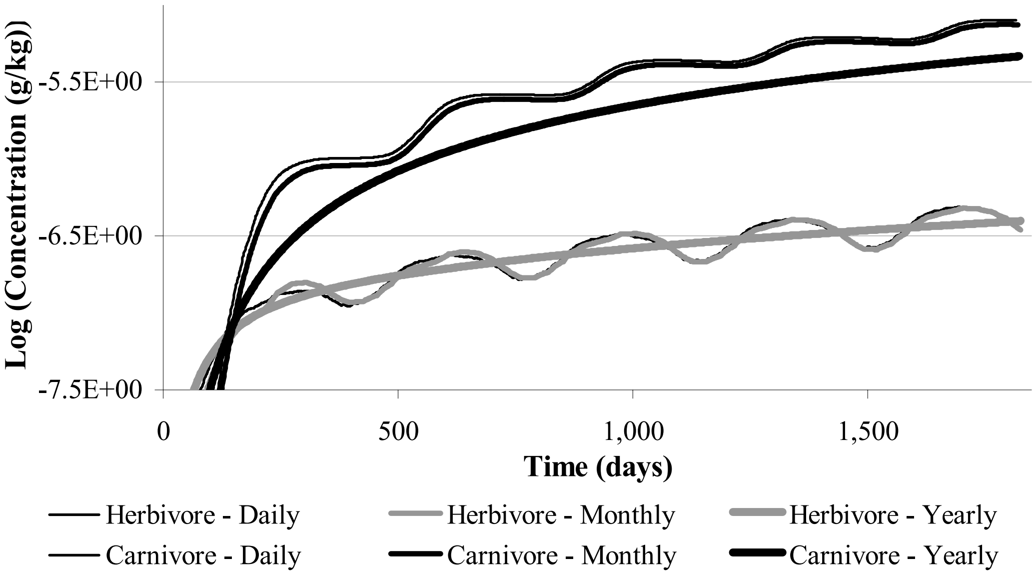


Figure 4-19
Methylmercury Concentrations in Water Column Herbivore and Carnivore Fish



4.5 SPATIAL COMPLEXITY EVALUATION

The spatial complexity evaluation examines how variations in parcel sizes, shapes, and configurations affect chemical concentrations estimated by TRIM.FaTE in surface soil and air. The evaluation is performed only for benzo(a)pyrene, and builds on the air parcel evaluation (Section 4.2) by considering transfers of this pollutant from the air parcel to surface soil. Specifically, the spatial complexity evaluation examines how predicted chemical concentrations are affected by four aspects of a hypothetical modeling configuration's design:

- The distance between source and target parcels;
- The number and size of parcels between the source and target parcels;
- The presence of boundary parcels surrounding the source and target parcels; and
- The size and configuration of the source parcel.

Each of the spatial complexity evaluations in this section compares predicted benzo(a)pyrene concentrations in the target parcels of various model scenarios. Except where otherwise noted, the only difference between the scenarios evaluated are the designs of the modeling configurations (e.g., the number and size of parcels between the source and target parcels). All scenarios included the following compartment types: lower air, surface soil, root soil, vadose soil, and grasses/herbs.

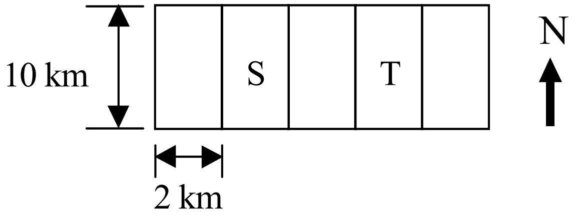
All scenarios were run with a controlled meteorological dataset. The meteorological conditions that varied in these data were wind direction, wind speed, rainfall, and temperature.

All scenarios included a constant one gram per second source of benzo(a)pyrene. The simulation period was six months for all scenarios.

4.5.1 Effect of Distance from Source

This section of the spatial complexity evaluation examines how predicted benzo(a)pyrene concentrations in surface soil are affected by the distance between the source and target parcels of the modeling configuration. The modeling configuration used for this section of the evaluation, shown in Figure 4-20, consists of five adjoining parcels, each of which is ten kilometers long by two kilometers wide. The benzo(a)pyrene source, which is represented by an "S" in Figure 4-20, is located in the second parcel from the west (i.e., left). The evaluation focuses on surface soil concentrations in a target parcel identified in Figure 4-20 with a "T."

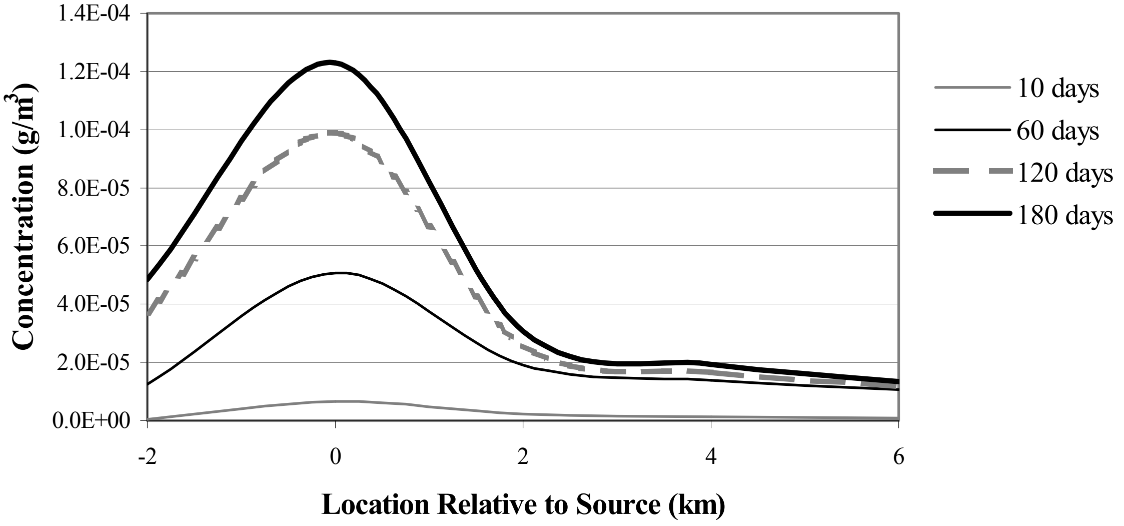
Figure 4-20
Modeling Configuration for the Evaluation of Effects of Distance From Source



Predicted benzo(a)pyrene concentrations in surface soil and air compartments of the target parcel are presented in Figure 4-21 and Figure 4-22, respectively. The concentrations are plotted for selected time intervals during the six-month simulation period. Distances are from the edge of the source parcel (i.e., distance zero).

Based on these results, the soil concentration accumulated over time with a fairly consistent profile. The concentrations in air were more variable than concentrations in soil, sometimes decreasing less rapidly with distance and at other times decreasing more rapidly. These differences were expected because the processes affecting estimates of mass in the air compartment are much more rapid, and therefore much more dynamic, than the processes affecting estimates of mass in the soil compartment. The estimates of mass in the soil compartment are less dependent than estimates of mass in the air compartment on current meteorological conditions.

Figure 4-21
Benzo(a)pyrene Concentrations in Surface Soil for Evaluation of Effects of Distance from Source[a]



[a] Although concentrations were calculated for each 20-day interval throughout the 180-day simulation period, only selected time intervals are plotted.

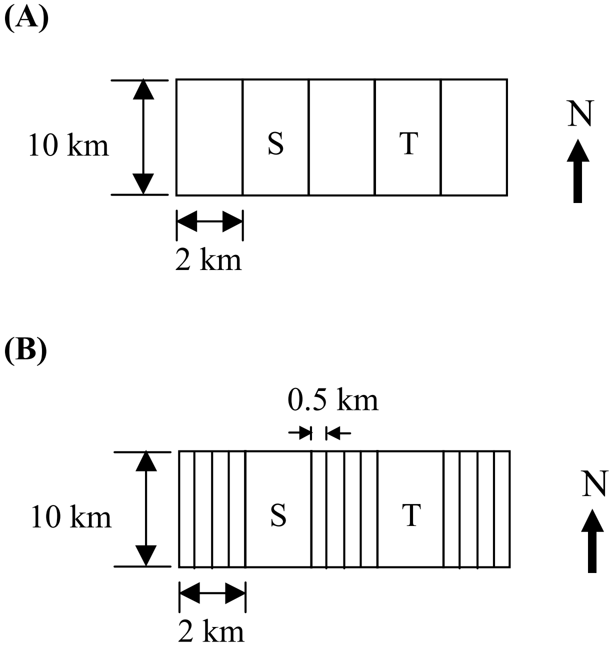
Figure 4-21 shows that estimated concentrations of benzo(a)pyrene in soil decreased by roughly 65 percent to 80 percent over the first two kilometers from the source. This indicates that concentrations in soil decreased more rapidly with distance from the source than was estimated previously (Bennett et al. 2000) based on the 30-kilometer characteristic travel distance (CTD) for benzo(a)pyrene. This difference was expected, however, based on differences between the spatial complexity analysis and the methods used to estimate the CTD. For example, the method used to develop the CTD assumed advection only in one direction, with no dispersive or advective losses in other directions. The TRIM.FaTE air compartment included advection in multiple directions, and the concentration was estimated to change with distance differently at each time step due to varying meteorological conditions. Because the TRIM.FaTE air compartment included advection in multiple directions, the rate of decrease in air concentrations, and thus deposition to the soil compartment, was more rapid than would be predicted based on the CTD's single-wind-direction method.

4.5.2 Effect of Horizontal Parcel Dimensions

This section of the spatial complexity evaluation examines how benzo(a)pyrene concentrations at the target parcel were affected by the horizontal dimensions of parcels between the source and target parcels. The distances between the source and target parcels are equal in the two modeling configurations developed for this evaluation, which are shown in Figure 4-23. In modeling configuration 4-23A, the source and target parcels are separated by a single parcel with a horizontal dimension of two kilometers. In modeling configuration 4-23B, the source and target parcels are separated by four parcels, each having a horizontal dimension of 0.5 kilometers.

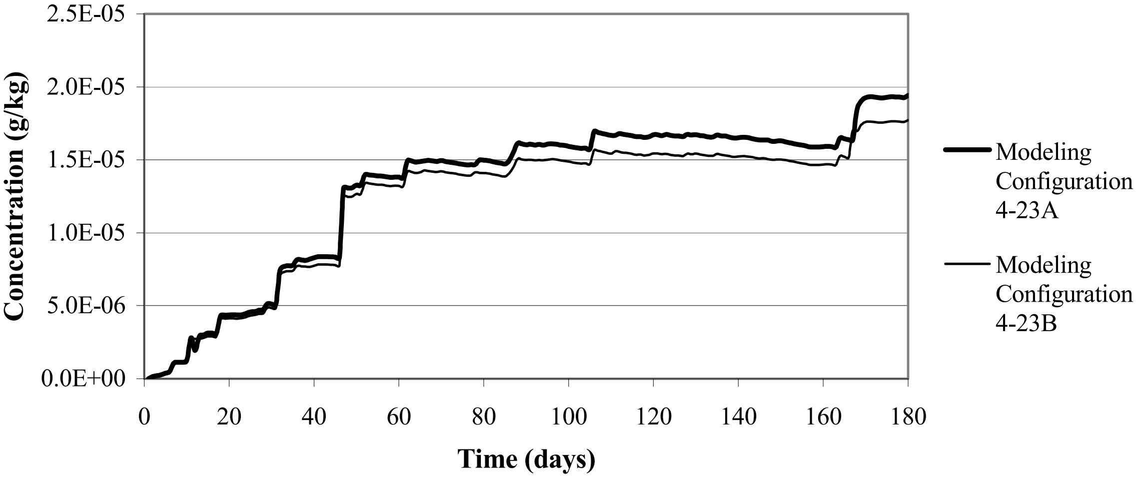
The predicted concentrations of benzo(a)pyrene in surface soil of the target parcels are plotted in Figure 4-24. The benzo(a)pyrene concentration in soil of the target parcel of modeling configuration 4-23A, in which the source and target parcels are separated by a single two-kilometer parcel, was slightly higher than the concentration in soil of the target parcel of modeling configuration 4-23B. Consideration of these results relative to the variance resulting from parameter uncertainty will inform next steps as to collection of additional parameter information and/or further evaluation of the effects observed here.

Figure 4-23
Modeling Configurations for Evaluation of the Effects of Horizontal Parcel Dimensions



Note: Not to scale

Figure 4-24
Benzo(a)pyrene Concentration in Surface Soil at Target Parcels of Modeling Configurations 4-23A and 4-23B



4.5.3 Effect of External Boundary Parcels

This section of the spatial complexity evaluation for benzo(a)pyrene examines how external boundary parcels surrounding internal parcels affect media concentrations in the internal parcels. It was expected that when boundary parcels were added, changes in wind direction could result in higher media concentrations in the internal parcels in some cases. For example, if the wind shifted a full 180-degrees, there would be advection of chemical mass directly back into the internal parcels. Shifts of less than 180 degrees but more than 90 degrees would result in advection of a lesser amount of contaminant mass back into the internal parcel. This evaluation compares the predicted benzo(a)pyrene concentrations in the target parcels of the modeling configurations in Figure 4-25, which have progressively increasing numbers of boundary parcels.

Figure 4-25
Modeling Configuration for Evaluation of Effects of External Boundary Parcels

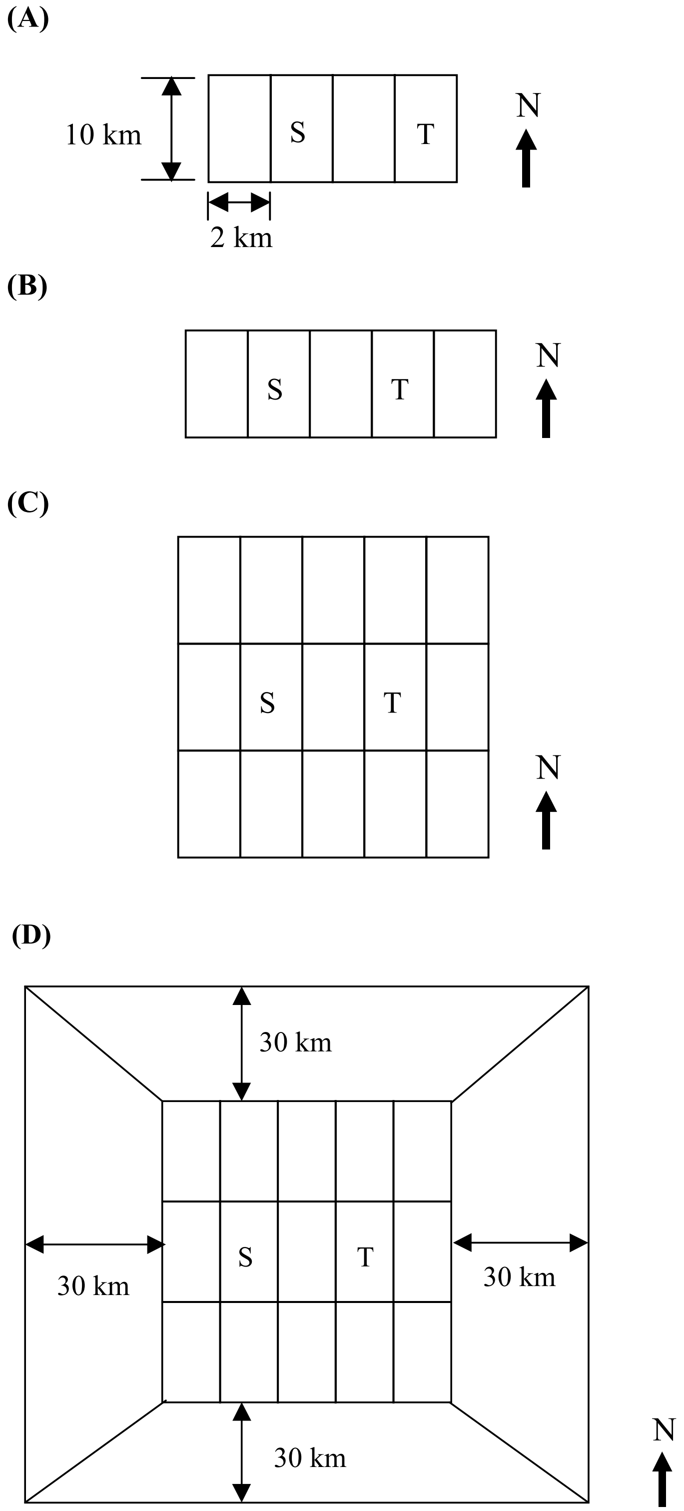


Table 4-18 presents the concentrations of benzo(a)pyrene predicted in air in the target parcels of each modeling configuration. Concentration estimates are presented for each of the first 22 days, as well as the daily averages for the first 22 days of the simulation period. Because the results were fairly consistent throughout the simulation period, daily results after the 22nd day are not presented. Ratios of the air concentrations predicted under various scenarios are included in Table 4-18 to facilitate comparison of the effects of the scenarios.

In all four modeling configurations, the average predicted benzo(a)pyrene concentration in air in the target parcel was approximately 3.1E-8 g/m^3. Daily predicted concentrations in the target parcel were equivalent in all four modeling configurations during 17 of the first 22 days of the simulation period. On the five days when winds were from the east (i.e., the target parcel was upwind from the source parcel) predicted concentrations in the target parcel differed as much as 88 percent among the four modeling configurations. However, the concentrations in the target parcel during these days were much lower than on days when winds blew from the west, and did not appear to significantly affect the average concentrations for the full simulation period.

Simulations for modeling configurations 4-25A and 4-25D were also compared without degradation included in the air compartment. The average air concentration in the target parcel of modeling configuration 4-25D (4.4E-8 g/m^3) was nearly identical to the average air concentration in the target parcel of modeling configuration 4-25A (4.3E-8 g/m^3). In this evaluation, adding border parcels to the modeling configuration did not greatly affect the average benzo(a)pyrene concentration predicted in the target parcel.

Table 4-18
Target Air Parcel Concentrations for Modeling Configurations 4-25A, B, C, and D (With Degradation)[a]

Time (Day)	Predicted Concentration in Air (g/m^3)				Scenario Ratios		
	4-25A	4-25B	4-25C	4-25D	4-25B/ 4-25A	4-25C/ 4-25A	4-25D/ 4-25A
1	0.0E+00	0.0E+00	0.0E+00	0.0E+00	--	--	--
2	3.4e-08	3.4E-08	3.4E-08	3.4E-08	1.0	1.0	1.0
3	5.1e-08	5.1E-08	5.1E-08	5.1E-08	1.0	1.0	1.0
4	2.2E-08	2.2E-08	2.2E-08	2.2E-08	1.0	1.0	1.0
5	4.5E-08	4.5E-08	4.5E-08	4.5E-08	1.0	1.0	1.0
6	5.7E-08	5.7E-08	5.7E-08	5.7E-08	1.0	1.0	1.0
7	4.1E-08	4.1E-08	4.1E-08	4.1E-08	1.0	1.0	1.0
8	6.1E-08	6.1E-08	6.1E-08	6.1E-08	1.0	1.0	1.0
9	8.9E-13	1.3E-12	1.4E-12	1.5E-12	1.4	1.5	1.6
10	6.9E-08	6.9E-08	6.9E-08	6.9E-08	1.0	1.0	1.0
11	4.3E-08	4.3E-08	4.3E-08	4.3E-08	1.0	1.0	1.0
12	2.6E-08	2.6E-08	2.6E-08	2.6E-08	1.0	1.0	1.0
13	6.6E-13	1.0E-12	1.0E-12	1.2E-12	1.5	1.6	1.8
14	3.2E-08	3.2E-08	3.2E-08	3.2E-08	1.0	1.0	1.0
15	9.5E-08	9.5E-08	9.5E-08	9.5E-08	1.0	1.0	1.0
16	7.3E-12	9.6E-12	1.1E-11	1.1E-11	1.3	1.5	1.6
17	1.5E-12	2.3E-12	2.5E-12	2.8E-12	1.5	1.7	1.9
18	2.4E-08	2.4E-08	2.4E-08	2.4E-08	1.0	1.0	1.0
19	1.7E-08	1.7E-08	1.7E-08	1.7E-08	1.0	1.0	1.0
20	2.2E-08	2.2E-08	2.2E-08	2.2E-08	1.0	1.0	1.0
21	1.0E-08	1.0E-08	1.0E-08	1.0E-08	1.0	1.0	1.0
22	9.9E-13	1.4E-12	1.4E-12	1.6E-12	1.4	1.4	1.6
Average	**3.1E-08**	**3.1E-08**	**3.1E-08**	**3.1E-08**	**1.0**	**1.0**	**1.0**

[a] Results are presented for the first 22 days of the simulation period. Similar results were observed after 22 days.

4.5.4 Effect of Source Parcel Size and Configuration

The effects of the size and configuration of the source parcel on benzo(a)pyrene concentrations in the target parcel were evaluated with the four modeling configurations shown in Figure 4-26. In modeling configuration 4-26A, the source is located in a 2 kilometer by 10 kilometer parcel. In modeling configuration 4-26B, the source is located in a smaller parcel within a 2 kilometer by 10 kilometer parcel. This modeling configuration allows the model to provide benzo(a)pyrene concentration estimates immediately adjacent to the source but in a separate parcel. Modeling configuration 4-26C includes two concentric parcels within the 2 kilometer by 10 kilometer parcel. In modeling configuration 4-26D, the source parcel is surrounded by four trapezoidal boundary parcels. Simulations for each modeling configuration were run for a 180-day modeling period.

Among the four modeling configurations, there was very little difference between the daily average benzo(a)pyrene concentrations in both the air and surface soil compartments. For example, the 180-day average benzo(a)pyrene concentrations in air of the target parcels of modeling configurations 4-26A and 4-26B were 2.4E-8 g/kg and 2.3E-8 g/kg, respectively. The 180-day average benzo(a)pyrene concentration surface soil of the target parcel was 1.3E-5 g/kg for both modeling configurations 4-26A and 2-26B (see Figure 4-27). Concentrations in the air and surface soil of the target parcels of modeling configurations 4-26C and 4-26D also were slightly lower than for modeling configuration 4-26A. Thus, among the simple modeling configurations used for this evaluation, the size and configuration of parcels did not appear to significantly affect air and soil concentrations in a common target parcel.

Figure 4-26
Modeling Configuration Evaluation of Effects of Source Parcel Size

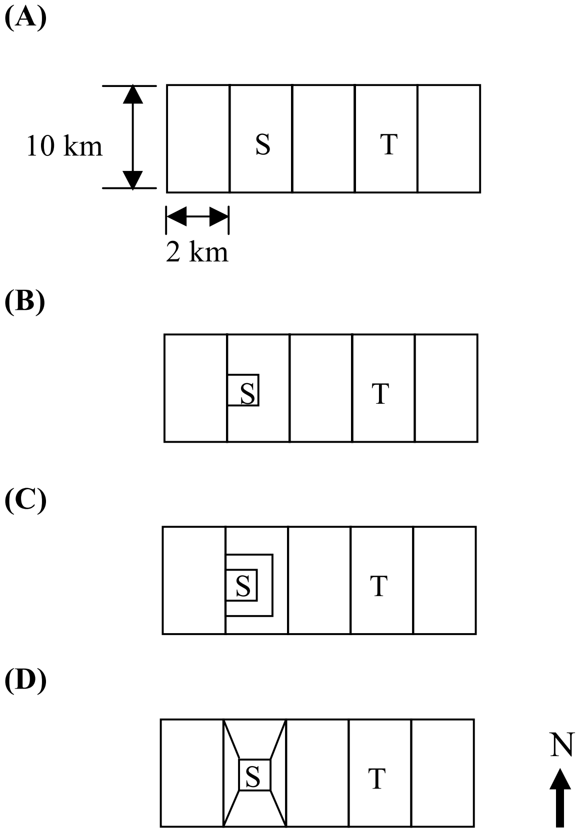
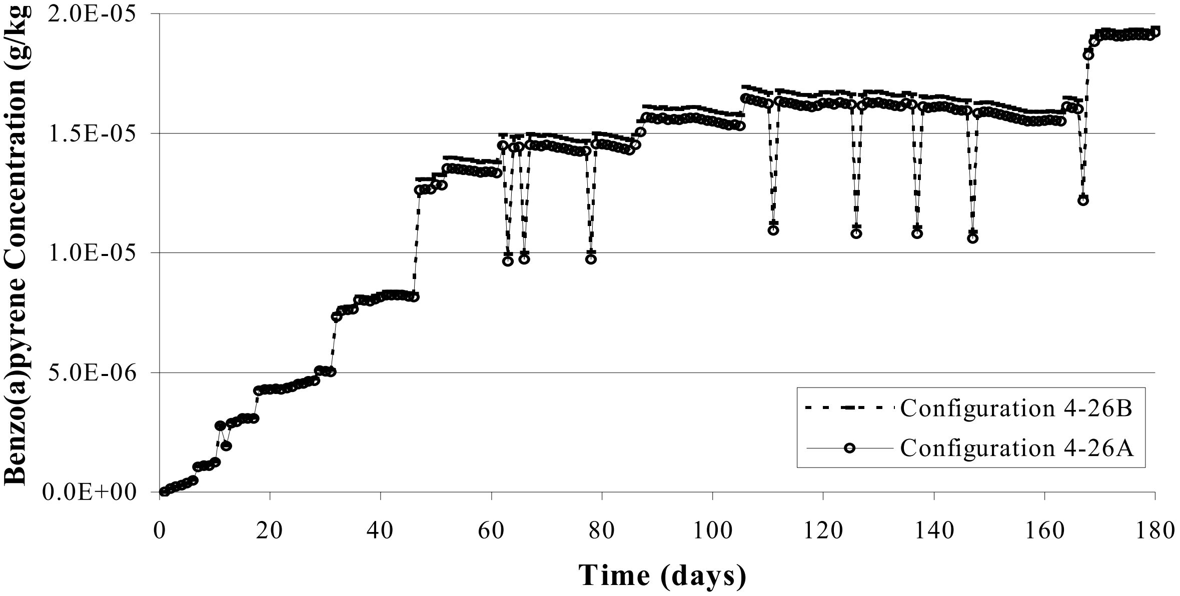


Figure 4-27
Surface Soil Concentrations in the Target Parcels of Modeling Configurations 4-26A and 4-26B



[This page intentionally left blank.]

5. REFERENCES FOR VOLUME I

Ambrose, R.A., Jr., T.A. Wool, and J.L. Martin. 1995. The Water Quality Analysis Simulation Program, WASP5. Part A: Model Documentation. Athens, GA: U.S. EPA National Exposure Research Laboratory, Ecosystems Division.

Arnold, J.R., R.L. Dennis, and G.S. Tonneson. 1998. Advanced techniques for evaluating Eulerian air quality models: Background and methodology. Presented at the 10th Joint Conference on the Applications of Air Pollution Meteorology with the A&WMA. Phoenix, Arizona, January 11-16, 1998.

Barr, J.F. 1996. Aspects of common loon (*Gavia immer*) feeding biology on its breeding ground. Hydrobiologia. 321:119-144.

Beck, M.B. and J. Chen. 2000. Assuring the quality of models designed for predictive tasks. In Handbook of Sensitivity Analysis, eds. A. Saltelli, K. Chan, and E.M. Scott (401-420). Chichester: John Wiley and Sons.

Beck, M.B. 1997. Water quality monitoring: A review of the analysis of uncertainty. Water Resources Research. 23(8):1393-1442.

Bennett, D.H., T.E. McKone, and R.G. Hetes. 2000a. Determining the appropriate level of model complexity [abstract]. Presented at the 21st Annual Meeting of the Society of Environmental Toxicology and Chemistry. Nashville, TN, November 12-16, 2000.

Bennett, D.H., D.F. Burch, R.M. Lee, B.F. Lyon, and D.L. Murphy. 2000b. Spatial resolution of TRIM.FaTE, a fate, transport, and ecological exposure model for air pollutants [abstract]. Presented at the 21st Annual Meeting of the Society of Environmental Toxicology and Chemistry. Nashville, TN, November 12-16, 2000.

Bennett, D.H., T.E. McKone, and W.E. Kastenberg. 2000. Characteristic time, characteristic travel distance, and population based potential dose in a multimedia environment: a case study. In Human and Ecological Risk Assessment: Theory and Practice, ed. D.J. Paustenbach. New York, NY: John Wiley and Sons.

Bennett, D.H., T.E. McKone, M. Matthies, and W.E. Kastenberg. 1998. General formulation of characteristic travel distance for semivolatile organic chemicals in a multimedia environment. Environ. Sci. Technol. 32:4023-4030.

Bennett, D.H., T.E. McKone, and M.G. Dusetzina. 1997. Building uncertainty and sensitivity analysis into the TRIM framework. Presented at the Annual Meeting of the Society of Risk Analysis. Washington, DC, December 7-10, 1997.

Biester, H., and C. Scholz. 1997. Determination of mercury phases in contaminated soils: mercury pyrolysis versus sequential extractions. Environ. Sci. Technol. 31:233-239.

Briggs, G.G., R.H. Bromilow, A.A. Evans, and M.R. Williams. 1983. Relationships between lipophilicity and the distribution of non-ionized chemicals in barley shoots following uptake by the roots. Pestic. Sci. 14:492-500.

Briggs, G.G., R.H. Bromilow, and A.A. Evans. 1982. Relationship between lipophilicity and root uptake and translocation of non-ionized chemicals by barley. Pestic. Sci. 13:495-504.

Bull, K.R., R.D. Roberts, M.J. Inskip, and G.T. Goodman. 1977. Mercury concentrations in soil, grass, earthworms and small mammals near an industrial emissions source. Environ. Pollut. 12:135-140.

Burch, D.F., R.M. Lee, B.F. Lyon, and D.L. Murphy. 2000. Model performance evaluation of TRIM.FaTE, a fate, transport, and ecological exposure model for air pollutants [abstract]. Presented at the 21st Annual Meeting of the Society of Environmental Toxicology and Chemistry. Nashville, TN, November 12-16, 2000.

Burken, J.G. and J.L. Schnoor. 1998. "Predictive Relationships for the Uptake of Organic Contaminants by Hybrid Poplar Trees," Environmental Science and Technology, 32 (21) 3379-3385.

CalTOX. 1993. CalTOX, A Multimedia Total-Exposure Model for Hazardous-Waste Sites. Background documentation prepared for California Environmental Protection Agency, the Office of Scientific Affairs, Department of Toxic Substances Control. December 1993.

Chamberlain, A.C. 1970. Interception and retention of radioactive aerosols by vegetation. Atmospheric Environment. 4:57-78.

Chen, J. and M.B. Beck. 1999. Quality Assurance of Multi-Media Model for Predictive Screening Tasks. U.S. Environmental Protection Agency, Athens, GA. Publication No. EPA/600/R-98/106.

Cohn, R.D. and R.L. Dennis. 1994. The evaluation of acid deposition models using principal component spaces. Atmospheric Environment. 28(15):2513-2543.

Cole, J.G. and D. Mackay. 2000. Correlating environmental partitioning properties of organic compounds: The three solubility approach. Environmental Toxicology and Chemistry. 19(2): 265-270.

Cousins, I. and D. Mackay. 2000. Correlating the physical-chemical properties of phthalate esters using the 'three solubility' approach. Chemosphere. 41(9):1389-1399.

Cowan, C.E., D. Mackay, T.C.J. Feijtel, D. van de Meent, A. DiGuardo, J. Davies, and N. Mackay. 1995. The Multi-Media Fate Model: A Vital Tool for Predicting the Fate of Chemicals. Pensacola, FL: SETAC Press.

Decisioneering. 1996. Crystal Ball Version 4.0 User Manual. Denver, CO: Decisioneering, Inc.

Dennis, R.L., W.R. Barchet, T.L. Clark, S.K. Seilkop, and P.M. Roth. 1990. Acid Deposition: State of Science and Technology, Report 5, Evaluation of Regional Acidic Deposition Models (Part I) and Selected Applications of RADM (Part II). National Acid Precipitation Assessment Program.

DiGiulio, R.T., and E.A. Ryan. 1987. Mercury in soils, sediments and clams from a North Carolina peatland. Water, Air, and Soil Pollution. 33:205-219.

Ebinghaus, R., S.G. Jennings, et al. 1999. International field intercomparison measurements of atmospheric mercury species at Mace Head, Ireland. Atmospheric Environment. 33(18): 3063-3073.

Efroymson, R.A. and D.L. Murphy. 2001. Ecological risk assessment of multimedia hazardous air pollutants: Estimating exposure and effects. Sci Total Environ. 274:219-230.

Efroymson, R.A., D.S. Jones, B.F. Lyon, D.H. Bennett, R.L. Maddalena, and D.L. Murphy. 2000. Biotic compartments in TRIM.FaTE, a fate, transport, and ecological exposure model for air pollutants. [abstract] Presented at the 21st Annual Meeting of the Society of Environmental Toxicology and Chemistry. Nashville, TN, November 12-16, 2000.

Efroymson, R.A., D.S. Jones, and A. Vasu. 1999. An ecological risk assessment methodology for hazardous air pollutants [abstract]. Presented at the 20th Annual Meeting of the Society of Environmental Toxicology and Chemistry. Philadelphia, PA, November 14-18, 1999.

Efroymson, R., B. Sample, C. Hunsaker, B. Lyon, A. Simcock, and G. Suter. 1997. A dynamic model for terrestrial ecological exposure to toxic air pollutants. Presented at the 18th Annual Meeting of the Society of Environmental Toxicology and Chemistry. San Francisco, CA, November 16-20, 1997.

Eisenberg, N., M. Federline, B. Sagar, G. Wittmeyer, J. Andersson, and S. Wingefors. 1995. Model validation from a regulatory perspective: A summary. In GEOVAL '94: Validation through model testing, OECD documents, safety assessment of radioactive waste repositories, Nuclear Energy Agency, Proceedings of an NEA/SKI Symposium. Paris, France, October 11-14, 1994.

EPRI. 1998. Mercury flux measurements: an intercomparison and assessment: Nevada mercury emissions project. Report TR-111346. Palo Alto, CA.

Fine, S.S., A.M. Eyth, B.F. Lyon, and T. Palma. 2000. The TRIM computer framework [abstract]. Presented at the 21st Annual Meeting of the Society of Environmental Toxicology and Chemistry. Nashville, TN, November 12-16, 2000.

Gnamuš, A., A. R. Byrne, and M. Horvat. 2000. Mercury in the soil-plant-deer-predator food chain of a temperate forest in Slovenia. *Environ. Sci. Technol.* 34:3337-3345.

Gonzalez, H. 1991. Mercury pollution caused by a chloralkali plant. Water, Air, Soil Pollut. 56:83-93.

Guha, S., S. Forbes, T.E. McKone, D.H. Bennett, and B.F. Lyon. 1997. A generalized, mass-conserving multimedia transport and transformation model: Development of transfer factors. Presented at the Annual Meeting of the Society of Risk Analysis, Washington, DC, December 7-10, 1997.

Habicht, F.H. 1992. Memorandum from the Deputy Administrator of the U.S. EPA. U.S. EPA, Office of the Administrator, Task Force on Environmental Regulatory Modeling. Washington, DC, March 7.

Hetes, R.G. and J.E. Langstaff. 2000. Estimation of uncertainty and variability within the total risk integrated methodology (TRIM) [abstract]. Presented at the 21st Annual Meeting of the Society of Environmental Toxicology and Chemistry. Nashville, TN, November 12-16, 2000.

Hodges, J.S. and J.A. Dewar. Is It You or Your Model Talking? A Framework for Model Validation. RAND Corporation, Santa Monica, CA, 1992. ISBN: 0-8330-1223-1.

Hoyer, M., J. Burke, et al. 1995. Atmospheric sources, transport and deposition of mercury in Michigan: Two years of event precipitation. Water Air and Soil Pollution. 80(1-4):199-208.

ICF Consulting. 2002. TRIM.FaTE Algorithm and Compartment Audit. Prepared by ICF Consulting for U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, October 2002.

Johnson, T., G.W. Suter, and T. Palma. 1997. TRIM.FaTE: A TRIM module for linking multimedia environmental systems with biotic domains. Presented at the Annual Meeting of the Society of Risk Analysis. Washington, DC, December 7-10, 1997.

Kelso, J.R.M. and M.G. Johnson. 1991. Factors related to the biomass and production of fish communities in small, oligotrophic lakes vulnerable to acidification. Canadian Journal of Fisheries and Aquatic Sciences. 48:2523-2532.

Konikow, L.F. and J.D. Bredehoeft. 1992. Ground-water models cannot be validated. Adv. Water Resour. 15(1):75-83.

Lin, C.J. and S.O. Pehkonen. 1999. Aqueous phase reactions of mercury with free radicals and chlorine: Implications for atmospheric mercury chemistry. Chemosphere. 38(6):1253-1263.

Lindberg, S.E. and W.J. Stratton. 1998. Atmospheric mercury speciation: Concentrations and behavior of reactive gaseous mercury in ambient air. Environmental Science & Technology. 32(1):49-57.

Lindberg, S.E., T.P. Meyers, et al. 1992. Atmosphere-surface exchange of mercury in a forest: Results of modeling and gradient approaches. Journal of Geophysical Research-Atmospheres. 97(D2):2519-2528.

Lindqvst, O., K. Johansson, M. Aastrup, A. Andersson, L. Bringmark, G. Hovsenius, L. Hakanson, A. Iverfeldt, M. Meili, and B. Timm. 1991. Mercury in the Swedish environment: recent research on causes, consequences and corrective methods. Water, Air, and Soil Pollution. 55(1-2):iii-261.

Lu, J.Y. and W.H. Schroeder. 1999. Sampling and determination of particulate mercury in ambient air: A review. Water, Air, and Soil Pollution. 112(3-4):279-295.

Lyon, B.F., T.E. McKone, and D.H. Bennett. 2000. Conceptual design and mass balance framework for TRIM.FaTE [abstract]. Presented at the 21st Annual Meeting of the Society of Environmental Toxicology and Chemistry. Nashville, TN, November 12-16, 2000.

Lyon, B.F., S. Guha, and T.E. McKone. 1997. TRIM: Mathematical and numerical aspects. Presented at the Annual Meeting of the Society of Risk Analysis. Washington, DC, December 7-10, 1997.

Mackay, K. 1991. Multimedia Environmental Models: The Fugacity Approach. Chelsea, MI: Lewis Publishers.

Maddalena, R.L., T.E. McKone, D.P.H. Hsieh, and S. Geng. 2001. Influential input classification in probabilistic multimedia models. Stochastic Environmental Research and Risk Assessment. 15(1):1-17.

Maddalena, R.L., D. H. Bennett, D. Murphy, and R.G. Hetes. 2000. Evaluation of a complex environmental model: the TRIM.FaTE example [abstract]. Presented at the 21st Annual Meeting of the Society of Environmental Toxicology and Chemistry. Nashville, TN, November 12-16, 2000.

McKone, T.E., S. Guha, T. Johnson, B. Lyon, G. Suter, and A. Vasu. 1997a. A multimedia health and ecological risk assessment methodology for air pollutants. Presented at the 18th Annual Meeting of the Society of Environmental Toxicology and Chemistry. San Francisco, CA, November 16-20, 1997.

McKone, T.E., T. Johnson, G.W. Suter II. 1997b. Estimating multi-pathway human and ecosystem exposures within the total risk integrated model (TRIM). Presented at the Annual Meeting of the Society of Risk Analysis. Washington, DC, December 7-10, 1997.

McKone, T. E. 1993. CalTOX, A Multimedia Total-Exposure Model for Hazardous-Wastes Sites Part II: The Dynamic Multimedia Transport and Transformation Model. Livermore, CA, prepared for the State of California, Department of Toxic Substances Control, Lawrence Livermore National Laboratory.

McKone, T.E. 1993a. CalTOX, A multimedia total-exposure model for hazardous-wastes sites Part I: Executive Summary. Laboratory. UCRL-CR-111456PtI. Livermore, CA: Lawrence Livermore National Laboratory.

McKone, T.E. 1993b. CalTOX, A multimedia total-exposure model for hazardous-wastes sites Part II: The dynamic multimedia transport and transformation model. UCRL-CR-111456PtII. Livermore, CA: Lawrence Livermore National Laboratory.

McKone, T.E. 1993c. CalTOX, A multimedia total-exposure model for hazardous-wastes sites Part III: The multiple-pathway exposure model. UCRL-CR-111456PtIII. Livermore, CA: Lawrence Livermore National Laboratory.

Muller, H., and G., Prohl. 1993. Ecosys-87: A dynamic model for assessing radiological consequences of nuclear accidents. Health Phys. 64:232-252.

Murphy, D.L., R.L. Maddalena, J. Langstaff, D.S. Jones, L.M. Lee, A.M. Eyth, B.F. Lyon, M. McVey, and G. Laniak. 2000. Evaluation of the TRIM.FaTE multi-media model: a mercury case study [abstract]. Presented at the Joint Meeting of the Society of Exposure and Analysis and the International Society of Environmental Epidemiology. Vancouver, Canada, August 11-15, 2002.

Murphy, D.L., T. Palma, R.G. Hetes, H.M. Richmond, and A.B. Vasu. 2000. Total risk integrated methodology (TRIM): focus on the fate, transport and ecological exposure module (TRIM.FaTE) [abstract]. Presented at the 21st Annual Meeting of the Society of Environmental Toxicology and Chemistry. Nashville, TN, November 12-16, 2000.

Nobel, Park S. 1999. Physicochemical and Environmental Plant Physiology, 2nd edition, Academic Press.

Oreskes, N., K. Shrader-Frechette, K. Belitz. 1994. Verification, validation, and confirmation of numerical models in the earth sciences. Science. 263:641-646.

Pai, P., S. Heisler, et al. 1998. An emissions inventory for regional atmospheric modeling of mercury. Water, Air, and Soil Pollution. 101(1-4):289-308.

Palma, T., A. Vasu, and R. Hetes. 1999. Total risk integrated methodology (TRIM). Air and Waste Management Association - EM Magazine. March 1999,30-34.

Park, R. A. 1998. AquaTOX for Windows: A modular toxic effects model for aquatic ecosystems. Draft. EcoModeling, Montgomery Village, MD.

Pleijel, K. and J. Munthe. 1995a. Modeling the atmospheric chemistry of mercury: The importance of a detailed description of the chemistry of cloud water. Water, Air, and Soil Pollution. 80(1-4):317-324.

Pleijel, K. and J. Munthe. 1995b. Modeling the atmospheric mercury cycle: Chemistry in fog droplets. Atmospheric Environment. 29(12):1441-1457.

Radhakrishnan, K. and A.C. Hindmarsh. 1993. Description and Use of LSODE, the Livermore Solver for Ordinary Differential Equations. LLNL report UCRL-ID-113855, December 1993.

Reiderer, M. 1995. Partitioning and transport of organic chemicals between the atmospheric environment and leaves. In: Plant Contamination: Modeling and Simulation of Organic Chemical Processes. eds. S. Trapp and J.C. McFarlane (153-190). Boca Raton: Lewis Publishers.

Revis, N.W. et al. 1989. Distribution of mercury species. Water, Air and Soil Pollution. 45(1-2): 105-113.

Schatzmann, M., S. Rafailidis, and M. Pavageau. 1997. Some remarks on the validation of small-scale dispersion models with field and laboratory data. Journal of Wind Engineering and Industrial Aerodynamics. 67(8):885-893.

Schroeder, W.H., J. Munthe, et al. 1989. Cycling of mercury between water, air, and soil compartments of the environment. Water, Air, and Soil Pollution. 48(3-4):337-347.

Schwarzenbach, R.P., P.M. Gschwend, and D.M. Imboden. 1993. Environmental Organic Chemistry. New York, NY: John Wiley and Sons.

Spear, C.R. 1997. Large simulation models: Calibration, uniqueness and goodness of fit. Environmental Modeling and Software. 12:219-228.

Talmage, S.S. and B. T. Walton. 1993. Food chain transfer and potential renal toxicity of mercury to small mammals at a contaminated terrestrial field site. Ecotoxicol. 2:243-256.

Taylor, A.C. 1993. Using objective and subjective information to develop distributions for probabilistic exposure assessment. Journal of Exposure Analysis and Environmental Epidemiology. 3:285-298.

U.S. EPA. 2002a. U.S. Environmental Protection Agency. TRIM.FaTE Technical Support Document Volume I: Description of Module. EPA-453/R-02-011a. Research Triangle Park, NC: Office of Air Quality Planning and Standards. September.

U.S. EPA. 2002b. U.S. Environmental Protection Agency. TRIM.FaTE Technical Support Document Volume II: Description of Chemical Transport and Transformation Algorithms. EPA-453/R-02-011b. Research Triangle Park, NC: Office of Air Quality Planning and Standards. September.

U.S. EPA. 2000. U.S. Environmental Protection Agency. An SAB Advisory on the Agency's "Total Risk Integrated Methodology (TRIM)." EPA-SAB-EC-ADV-00-004. Washington, DC: Science Advisory Board. May.

U.S. EPA. 1999a. U.S. Environmental Protection Agency. Total Risk Integrated Methodology Status Report. EPA-453/R-99-010. Research Triangle Park, NC: Office of Air Quality Planning and Standards. November.

U.S. EPA. 1999b. U.S. Environmental Protection Agency. TRIM.Expo Technical Support Document. External Review Draft. EPA-453/D-99-001. Research Triangle Park, NC: Office of Air Quality Planning and Standards. November.

U.S. EPA. 1999c. U.S. Environmental Protection Agency. TRIM.FaTE Technical Support Document Volume I: Description of Module. External Review Draft. EPA-453/D-99-002A. Research Triangle Park, NC: Office of Air Quality Planning and Standards. November.

U.S. EPA. 1999d. U.S. Environmental Protection Agency. TRIM.FaTE Technical Support Document Volume II: Description of Chemical Transport and Transformation Algorithms. External Review Draft. EPA-453/D-99-002B. Research Triangle Park, NC: Office of Air Quality Planning and Standards. November.

U.S. EPA. 1999e. U.S. Environmental Protection Agency. National air toxic program: the integrated urban strategy. Federal register 64: 38705-38740. July 19.

U.S. EPA. 1998a. U.S. Environmental Protection Agency. An SAB Advisory on the TRIM.FaTE Moesl of the Total Risk Integrated Methodology. EPA-SAB-EC-ADV-99-003. Washington, DC: Science Advisory Board. December.

U.S. EPA. 1998b. U.S. Environmental Protection Agency. Total Risk Integrated Methodology, Implementation of the TRIM Conceptual Design Through the TRIM.FaTE Module, A Status Report. EPA-452/R-98-001. Research Triangle Park, NC: Office of Air Quality Planning and Standards. March.

U.S. EPA. 1998c. U.S. Environmental Protection Agency. Study of hazardous air pollutants from electric utility steam generating units-final report to congress. EPA 453/R-989-004a. Office of Air Quality Planning and Standards. February.

U.S. EPA. 1998d. U.S. Environmental Protection Agency. The total risk integrated methodology: technical support document for the TRIM.FaTE module. Draft. EPA-452/D-98-001. Office of Air Quality Planning and Standards.

U.S. EPA. 1998e. U.S. Environmental Protection Agency. Methodology for assessing health risks associated with multiple exposure pathways to combustor emissions. External Review Draft. Update to EPA/600/6-90/003. NCEA-C-0238. National Center for Environmental Assessment.

U.S. EPA. 1998f. White Paper on the Nature and Scope of Issues on Adoption of Model Use and Acceptability Guidance. External Review Draft. Washington, DC: Science Policy Council.

U.S. EPA. 1997. U.S. Environmental Protection Agency. Mercury study report to congress (Volumes I-VIII). EPA-452/R-97-005. Office of Air Quality Planning and Standards.

U.S. EPA. 1997b. U.S. Environmental Protection Agency. Mercury study report to congress. Volume V: health effects of mercury and mercury compounds. U.S. EPA Office of Air Quality Planning and Standards, and Office of Research and Development.

U.S. EPA. 1994a. U.S. Environmental Protection Agency. Report of the agency task force on environmental regulatory modeling. Guidance, support needs, draft criteria and charter. EPA 500-R-94-001. Washington, DC: Office of Solid Waste and Emergency Response.

U.S. EPA. 1994b. U.S. Environmental Protection Agency. Review of draft "addendum to the methodology for assessing health risk associated with indirect exposure to combustor emissions". EPA-SAB-1AQC-94-009B. Washington, DC: Science Advisory Board.

U.S. EPA. 1989. Resolution on the Use of Mathematical Models by EPA for Regulatory Assessment and Decision Making. EPA-SAB-EEC-89-012. Washington, DC, Science Advisory Board, Environmental Engineering Committee.

Vasu, A.B., R.G. Hetes, T. Palma, and T.E. McKone. 1998. TRIM: a multimedia, multipathway framework for assessing human and ecological exposure and risk. Presented at the 19th Annual Meeting of the Society of Environmental Toxicology and Chemistry. Charlotte, NC, November 15-19, 1998.

Vasu, A., M. Dusetzina, R. Hetes, T. Palma, H. Richmond, T. McKone, and T. Johnson. 1997. Introduction to the total risk integrated methodology (TRIM). Presented at the Annual Meeting of the Society of Risk Analysis. Washington, DC, December 7-10, 1997.

Wagrowski, D.M., and R.A. Hites. 1997. Polycyclic aromatic hydrocarbon accumulation in urban, suburban, and rural vegetation. Environ. Sci. Technol, 31:279-282.

Wang, W. and C.T. Driscoll. 1995. Patterns of total mercury concentrations in Onondaga Lake, New York. Environ. Sci. Technol. 29:2261-2266.

Watras, C.J., K.A. Morrison, J.S. Host, and N.S. Bloom. 1995. Concentration of mercury species in relationship to other site-specific factors in the surface waters of northern Wisconsin lakes. Limnol. Oceanogr. 40:556-565.

Wren, C.D., H.R. Maccrimmon, and B.R. Loescher. 1983. Examination of bioaccumulation and biomagnification of metals in a Precambrian shield lake. Water, Air Soil Pollut. 19:277-291.

Xiao, Z., J. Sommar, et al. 1998. Atmospheric mercury deposition to grass in southern Sweden. Science of the Total Environment. 213(1-3):85-94.

Zimmer, R., J. Dee, D. Jones, B. Sample, and G. Suter. 1997. Use of EcoFaTE in modeling pollutant mass transfers and subsequent risks within aquatic systems. Presented at the 18th Annual Meeting of the Society of Environmental Toxicology and Chemistry. San Francisco, CA, November 16-20, 1997.

[This page intentionally left blank.]

APPENDIX I-A

TRIM.FaTE ALGORITHM PAIRING TABLES

[This page intentionally left blank.]

APPENDIX I-A
TRIM.FaTE ALGORITHM PAIRING TABLES[a]

PAIRED ALGORITHMS (TRANSFER FROM ONE COMPARTMENT TO ANOTHER AND THE REVERSE TRANSFER)

ALGORITHMS FOR EXCHANGES BETWEEN COMPARTMENTS OF THE SAME TYPE

1. **Algorithm: Advection from Air to Air** [all chemicals] [TF 3-1][b]	To reverse the direction of the flow, the receiving and sending compartments are switched (with the exception of erosion of surface soil to surface soil, or runoff from surface soil to surface soil, for which the processes occur in the down-gradient direction only). Diffusion of contaminants between soil compartments of the same type occurs only in the root-zone soil and vadose-zone soil compartments.
148. Algorithm: Runoff from Surface Soil to Surface Soil [all chemicals] (occurs in the down-gradient direction only) [TF 5-10a]	
50. Algorithm: Erosion from Surface Soil to Surface Soil [all chemicals] (occurs in the down-gradient direction only) [TF 5-11a]	
129. Algorithm: Percolation from Root Zone to Root Zone [all chemicals] [TF 5-9]	
133. Algorithm: Percolation from Vadose Zone to Vadose Zone [all chemicals] [TF 5-9]	
44. Algorithm: Dispersive Waterflow from Surface Water to Surface Water, General [all chemicals] [TF 4-12]	
169. Algorithm: Waterflow from Surface Water to Surface Water [all chemicals] (occurs in the downgradient direction only) [TF 4-9]	
134. Algorithm: Pore Water Diffusion from Sediment to Sediment [all chemicals] [TF 4-13]	

TWO-WAY TRANSFERS	
EXCHANGES BETWEEN AIR AND PLANT LEAVES, SURFACE SOIL, AND SURFACE WATER	
Diffusive Transfers	
31. Algorithm: Diffusion from Air to Plant Leaf [all chemicals except divalent mercury] [TF 7-9a]	**34. Algorithm: Diffusion from Plant Leaf to Air, Default** [all chemicals, except divalent mercury] [TF 7-8a]
32. Algorithm: Diffusion from Air to Surface Soil [all chemicals except divalent mercury] [TF 5-1]	**38. Algorithm: Diffusion from Surface Soil to Air** [all chemicals, except divalent mercury] [TF 5-2]
33. Algorithm: Diffusion from Air to Surface Water, Two Film [all chemicals, except divalent mercury] [TF 3-2]	**40. Algorithm: Diffusion from Surface Water to Air, Two Film** [all chemicals, except divalent mercury] [TF 3-3]
Air Deposition of Vapors and Particles and Resuspension/Washoff of Same	
On and Off Plant Leaves	
172. Algorithm: Wet deposition of vapor phase to Plant Leaf from Air, Organics [TF 7-7b] (The remainder is wet deposited to the soil, #172b, a new algorithm)	Algorithm # 34 [TF 7-8] (diffusion algorithm, see above) is the only instance of the reverse transfer, from plant leaf to air for the vapor phase.
173. Algorithm: Wet deposition of vapor phase to Plant Leaf from Air [divalent and elemental mercury only] [TF 7-7a] (The remainder is wet deposited to the soil, #174)	
46b. [NEW] Algorithm: Dry deposition of vapor from air to plant leaf [= net deposition; divalent mercury only] [TF A-3]	
48b. Algorithm: Dry Deposition of particles to plant leaf [, i.e., to leaf particle compartment] [new] [all chemicals] [TF 7-1] (the remainder is dry deposited on the soil, #48)	**126. Algorithm: Particles Blown off from Plant Leaf to Air (DRY)** [all chemicals] [TF 7-2]
177b. Algorithm: Wet deposition of particles to plant leaf [i.e., to leaf particle compartment] [new] [all chemicals] [TF 7-3] (the remainder is wet deposited to the soil, #177)	**128. Algorithm: Particles washed off leaf onto ground** [all chemicals] [TF 7-4]
164. Algorithm: Transfer from Leaf Particle on surface to leaf [all chemicals] [TF 7-5]	**165. Algorithm: Transfer from Leaf to Leaf Particle on surface** [all chemicals] [TF 7-6]

Between Air and Soil	
172b. Algorithm: Wet deposition of vapor phase to soil for organics [new] [TF 5-5a] (Some is intercepted by the plant leaves, #172.)	Algorithm # 38 [TF 5-2] (diffusion algorithm, see above) is the only instance of the reverse transfer, from soil to air for the vapor phase.
174. Algorithm: Wet deposition of vapor phase to Soil [elemental and divalent mercury] [TF 5-5b] (Some is intercepted by the plant leaves, #173.)	
46. Algorithm: Dry deposition of vapor from air to surface soil [divalent mercury] [TF A-2] (Some is intercepted by plant leaves, #46b)	
48. Algorithm: Dry Deposition to soil of particles [all chemicals][TF 5-3] (Some of the dry deposition is intercepted by plants, #48b.)	**147. Algorithm: Resuspension from Surface Soil to Air, Set to Deposition rate of particles** [all chemicals][TF 5-6]
177. Algorithm: Wet deposition to soil of particles [all chemicals] [TF 5-4] (Some of the wet deposition of particles is intercepted by plants, # 177b.)	
Between Air and Surface Water	
171. Algorithm: Wet Deposition of Vapor from Air to Surface Water Organics [TF 4-3a]	Algorithm # 40 (diffusion algorithm, see above) is the only instance of the reverse transfer, from surface water to air for the vapor phase.
175. Algorithm: Wet deposition of vapor phase to Surface water [elemental and divalent mercury] [TF 4-3b]	
47. Algorithm: Dry deposition of vapor from air to surface water [= net deposition; divalent mercury only] [TF A-1]	
45. Algorithm: Dry Deposition of Particles from Air to Surface Water [all chemicals][TF 4-1b]	There is no "reverse" process. Particles in the surface water can be deposited to sediments (#151) and resuspended into the surface water (#146).
170. Algorithm: Wet Deposition of Particles from Air to Surface Water [all chemicals][TF 4-2b]	

EXCHANGES BETWEEN SOIL LAYERS AND SOIL BIOTA (ROOTS AND SOIL INVERTEBRATES)	
Vertical Exchanges between Soil Compartments	
43a. Algorithm: Diffusion downward from higher Vadose Zone to lower Vadose Zone [all chemicals] [TF 5-7]	**43b. Algorithm: Diffusion upward from lower Vadose Zone to higher Vadose Zone** [all chemicals] [TF 5-8]
43c. Algorithm: Diffusion downward from higher Root-zone Soil to lower Root-zone Soil [all chemicals] [TF 5-7]	**43d. Algorithm: Diffusion upward from lower Root-zone Soil to higher Root-zone Soil** [all chemicals] [TF 5-8]
Between Soil and Soil Biota	
158. Algorithm: Time-dependent partition from root zone [soil] to root, Interacts with bulk soil [for all three mercury species] [TF 7-10a]	**155. Algorithm: Time-dependent partition from root to root zone [soil], Interacts with bulk soil** [for all three mercury species]
159. Algorithm: Time-dependent partition from root zone [soil] to root, Interacts with soil pore water [for organics only] [TF 7-10b]	**156. Algorithm: Time-dependent partition from root to root zone [soil], Interacts with soil pore water** [for organics only]
167. Algorithm: Transfer from root zone bulk soil to stem [for all chemicals] [TF 7-12a]	No match for transfer in the reverse direction.
167b. Algorithm: Transfer from root-zone soil pore water to stem, for organic chemicals [TF 7-12b1] [not in current library]	**167c. Algorithm: Transfer from stem root-zone soil pore water**, for organic chemicals] [TF 7-12b2] [not in current library]
157. Algorithm: Time-dependent partition from Root Zone to arthropod [bulk soil] [all chemicals] [TF 7-19]	**152. Algorithm: Time-dependent partition from arthropod to Root Zone [bulk soil]** [all chemicals] [TF 7-20]
160. Algorithm: Time-dependent partition from Root Zone to Worm, Interacts with bulk soil [all mercury species] [TF 7-17a]	**163. Algorithm: Time-dependent partition from worm to Root Zone, Interacts with bulk soil** [all mercury species] [TF 7-18a]
160b. Algoirthm: Time-dependent partition from Root Zone to Worm, Interacts with soil pore water [organics] [TF 7-17b]	**163b. Algoirthm: Time-dependent partition from Worm to Root Zone, Interacts with soil pore water** [organics] [TF 7-18b]

Between Soil Compartments, Diffusion, Percolation to Ground Water, and GW Recharge to Surface Water	
39. Algorithm: Diffusion from Surface Soil to Root Zone [all chemicals] [TF 5-7]	**35. Algorithm: Diffusion from Root Zone to Surface Soil** [all chemicals] [TF 5-8]
36. Algorithm: Diffusion from Root Zone to Vadose Zone [all chemicals] [TF 5-7]	**42. Algorithm: Diffusion from Vadose Zone to Root Zone** [all chemicals] [TF 5-8]
131. Algorithm: Percolation from Surface Soil to Root Zone [all chemicals] [TF 5-9]	Percolation is a one-way process (down). Diffusion works both up and down through the soil column. **135. Algorithm: Recharge from GW to Surface Water** [TF 5-13]
130. Algorithm: Percolation from Root Zone to Vadose Zone [all chemicals] [TF 5-9]	
132. Algorithm: Percolation from Vadose Zone to GW [all chemicals] [TF 5-12]	
EXCHANGES BETWEEN SURFACE WATER, SEDIMENTS, AND BIOTA	
151. Algorithm: Sediment deposition from surface water to sediment [all chemicals] [TF 4-4]	**146. Algorithm: Resuspension from Sediment to Surface Water** [all chemicals] [TF 4-5]
2. Algorithm: Algae deposition from surface water to sediment [all chemicals] [TF 4-6]	
37. Algorithm: Diffusion from Sediment to Surface Water, Fugacity-based [all chemicals] [TF 4-10]	**41. Algorithm: Diffusion from Surface Water to Sediment, Fugacity-based** [all chemicals] [TF 4-11]
49. Algorithm: Elimination from fish to surface water [all three mercury species] [TF A-4]	No significant uptake of mercury directly from surface water by fish.
56. Algorithm: Exchange from fish to surface water, organics [TF 6-8]	**52. Algorithm: Exchange from surface water to fish,** organics [TF 6-5]
53. Algorithm: Exchange from macrophyte to surface water [organics only] [TF 6-2a]	**57. Algorithm: Exchange from surface water to macrophyte** [organics only] [TF 6-1a]
153. Algorithm: Time-dependent Partition from macrophyte to surface water [all three mercury species] [TF 6-2b]	**162. Algorithm: Time-dependent Partition from surface water to macrophyte** [all three mercury species] [TF 6-1b]
54. Algorithm: Exchange from benthic invertebrate to sediment [pore water] [organics only] [TF 6-4a]	**55. Algorithm: Exchange from sediment to benthic invertebrate [pore water]** [organics only][TF 6-3a]

154. Algorithm: Time-dependent Partition from benthic invertebrate to sediment [all three mercury species only] (TSD Equation 7-106) [TF 6-4b]	**161. Algorithm: Time-dependent Partition from sediment to benthic invertebrate** [all three mercury species only] (TSD Equation 7-107) [TF 6-3b]
DEMETHYLATION AND METHYLATION REACTIONS FOR MERCURY	
21. Algorithm: Demethylation (MHg->Hg2) rate in air [TF A-8]	**104. Algorithm: Methylation(Hg2 -> MHg) in air** [TF A-7]
22. Algorithm: Demethylation (MHg->Hg2) in birds [TF A-8]	**105. Algorithm: Methylation (Hg2->MHg) in birds** [TF A-7]
25. Algorithm: Demethylation (MHg->Hg2) in mammals [TF A-8]	**108. Algorithm: Methylation (Hg2->MHg) in mammals** [TF A-7]
20. Algorithm: Demethylation(Hg2 -> MHg) in plant [leaf] [TF A-8]	**109. Algorithm: Methylation(Hg2 -> MHg) in plant leaves** [TF A-7]
20. Algorithm: Demethylation(Hg2 -> MHg) in plant [stem] [TF A-8]	**110. Algorithm: Methylation(Hg2 -> MHg) in plant stem** [TF A-7]
No apparent demethylation in plant roots.	No apparent methylation in plant roots.
28. Algorithm: Demethylation(MHg -> Hg2) in surface soil [TF A-8]	**113. Algorithm: Methylation(Hg2 -> MHg) in surface soil** [TF A-7]
26. Algorithm: Demethylation(MHg -> Hg2) in root zone [TF A-8]	**111. Algorithm: Methylation(Hg2 -> MHg) in root zone** [TF A-7]
30. Algorithm: Demethylation(MHg -> Hg2) in vadose zone [TF A-8]	**115. Algorithm: Methylation(Hg2 -> MHg) in vadose zone** [TF A-7]
24. Algorithm: Demethylation(MHg -> Hg2) in GW [TF A-8]	**107. Algorithm: Methylation(Hg2 -> MHg) in GW** [TF A-7]
29. Algorithm: Demethylation(MHg -> Hg2) in surface water [TF A-8]	**114. Algorithm: Methylation(Hg2 -> MHg) in surface water** [TF A-7]
23. Algorithm: Demethylation (MHg->Hg2) in fish [TF A-8]	**106. Algorithm: Methylation (Hg2->MHg) in fish** [TF A-7]
27. Algorithm: Demethylation(MHg -> Hg2) in sediment [TF A-8]	**112. Algorithm: Methylation(Hg2 -> MHg) in sediment** [TF A-7]
Demethylation in benthic invertebrates not included owing to lack of data.	No apparent methylation in benthic invertebrates.
OXIDATION AND REDUCTION REACTIONS FOR MERCURY	
116. Algorithm: Oxidation(Hg0 -> Hg2) in air [TF A-6]	**136. Algorithm: Reduction(Hg2 -> Hg0) in air** [TF A-5]
117. Algorithm: Oxidation(Hg0 -> Hg2) in birds [TF A-6]	**137. Algorithm: Reduction(Hg2 -> Hg0) in birds** [TF A-5]
120. Algorithm: Oxidation(Hg0 -> Hg2) in mammals [TF A-6]	**140. Algorithm: Reduction(Hg2 -> Hg0) in mammals** [TF A-5]
No apparent oxidation in plant leaves, stems, or roots.	No apparent reduction in plant leaves, stems, or roots.
123. Algorithm: Oxidation(Hg0 -> Hg2) in surface soil [TF A-6]	**143. Algorithm: Reduction(Hg2 -> Hg0) in surface soil** [TF A-5]

121. Algorithm: Oxidation(Hg0 -> Hg2) in root zone [TF A-6]	**141. Algorithm: Reduction(Hg2 -> Hg0) in root zone** [TF A-5]
125. Algorithm: Oxidation(Hg0 -> Hg2) in vadose zone [TF A-6]	**145. Algorithm: Reduction(Hg2 -> Hg0) in vadose zone** [TF A-5]
119. Algorithm: Oxidation(Hg0 -> Hg2) in GW [TF A-6]	**139. Algorithm: Reduction(Hg2 -> Hg0) in GW** [TF A-5]
124. Algorithm: Oxidation(Hg0 -> Hg2) in surface water [TF A-6]	**144. Algorithm: Reduction(Hg2 -> Hg0) in surface water** [TF A-5]
new. Algorithm: Oxidation(Hg0 -> Hg2) in macrophytes [TF A-6]	No apparent reduction in macrophytes.
118. Algorithm: Oxidation(Hg0 -> Hg2) in fish [TF A-6]	**138. Algorithm: Reduction(Hg2 -> Hg0) in fish** [TF A-5]
122. Algorithm: Oxidation(Hg0 -> Hg2) in sediment [TF A-6]	**142. Algorithm: Reduction(Hg2 -> Hg0) in sediment** [TF A-5]
Oxidation in benthic invertebrates not included due to lack of data.	No apparent reduction in benthic invertebrates.
MOVEMENT WITHIN PLANTS	
166. Algorithm: Transfer from leaf to stem [all chemicals][TF 7-13]	**168. Algorithm: Transfer from stem to leaf** [all chemicals] [TF 7-14]
No movement from root to stem, just from soil to stem as a short-cut.	No movement from stem to root.

ONE-WAY TRANSFERS	
DEGRADATION/REACTION SINKS [These Transfer Factors are not numbered in TSD II]	**RUNOFF AND EROSION FROM SOIL TO SURFACE WATER**
5. Algorithm: Degradation/Reaction sink in Air [organic chemicals] [TF 2-1]	**149. Algorithm: Runoff from Surface Soil to Surface Water** [all chemicals] [TF 5-10b]
6. Algorithm: Degradation/Reaction sink in Birds [organic chemicals] [TF 2-1]	**51. Algorithm: Erosion from Surface Soil to Surface Water** [all chemicals] [TF 5-11b]
10. Algorithm: Degradation/Reaction sink in Mammals [organic chemicals] [TF 2-1]	**TERRESTRIAL ANIMAL EXCRETION TO SOIL OR SW**
9. Algorithm: Degradation/Reaction sink in Leaf [organic chemicals] [TF 2-1]	**58. Algorithm: First-order excretion to soil, birds** [all chemicals] [TF 7-31]
15. Algorithm: Degradation/Reaction sink in Stem [organic chemicals] [TF 2-1]	**59. Algorithm: First-order excretion to soil, mammals** [all chemicals] [TF 7-31]
12. Algorithm: Degradation/Reaction sink in Root [organic chemicals] [TF 2-1]	**60. Algorithm: First-order excretion to water (General), birds** [all chemicals] [TF 7-32]
19. Algorithm: Degradation/Reaction sink in Worm [organic chemicals] [TF 2-1]	**61. Algorithm: First-order excretion to water (General), mammals** [all chemicals] [TF 7-32]
Note: No degradation/reaction sink in soil arthropods.	**TERRESTRIAL ANIMAL DIRECT INGESTION OF SOIL OR SW**
16. Algorithm: Degradation/Reaction sink in Surface Soil [organic chemicals] [TF 2-1]	**94. Algorithm: Ingestion of soil by birds, General** [all chemicals] [TF 7-22]
13. Algorithm: Degradation/Reaction sink in Root Zone [organic chemicals] [TF 2-1]	**95. Algorithm: Ingestion of soil by mammals, General (surface soil)** [all chemicals] [TF 7-22]
18. Algorithm: Degradation/Reaction sink in Vadose Zone [organic chemicals] [TF 2-1]	**97. Algorithm: Ingestion of water by birds, General (surface water)** [all chemicals] [TF 7-21]
8. Algorithm: Degradation/Reaction sink in Groundwater [organic chemicals] [TF 2-1]	**98. Algorithm: Ingestion of water by mammals, General (surface water)** [all chemicals]] [TF 7-21]
17. Algorithm: Degradation/Reaction sink in Surface Water [organic chemicals] [TF 2-1]	**84b. Ingestion of leaf particles by birds [new]** - applies only to certain birds, depending on their diet. [TF 7-24]

7. Algorithm: Degradation/Reaction sink in Fish [organic chemicals] [TF 2-1]	**84c. Ingestion of leaf particles by mammals [new]** - applies only to certain mammals, depending on their diet. [TF 7-24]
14. Algorithm: Degradation/Reaction sink in Sediment [organic chemicals] [TF 2-1]	**TERRESTRIAL ANIMAL INHALATION**
11. Algorithm: Degradation/Reaction sink in Benthic Invertebrates [organic chemicals] [TF 2-1]	**100. Algorithm: Inhalation by birds, General** [all chemicals] [TF 7-30]
BULK ADVECTION TO ADVECTION SINK	**101. Algorithm: Inhalation by mammals, General** [all chemicals] [TF 7-30]
3. Algorithm: Bulk advection from air to advection sink [all chemicals] [TF 3-1b]	**LITTER FALL**
4. Algorithm: Bulk advection from surface water to flush-rate advection sink [all chemicals][TF 4-7a,b]	**102. Algorithm: Litter fall to soil from leaf particle** [all chemicals] [TF 7-16]
OTHER SINKS	**103. Algorithm: Litter fall to soil from leaves** [all chemicals] [TF 7-15]
179. Algorithm: Runoff from Surface Soil to Surface Soil Sink [all chemicals] [new] [TF 5-10c]	
178. Algorithm: Erosion from Surface Soil to Surface Soil Sink [all chemicals] [new] [TF 5-11c]	
150. Algorithm: Sediment burial from sediment to sediment burial sink, Zero net deposition, [all chemicals][TF 4-8]	

[a] Food ingestion algorithms are not presented in this table.

[b] Numbers in brackets (*e.g.,* [TF 3-1]) refer to the numbered transfer factor algorithms in the *TRIM.FaTE Technical Support Document Volume II: Description of Chemical Transport and Transformation Algorithms*, September 2002 (EPA-453/R-02-011b).

[This page intentionally left blank.]

APPENDIX I-B

BIOMASS OF FISH

[This page intentionally left blank.]

APPENDIX I-B
BIOMASS OF FISH

The mass of fish in each trophic level is derived from studies of the biomass of individual species in various systems and studies of feeding strategies of those species. Kelso and Johnson (1991) reported the biomass of individual species in 19 central Ontario lakes. Only adult fish ($\geq$1 year of age) were retained by the traps and nets used for this study. Population biomass was estimated using the mark and recapture method. The biomass of rare species could not be quantitatively estimated and are not included in the estimates of total biomass per lake or per area. Thus, these methods likely underestimate the total and species-specific biomass.

The most significant impact of this bias on TRIM.FaTE is that the young-of-the-year (YOY) of many species (e.g., perch and bass) are planktivorous. Thus, YOY biomass had to be approximated in order to populate the water column herbivore (planktivore) domain. Robust estimates of YOY biomass have not yet been found, though future efforts will focus on this task. The ratio of YOY to adult biomass for rainbow and brown trout in the Tule River, California (H. Yagger, personal communication) was used as a first approximation for the species quantitatively surveyed by Kelso and Johnson (1991). The reproductive strategies of most freshwater fish rely on the production of large numbers of eggs, with relatively few individuals progressing to adulthood. The result is that the YOY biomass may equal or exceed the total adult biomass. In the Tule River, the YOY:adult ratio for rainbow trout ranged from 1.0 to 1.66. The brown trout population was less stable and the YOY:adult ratio ranged from 0.002 to 0.4. A YOY:adult biomass ratio of 1.0 is used for the current version of TRIM.FaTE. Thus, the total biomass estimates for each species were doubled.

The trophic status of each species was preliminarily assigned according to the designations used by EPA for evaluating the biological integrity of surface waters (U.S.EPA 1993). Those designations are based on reviews of feeding studies, with each species assigned to the one trophic level that best describes the feeding habits of adult fish. However, most fish species occupy more than one trophic level. This is especially true when YOY fish are included. But even adults of some species will feed opportunistically on a range of prey. Therefore, dietary studies of selected species were used to refine and confirm the preliminary trophic level designations (Etnier and Starnes 1993).

Exhibit I-B-1 presents the current TRIM.FaTE trophic level designations for the species quantitatively surveyed by Kelso and Johnson (1991). These levels correspond to the current fish domains in each of the two food chains (e.g., water column omnivore and benthic omnivore). Species occupying more than one trophic level were fractionally assigned to multiple domains. For example, the stomach contents of yellow perch have been found to consist of approximately 70 percent invertebrates and 30 percent fish (Hayes et al. 1992). Therefore, 70 percent of the adult yellow perch population (based on biomass) is assigned to the benthic omnivore domain and 30 percent of the population is assigned to the water column omnivore domain. The water column omnivore domain was selected instead of the piscivore domains because yellow perch consume relatively small fish, which are assigned to the water column herbivore (planktivore) domain.

Biomass of the species categorized as carnivores was similarly modified to reflect changes in diet with size. That is, older, larger carnivores (e.g., bass) are assumed to prey on omnivores, whereas younger, smaller members of the population are assumed to prey on herbivores. Data have not yet been found with which to estimate the fraction of bass (or other species identified as carnivores) to be reassigned to the omnivore categories As a first approximation, the water column carnivore biomass was split as 30 percent carnivore and 70 percent omnivore. These are the values Hayes (1992) presented for yellow perch consumption of fish (30 percent) and invertebrates (70 percent). While these data are not for a species included in the carnivore categories, the inherent assumptions are reasonably analogous. Therefore, the final water column carnivore biomass is 0.3 times the initial, literature-derived water column carnivore biomass. The new water column omnivore biomass is the sum of the initial, literature-derived water column omnivore biomass and 0.7 times the initial, literature-derived water column carnivore biomass. This appears to produce a reasonable apportionment of biomass among the water column trophic levels (7.43 percent water column carnivores; 24.26 percent water column omnivores; 68.31 percent water column herbivores; ratio of 1:3:9)

Benthic carnivores were similarly assigned as 30 percent benthic carnivores and 70 percent benthic omnivores. Thus, the new benthic carnivore biomass is 0.3 times the initial, literature-derived benthic carnivore biomass The new benthic omnivore biomass is the sum of the initial, literature-derived benthic omnivore biomass and 0.7 times the initial, literature-derived benthic carnivore biomass. Benthic herbivores are comprised of benthic invertebrates rather than fish. The current default value for benthic invertebrates is a total biomass per area (kg m^{-2}) of 3.7E-03 (value for Brewer Lake, Maine, from D. Courtemanch). These values appear to produce a fairly reasonable apportionment of biomass among the benthic trophic levels (3.69 percent benthic carnivores; 32.53 percent benthic omnivores; 63.78 percent benthic invertebrates; ratio of 1:3:17). Although four percent benthic carnivores seems low, there is not a good rationale for apportioning the benthic carnivore biomass differently than the water column carnivore biomass (i.e., 30/70).

Exhibit I-F-2 presents the current default estimates of biomass per area by trophic level for TRIM.FaTE. Only data reported by Kelso and Johnson (1991) for lakes with pH > 6.0 in which both food chains are represented are included.

Exhibit I-B-1
Trophic Level Designations for Species Quantitatively Surveyed by Kelso and Johnson (1991)

Species	Species ID	EPA Trophic Level	TRIM Trophic Level	% of Biomass
Creek chub	CC	G	BO	100
Creek chub	CC-yoy	G	BO	100
Pearl dace	PD	G	BO	100
Pearl dace	PD-yoy	G	BO	100
Northern redbelly dace	RD	H	BO	100
Northern redbelly dace	RD-yoy	H	BO	100
Brown bullhead	BB	I	BO	100
Brown bullhead	BB-yoy	I	BO	100
Brook trout	BT	I	BO	100
Brook trout	BT-yoy	I	BO	100
Common shiner	CS	I	BO	100
Common shiner	CS-yoy	I	BO	100
Pumpkinseed	PS	I	BO	100
Yellow perch	YP	I	BO	70
White sucker	WS	O	BO	100
White sucker	WS-yoy	O	BO	100
Largemouth bass	LB	P	BO	35
Northern pike	NP	P	BO	35
Northern pike	NP-yoy	P	BO	35
Rockbass	RB	P	BO	35
Smallmouth bass	SB	P	BO	35
Largemouth bass	LB	P	BC	15
Northern pike	NP	P	BC	15
Northern pike	NP-yoy	P	BC	15
Rockbass	RB	P	BC	15
Smallmouth bass	SB	P	BC	15
Largemouth bass	LB-yoy		WCH	100
Pumpkinseed	PS-yoy		WCH	100
Rockbass	RB-yoy		WCH	100
Smallmouth bass	SB-yoy		WCH	100
Yellow perch	YP-yoy		WCH	100
Yellow perch	YP	I	WCO	30
Largemouth bass	LB	P	WCO	35
Northern pike	NP	P	WCO	35
Northern pike	NP-yoy	P	WCO	35
Rockbass	RB	P	WCO	50
Smallmouth bass	SB	P	WCO	35
Largemouth bass	LB	P	WCC	15
Northern pike	NP	P	WCC	15
Northern pike	NP-yoy	P	WCC	15
Smallmouth bass	SB	P	WCC	15

Exhibit I-B-2
Biomass (kg/ha) by Trophic Level for All Lakes with pH > 6.0 in Which Both Food Chains Are Represented

	TRIM Trophic Level					
Lake	**BO**	**BC**	**WCH**	**WCO**	**WCC**	**Grand Total**
04	13.27	2.15	15.89	5.48	2.15	38.95
20	39.47	2.20	16.63	6.60	1.33	66.22
33	5.95	1.46	13.35	4.49	1.46	26.70
A1	14.80	4.08	27.18	9.51	4.08	59.65
C1	22.43	1.22	11.10	4.07	0.00	38.82
P1	17.32	1.75	14.59	4.93	1.73	40.32
Grand Total	320.31	12.85	98.75	35.08	10.74	477.73
Mean	18.87	2.14	16.46	5.85	1.79	45.11
Min	5.95	1.22	11.10	4.07	0.00	26.70
Max	39.47	4.08	27.18	9.51	4.08	66.22
Ave Biomass (kg/m^2)	**1.89E-03**	**2.14E-04**	**1.65E-03**	**5.85E-04**	**1.79E-04**	**4.51E-03**
Typical mass (kg)	**0.5**	**2**	**0.025**	**0.5**	**2**	
Population (#/m^2)	**3.77E-03**	**1.07E-04**	**6.58E-02**	**1.17E-03**	**8.95E-05**	

References for Appendix I-B

Etnier, D. A., and W. C. Starnes. 1993. The fishes of Tennessee. University of Tennessee Press, Knoxville, TN.

Hayes, D. B., W. W. Taylor, and J. C. Schneider. 1992. Response of yellow perch and the benthic invertebrate community to a reduction in the abundance of white suckers. Transactions of the American Fisheries Society 121:36-53.

Kelso, J.R.M. and M.G. Johnson. 1991. Factors related to the biomass and production of fish communities in small, oligotrophic lakes vulnerable to acidification. Canadian Journal of Fisheries and Aquatic Sciences. 48:2523-2532.

U.S. EPA (U.S. Environmental Protection Agency). 1993. Wildlife Exposure Factors Handbook, Volume I. EPA/600/R-93/187a. Washington, D.C.: Office of Water and Office of Research and Development. December.

TECHNICAL REPORT DATA

(Please read Instructions on reverse before completing)

1. REPORT NO. EPA-453/R-02-012	2.	3. RECIPIENT'S ACCESSION NO.
4. TITLE AND SUBTITLE Evaluation of TRIM.FaTE. Volume I: Approach and Initial Findings		5. REPORT DATE September, 2002 6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S)		8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS		10. PROGRAM ELEMENT NO. 11. CONTRACT/GRANT NO.
12. SPONSORING AGENCY NAME AND ADDRESS U.S. Environmental Protection Agency Office of Air Quality Planning and Standards Emissions Standards & Air Quality Strategies and Standards Divisions Research Triangle Park, NC 27711		13. TYPE OF REPORT AND PERIOD COVERED Technical Report 14. SPONSORING AGENCY CODE EPA/200/04

15. SUPPLEMENTARY NOTES

16. ABSTRACT

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. This report describes a set of evaluation analyses performed on the Environmental Fate, Transport, and Ecological Exposure module of TRIM (TRIM.FaTE), primarily during 2000, with some spanning into 2002.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Risk Assessment Multimedia Modeling Exposure Assessment Air Pollutants	Air Pollution	

18. DISTRIBUTION STATEMENT Release Unlimited	19. SECURITY CLASS *(Report)* Unclassified	21. NO. OF PAGES 151
	20. SECURITY CLASS *(Page)* Unclassified	22. PRICE

EPA Form 2220-1 (Rev. 4-77) PREVIOUS EDITION IS OBSOLETE

United States
Environmental Protection
Agency

Office of Air Quality Planning and Standards
Emissions Standards & Air Quality Strategies and Standards Divisions
Research Triangle Park, NC

Publication No. EPA-453/R-02-012
September 2002