2. INTRODUCTION TO TRIM.FaTE

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

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

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

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

2.1 REVIEW OF EXISTING FATE AND TRANSPORT MODELS

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

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

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

The initial literature searches identified several models/approaches for multimedia, multipathway modeling, including EPA's Indirect Exposure Methodology (IEM), the California Department of Toxic Substance Control's Multimedia Risk Computerized Model (CalTOX), the Dutch model SimpleBOX, the Integrated Spatial Multimedia Compartmental Model (ISMCM), and the Multimedia Environmental Pollutant Assessment System (MEPAS).

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

- **Indirect Exposure Methodology (IEM)**. The version of IEM reviewed by OAQPS during initial TRIM development efforts consisted of a set of multimedia fate and exposure algorithms developed by EPA’s Office of Research and Development. This methodology was, and remains today, a significant Agency methodology for multimedia, multipathway modeling for pollutants for which indirect (*i.e.,* non-inhalation) impacts may be important (*i.e.,* organic and inorganic pollutants that tend to be long-lived, bioaccumulating, non- (or at most semi-) volatile, and more associated with soil and sediment than with water).

  An interim document describing this methodology was published in 1990 (U.S. EPA 1990), a major addendum was issued in 1993 (U.S. EPA 1993), and an updated guidance document was published in 1999 (U.S. EPA 1999d).[1] The IEM assessed by OAQPS had undergone extensive scientific review, including review by SAB, which was useful in focusing efforts in the development of TRIM. The SAB identified several limitations of IEM that were pertinent to its application to the design qualifications for TRIM (U.S. EPA 1994b). Concurrently with IEM development, EPA also developed and applied a closely related set of multimedia models in a variety of dioxin assessments (U.S. EPA 1994c).

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

During its review of the IEM methodology, OAQPS identified several limitations in the IEM approach relative to the TRIM.FaTE design criteria and OAQPS' needs. For example, the version of IEM evaluated could be applied only to chemicals that were emitted to the air. This limited its ability to provide assessment of media concentrations resulting from air emissions when other pollutant sources might have a significant impact on the results. However, IEM is an evolving and emerging methodology that has moved EPA beyond analyzing the potential effects associated with only one medium (air) and exposure pathway (inhalation) to the consideration of multiple media and exposure pathways. It was crucial in the initial development of TRIM, and remains true today, that a sense of continuity be maintained between IEM and TRIM methodologies.

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

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

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

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

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

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

  The multipathway exposure model reviewed at the time of initial TRIM development encompassed 23 exposure pathways to estimate average daily doses within a human population in the vicinity of a hazardous substances release site. The exposure assessment process consisted of relating contaminant concentrations in the multimedia model compartments to contaminant concentrations in the media with which a human population has contact (*e.g.*, personal air, tap water, foods, household dusts/soils). The explicit treatment of differentiating environmental media pollutant concentration and the pollutant concentration to which humans are exposed favorably distinguished CalTOX from many other exposure models. In addition, all parameter values used as inputs to CalTOX were distributions, described in terms of mean values and a coefficient of variation, rather than point estimates (central tendency or plausible upper values) such as most other models employed. This stochastic approach allowed both sensitivity and uncertainty to be directly incorporated into the model operation.

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

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

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

  OAQPS review found that the version of ISMCM available during early TRIM efforts considered all media, biological and non-biological, in one integrated system and included both spatial and compartmental modules to account for complex transport of pollutants through an ecosystem. Assuming mass conservation, ISMCM was able to predict transport based on a sound mechanistic description of environmental processes, including estimation of intermedia transfer factors.

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

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

  Based on OAQPS review during initial TRIM efforts, the mathematical design of this model did not include mass balance and could not be integrated into TRIM. As with IEM, MEPAS represented a "linked" model system that utilized a one-way process through a sequence of models that individually describe a specific environmental process or medium. These types of models are not mass conservative and did not allow for the temporal tracking of the pollutants and concomitant exposure necessary to meet the needs of TRIM.

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

2.2 APPROACH TO DEVELOPING TRIM.FaTE

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

Multimedia models existing at the time of initial TRIM development could be divided into two basic categories: "linked" single medium model systems and mass-conserving models. Mass-conserving models could be further classified as fugacity-based, concentration-based, or inventory-based models depending on the choice of state variable (*i.e.*, fugacity, concentration, or inventory). OAQPS concluded that the linked single medium and mass-conserving models each had their own strengths and limitations.

"Linked" single medium modeling systems were identified as those composed of several independent single medium models. The linked system typically calculated fate and transport by running a single medium model (*e.g.*, an atmospheric model) and using the output from each time step as the input for the corresponding time step of another single medium model (*e.g.*, a soil or surface water model). There were several highly sophisticated single medium models to choose from when constructing a linked system. However, the linked design did not assure conservation of mass because the dynamic feedback loops and secondary pollutant transfers were not treated in a fully coupled manner. In addition, the level of detail provided by the linked model system could not be easily adjusted to suit the needs of different modeling objectives.

Mass-conserving multimedia models were developed to fully account for the distribution of mass within a compartmentalized system. The fugacity type multimedia models were introduced by Mackay (1979, 1991) as screening tools to assess the relative distribution of chemicals in air, water, sediment, and soil. Although the fugacity concept provides a convenient method for quantifying the multimedia fate of chemicals (Cowen *et al.* 1995),[2] models that use fugacity as the state variable are limited in application only to organic chemicals. Concentration-based models like Simple Box and inventory-based models like CalTOX could technically handle inorganic chemicals, but temporal and spatial resolution would be limited by the rigid compartmentalized structure or boxes used to represent the environmental media. Spatial compartmental models (*e.g.*, ISMCM) represented the closest current models to an integrated multimedia system. However, as previously described, ISMCM did not meet the TRIM design criterion for a flexible architecture.

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

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

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

2.3 KEY CAPABILITIES OF TRIM.FaTE

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

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

To accommodate these characteristics, the Agency developed a new model framework that expanded upon the mass balance and compartmental framework used by CalTOX and the system of equations used in ChemCan[3] and SimpleBOX to produce a modeling system that incorporates a flexible level of spatial and temporal resolution while maintaining a complete multimedia mass balance. Development of the TRIM.FaTE framework required the TRIM team to design several features not available in existing multimedia models at the time of initial TRIM development. These key features included:

- Implementation as a truly coupled multimedia model framework;

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

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

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

2.3.1 TRULY COUPLED MULTIMEDIA FRAMEWORK

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

2.3.2 SCALABLE COMPLEXITY

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

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

2.3.3 FLEXIBLE ALGORITHM LIBRARY

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

Another advantage in the algorithm implementation is the potential to choose from a set of algorithms for each of the types of chemical mass transfers. The primary benefit would be in performing sensitivity analyses when there are uncertainties regarding the model approach for some transport or transformation processes. If there were several different algorithms available for a given process, the user could perform analyses using the different algorithms, thus allowing decision-makers to consider the impact of algorithms selection on predicted values.

2.3.4 FULL MASS BALANCE

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

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

2.3.5 EMBEDDED PROCEDURE FOR UNCERTAINTY AND VARIABILITY ANALYSIS

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

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

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

2.3.6 EXPOSURE MODEL FOR ECOLOGICAL RECEPTORS

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

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

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