Chapter 18 Quantification of Exposure: Multimedia Modeling

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18.1 Introduction

This chapter summarizes the concepts and tools available for multimedia modeling to support a multipathway human health risk assessment. The discussion is divided into three sections:

- Section 18.2 discusses multimedia fate and transport modeling used to estimate chemical concentrations in abiotic and biotic media that indirectly result from air emissions;

- Section 18.3 discusses key parameters used as inputs to multimedia models; and

- Section 18.4 presents examples of the use of multimedia models in air toxics risk assessments.

18.2 Multimedia Fate and Transport Modeling

Although the primary route of exposure to many air toxics is via inhalation, non-inhalation exposure through soil, water, and food pathways can be a potential health concern for those air toxics that persist and which also may bioaccumulate (see Chapter 4 for the list of persistent bioaccumulative hazardous air pollutants (PB-HAP) chemicals). Therefore, risk assessments for these substances often include multimedia modeling to predict the movement of these air toxics in the environment. This section provides an overview of the multimedia fate and transport models commonly used by EPA.

18.2.1 Basis of Multimedia Models

Multimedia fate and transport models take into account various physical and chemical processes to predict the movement of pollutants within and between environmental media. Multimedia models can be grouped into the following basic categories.

- **Linked modeling systems** are composed of several independent single-medium models. These systems typically consist of a "one-way" process through a series of linked single-medium models or algorithms; that is, they calculate fate and transport by running a single-medium model (e.g., an atmospheric model) and using the output as the input for the next single-medium model (e.g., a soil or surface water model). One of the primary advantages of linked modeling systems is that they can incorporate several highly sophisticated single-medium models into a single modeling system. The primary drawbacks of these types of models are (1) they do not always assure conservation of mass; (2) they lack dynamic "feedback" loops; and (3) secondary pollutant transfers are not treated in a fully coupled manner.

- **Fully coupled, mass-conserving models** estimate the fate and transport of pollutants between and within media and are able to fully account for the distribution of pollutant mass within a defined modeling region. In these types of models, each of the included media (e.g., soil, air, biota) are modeled simultaneously (i.e., fully coupled), and thus these models can simulate dynamic "feedback" loops and secondary pollutant transfers. The primary drawback of these types of models is that they typically involve some simplification relative to sophisticated single-medium models due to the computational demands associated with modeling multiple media simultaneously.

18.2.2 Multimedia Exposure Models

To date, EPA has used primarily the Multiple Pathways of Exposure (MPE) model and variations of the MPE approach to conduct multimedia fate and transport modeling for air toxics. More recently, EPA developed the Fate, Transport, and Ecological Exposure (TRIM.FaTE) model as a component of the Total Risk Integrated Methodology (TRIM).[(1)] This section provides a summary of the MPE model, the variations of the MPE approach, and the TRIM.FaTE model. During the development of the TRIM.FaTE model, EPA conducted a comprehensive review of those multimedia fate and transport models that estimate exposures and risks from emissions of air toxics that EPA and other organizations in the United States use. Exhibit 18-1 provides a summary of the models included in this review, with models grouped into the two basic categories described in the previous section. The TRIM.FaTE documentation provides a description of each of these models. Also presented at the end of this section is a multimedia model developed by the State of California called CalTOX.[(2)]

Exhibit 18-1. Multimedia Models Reviewed During TRIM.FaTE Development

Linked Modeling Systems	Fully Coupled, Mass-Conserving Models
• Indirect Exposure Methodology (IEM)/Multiple Pathways of Exposure (MPE), developed by EPA's National Center for Environmental Assessment • Multimedia Environmental Pollutant Assessment System (MEPAS), developed by the U.S. Department of Energy	• CalTOX, California Department of Toxic Substance Control's Multimedia Risk Computerized Model • SimpleBOX, developed by the Netherlands National Institute of Public Health and the Environment • Modeling Multimedia Environmental Distribution for Toxics (Mend-Tox)/ISMCM), developed by EPA's Office of Research and Development

<u>**Multiple Pathways of Exposure Model (MPE)**</u>

The Multiple Pathways of Exposure model, formerly known as the Indirect Exposure Methodology (IEM), primarily consists of a set of multimedia fate and exposure algorithms developed by EPA's Office of Research and Development (ORD).[(a)] ORD issued an interim document describing this methodology in 1990, a major addendum was issued in 1993, and an updated guidance document was issued in 1999 in response to comments it received during a 1994 Science Advisory Board review of the addendum.[(3)] The MPE documentation describes fate and transport algorithms, exposure pathways, receptor scenarios, and dose algorithms.

The MPE approach includes procedures for estimating human exposures and health risks resulting from the transfer of emitted pollutants from air to soil and surface water bodies and the

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[a] Note that the MPE model and many of its variations are conceptual models used to describe fate and transport, not "ready-to-run" computer models. Typically, users incorporate these conceptual models into spreadsheets or other computer frameworks to create a usable model.

subsequent uptake by vegetation, animals, and humans. The methodology specifically addresses exposures via inhalation; ingestion of food, water, and soil; and dermal contact. The MPE model was designed to predict long-term, steady-state impacts from continuous sources, rather than short-term, time-series estimates. It consists of a "one-way process" through a series of linked models and algorithms, beginning with the modeling of the transport of pollutant emissions in air and the subsequent deposition to soil and surface water and culminating in the uptake of the emitted pollutant(s) into biota. The aspects of the MPE model that address exposure estimation are described in more detail in Section 18.4 below.

The *Draft Guidance on the Development, Evaluation, and Application of Regulatory Environmental Models* recommends best practices to help determine when a model, despite its uncertainties, can be appropriately used to inform a decision. The Knowledge Base (KBase) is a web-accessible database of information on some of EPA's most frequently used models. The draft guidance recommends what information about models to document, while the Knowledge Base is the repository where this information is documented. Both products are available at the CREM internet site at http://www.epa.gov/crem.

EPA designed the MPE model to assess human exposures to air toxics emitted from stationary combustors, although analysts can apply most aspects of the approach to other types of stationary sources. One can apply this model to one or more sources at a single facility simultaneously to estimate exposures within 50 kilometers of the facility. The MPE model will allow modeling of only one chemical at a time, and there is no tracking (i.e., carry through the analysis) of transformation products of the modeled chemical. To apply the MPE approach, users must provide a significant number of site-specific inputs, such as source emission rate, wind speed and direction, soil loss constant, and pollutant degradation rate.

EPA modified the MPE approach to multimedia fate and transport modeling for use in two additional EPA models and modeling approaches. These models and approaches are as follows.

- **IEM2M**. In 1997, Office of Air Quality Planning and Standards (OAQPS) modified the then-current version of the IEM model to create IEM2M. This revised version of IEM added the functionality necessary to model transformation between the three key species of mercury and track the concentrations throughout the modeled system for each of these species. This model was applied to estimate nationwide exposures to mercury for the *Mercury Study Report to Congress*.[4]

- **Human Health Risk Assessment Protocol (HHRAP)**. EPA's Office of Solid Waste and Emergency Response (OSWER) developed the HHRAP to provide guidance for conducting multipathway exposure and risk assessments of emissions of air toxics from hazardous waste combustion facilities. The suggested protocol for assessing multipathway exposures was adapted from the MPE approach and the documentation of this protocol[5] compiles detailed information on many of MPE's input parameters and algorithms.

Two additional models and approaches used by EPA to assess multipathway exposures to air toxics use many of the same fate and exposure algorithms and methodologies used in the MPE model.

- **Dioxin Reassessment Methodology**. Many of the algorithms used in the MPE model have been used for ongoing EPA efforts to characterize exposure and risks from dioxins, particularly chlorinated dibenzodioxins and dibenzofurans, as part of the Dioxin Reassessment project.[6]

- **Multimedia, Multipathway, Multi-receptor Exposure and Risk Assessment Model (3MRA)**. The 3MRA model is currently being developed by EPA's Office of Solid Waste and Emergency Response to support their Hazardous Waste Identification Rule (HWIR). Many of the fate and exposure algorithms used in 3MRA are similar to those used in MPE.

<u>**TRIM.FaTE**</u>

EPA developed the TRIM Fate, Transport, and Ecological Exposure (TRIM.FaTE) model[7] to describe the movement and transformation of pollutants over time, through a user-defined, bounded system of environmental compartments (i.e., abiotic media and organisms). The design of the compartment system can encompass spatial interconnections (with some similarities to grid-type Eulerian models) and ecological exposure-related relationships. TRIM.FaTE is designed to generate both media concentrations relevant to human pollutant exposures and exposure estimates relevant to ecological risk assessment primarily for air pollutants for which non-inhalation exposures are important.

In contrast to the IEM/MPE approach, TRIM.FaTE is a fully coupled multimedia model that estimates the flow of pollutant through time among environmental compartments. TRIM.FaTE offers the following important features that are not available using IEM/MPE.

- TRIM.FaTE is able to model mass-balanced "feedback" loops between media as well as secondary emissions (e.g., re-emission of deposited pollutants).

- TRIM.FaTE has the ability to provide detailed time-series estimates of pollutant concentrations in the environmental compartments.

- TRIM.FaTE maintains a full mass balance of the pollutant mass in the system (i.e., all the pollutant introduced into the system is accounted for among all the environmental compartments).

- TRIM.FaTE can model sensitivity of model results to variations in input parameters and perform probabilistic modeling such that uncertainty and variability in model results can be characterized.

- TRIM.FaTE is designed with the flexibility to allow for implementation of nearly limitless configurations (e.g., spatial resolution, types of biota), algorithms, and approaches. Simulations can range from quite simple analyses of pollutant distribution across abiotic media and biota to more complex, spatially-refined assessments, with associated implications with regard to user requirements.

TRIM.FaTE can model multimedia fate and transport of air toxics from any type of stationary source. It can be applied to multiple facilities, sources, and chemicals simultaneously to track the fate and transport of emitted pollutants as well as transformation products of the emitted pollutants. The amount of input data required by TRIM.FaTE is directly related to the complexity of the user-specified modeling system; however, TRIM.FaTE analyses typically require more input data than similar analyses conducted using the MPE approach. As noted in Exhibit 18-2, TRIM.Expo is the exposure component of the TRIM modeling system (see Section 18.2.2.2).

California Total Exposure Model for Hazardous Waste Sites (CalTOX)

The Department of Toxic Substances Control (DTSC), within the California Environmental Protection Agency, has the responsibility for managing the State's hazardous-waste program. As part of this program, the DTSC funded the development of the CalTOX program.[2] CalTOX has been developed as a set of spreadsheet models and spreadsheet data sets to assist assessing human exposures and defining soil clean-up levels at uncontrolled hazardous wastes sites. More recently, CalTOX has been modified for use in establishing waste classification for landfills and hazardous waste facilities in California. CalTOX addresses contaminated soils and the contamination of adjacent air, surface water, sediments, and ground water. The modeling components of CalTOX include a multimedia transport and transformation model, exposure scenario models, and add-ins to quantify uncertainty and variability. The multimedia transport and transformation model is a dynamic model that can assess time-varying concentrations of pollutants introduced initially to soil layers or for pollutants released continuously to air, soil, or water. This model assists the user in examining how chemical and landscape properties impact both the ultimate route and quantity of human contact. Multimedia, multiple pathway exposure models are used in CalTOX to estimate average daily doses within a human population. The exposure modeling part of CalTOX is described further in Chapter 20.

18.3 Key Parameters/Inputs for Multimedia Models

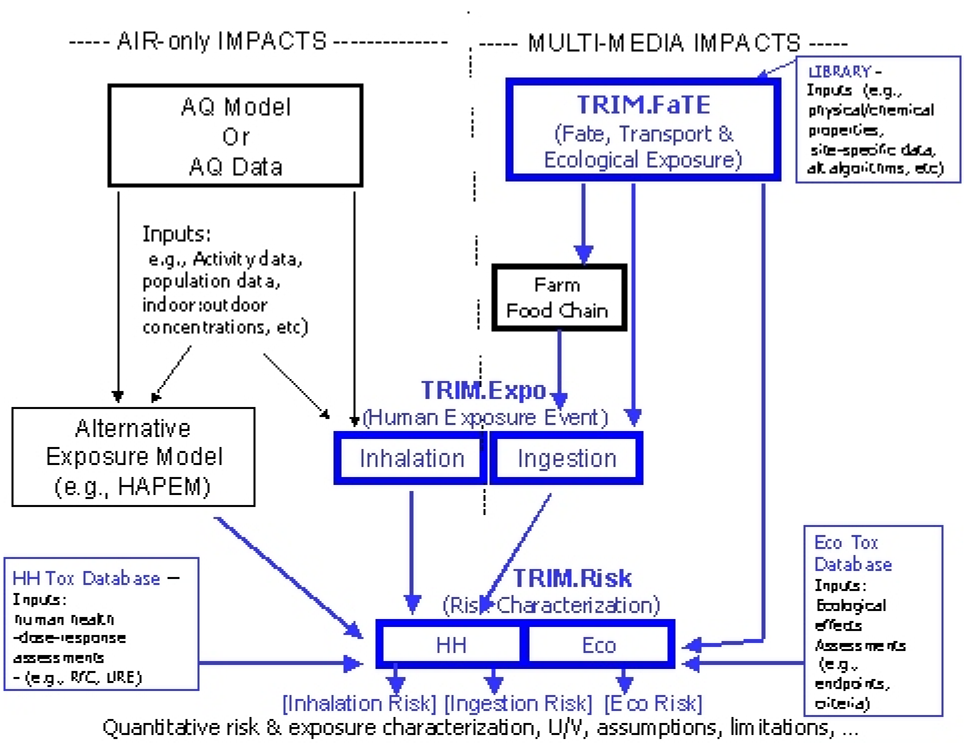
For most air risk applications, multimedia modeling results are strongly dependent on the **emission rate** of pollutants emitted to the air from the facility. For the MPE framework and TRIM.FaTE model, transport of modeled pollutants and accumulation in media of interest result directly from the emission of the chemical into the air from the facility, the dispersion or advection of chemical through the air, and the subsequent deposition of the chemical onto land, water, or other surfaces in the modeled region. In addition to emission rate, several other types of data are often required by multimedia models to characterize the pollutants and site being modeled. Generally, the data requirements for multimedia fate and transport models fall into the following categories.

- **Source characteristics** for the sources that are modeled, such as location, emission rates for the modeled pollutant(s), stack height, exit gas velocity, and exit gas temperature.

- **Environmental setting characteristics** for the abiotic media included in the modeling scenario, such as water body dimensions, surface soil characteristics (e.g., organic carbon content, porosity), and data related to local meteorology and hydrology (e.g., precipitation, erosion, runoff rates).

- **Abiotic chemical/physical data** for the chemicals included in the modeling scenario, such as Henry's law constant and soil-water partition coefficients. EPA's draft HHRAP provides default values for many of these parameters.[5]

Exhibit 18-2. Role of the TRIM Modeling System



The Total Risk Integrated Methodology (TRIM) modeling system can be used to assess human inhalation, human ingestion, and ecological risks. TRIM.FaTE accounts for movement of a chemical through a comprehensive system of discrete compartments (e.g., media and biota) that represent possible locations of the chemical in the physical and biological environments of the modeled ecosystem and provides an inventory, over time, of a chemical throughout the entire system. In addition to providing exposure estimates relevant to ecological risk assessment, TRIM.FaTE generates media concentrations relevant to human ingestion exposures that can be used as input to the ingestion component of the Exposure-Event module, TRIM.Expo. Measured concentrations also can be used as inputs to TRIM.Expo. In the inhalation component of TRIM.Expo, human exposures are evaluated by tracking randomly selected individuals that represent an area's population and their inhalation and ingestion through time and space. $\text{TRIM.Expo}_{\text{Inhalation}}$ can accept ambient air concentration estimates from an external air quality model or monitoring data. In the Risk Characterization module, TRIM.Risk, estimates of human exposures or doses are characterized with regard to potential risk using the corresponding exposure- or dose-response relationships. The TRIM.Risk module is also designed to characterize ecological risks from multimedia exposures. The output from TRIM.Risk is intended to include documentation of the input data, assumptions in the analysis, and measures of uncertainty/variability, as well as the results of risk calculations and exposure analysis. Information on TRIM can be accessed at: http://www.epa.gov/ttn/fera/.

- **Non-chemical-specific characteristics of biota** for any organisms included in the modeling scenario, such as feeding rates, body weight, and population density.

- **Biotic chemical-specific data** for any organisms included in the modeling scenario, such as bioaccumulation and/or bioconcentration factors or assimilation efficiency values.

The Multiple Pathways of Exposure (MPE) model,[8] a commonly used model for multipathway analyses, requires air concentrations, deposition rates, which are typically obtained via Industrial Source Complex (e.g., ISCST3) modeling (see Chapter 9 for descriptions of these models). Risk assessors would execute the ISCST3 modeling for multipathway in a similar fashion to how they executed the modeling for inhalation. Specifically, the sources would be characterized in the same way (e.g., vent height and diameter, release temperature and velocity, flow rate). The user would provide the inputs necessary to calculate the deposition rates properly (e.g., particle size distribution, scavenging coefficient). However, for multipathway analyses, the user should execute the ISCST3 model with the "depletion option" (i.e., telling the model to subtract out the mass of chemical deposited).

The user would need to know the particulate/particle-bound/vapor fractions of the emissions for ISCST3 to calculate wet and dry deposition of vapors and particles. These would probably be considered source-related, since although they are chemical-dependent, they also vary by source (i.e., the industrial process affects the emissions profile).

For dry deposition of particles, the user would supply the following inputs (in addition to the normal ISC inputs), including the:

- Array of particle diameters of the emissions;
- Array of mass fractions corresponding to the different particle diameters; and
- Array of particle densities corresponding to the different particle diameters.

For wet deposition of particles, the user would supply the following inputs (in addition to the normal ISC inputs), including the:

- Particle scavenging coefficients for liquid precipitation corresponding to the different particle diameters; and
- Particle scavenging coefficients for frozen precipitation corresponding to the different particle diameters.

For wet deposition of gases, the user would supply the following inputs (in addition to the normal ISC inputs), including the:

- Gaseous scavenging coefficient for liquid precipitation; and
- Gaseous scavenging coefficient for frozen precipitation.

The ISC user's guide[9] provides more detailed information on the deposition algorithms and required input data. There also is guidance for application of ISC for multipathway assessment in the latest MPE documentation.[8]

The only facility-related/source term data points used by the **TRIM Fate, Transport, and Ecological Exposure (TRIM.FaTE)** model are chemical emission rate, location (lat/long, UTM), and emission height, which are available from the inhalation modeling. TRIM.FaTE calculates all values internally for determining vapor/particle fractions and deposition rates based on chemical-specific (**not** source-specific) properties.

Other multimedia models may require specific source characterization data and other documentation that were not obtained for the inhalation analysis (the various user's guides for these models should be consulted for appropriate inputs).

It is important to note that the number and refinement of inputs to a multimedia model may vary depending on the outputs of interest and level of detail entailed in the modeling.

18.4 Examples of Multimedia Modeling

TRIM.FaTE Test Case Application. As a test case application, the TRIM.FaTE model was used to predict multimedia concentrations of mercury at a chlor-alkali facility in the northeastern United States. Speciated mercury concentrations were calculated for various abiotic media (e.g., surface soil, surface water, lake sediment) and biota (e.g., fish for various trophic levels, birds, mammalian predators) for the ecosystem surrounding the facility. A sensitivity and uncertainty analysis using TRIM.FaTE tools and a model comparison involving the 3MRA modeling system were also performed. The complete report on the test case will be available at the TRIM.FaTE page of EPA's Fate, Exposure, and Risk Analysis (FERA) website: http://www.epa.gov/ttn/fera/trim_fate.html.

Paints Hazardous Waste Listing Determination Analysis. On April 4, 2002, EPA issued a final determination not to list as hazardous certain wastes generated from the production of paint. EPA made this determination pursuant to the Resource Conservation and Recovery Act (RCRA), which directs EPA to determine whether certain wastes from the paint production industry may present a substantial hazard to human health or the environment. EPA proposed concentration-based listings for certain paint waste solids (K179) and liquids (K180) on February 13, 2001 (66 *Federal Register* 10060). However, following a review of the public comments and supplemental analyses based on public comments, EPA determined that the paint wastes identified in the February 13, 2001, proposal did not present a substantial hazard to human health or the environment. EPA conducted a multipathway risk assessment in support of this determination.[10] EPA used a series of models to estimate concentrations of Chemicals of Potential Concern (COPCs) in the environment with which human and ecological receptors may come into contact. The analysis used a source partioning model to estimate environmental releases of each COPC from a waste management unit for each waste stream, as appropriate. These estimated environmental releases provided input to the fate and transport models to estimate media concentrations in air, soil, surface water, and groundwater. A farm food chain model was used to estimate COPC concentrations in produce, beef, and dairy products. Aquatic bioconcentration factors were used to estimate concentrations in fish.

Chlorinated Aliphatics Hazardous Waste Listing Determination. In support of a hazardous waste listing determination for wastewaters and wastewater treatment sludges generated from the production of certain chlorinated aliphatic chemicals, EPA conducted a multipathway human health risk assessment.[11] EPA used the ISCST3 model to estimate dispersion and deposition of vapors emitted from wastewater treatment tanks and landfills, and vapors and particulates emitted from sludge land treatment units. EPA used a series of indirect exposure equations based on the MPE approach to quantify the concentrations of contaminants that pass from contaminated environmental media to the receptor indirectly. For example, EPA examined risks associated with contaminant transport in air; deposition onto plants and soil; accumulation in forage, grain, silage, and soil; subsequent ingestion by beef cattle and dairy cattle; and human ingestion of contaminated beef and dairy products.

Hazardous Waste Combustor MACT Standard Analysis. A human health and ecological risk assessment was performed in support of developing a Maximum Achievable Control Technology (MACT) standard for hazardous waste combustor facilities.[(12)] The risk analysis included a multimedia, multipathway assessment that addressed direct exposures to constituents released into the atmosphere by hazardous waste combustor units and indirect exposures due to the movement of air toxics in the food chain. The risk assessment addressed both human health risks (cancer effects and noncancer effects) as well as ecological risks. Constituents assessed were seven congeners of chlorinated dioxin and 10 congeners of chlorinated furan; three species of mercury; 14 metals (antimony, chromium III, chromium VI, arsenic, lead, barium, nickel, beryllium, selenium, cadmium, silver, thallium, cobalt, copper, and manganese); particulate matter; hydrochloric acid; and chlorine gas. To the maximum extent possible, this risk assessment followed the latest risk guidelines adopted by EPA and used the most recent data available.

Columbus Waste-to-Energy Study. A risk assessment study using fate modeling was performed by EPA's NCEA for dioxin emissions at the Columbus, Ohio, Waste-to-Energy incinerator facility.[(13)] In 1994, EPA headquarters, the Office of Research and Development, and Region 5 conducted a screening assessment of indirect impacts, leading to the conclusion that continued emissions "may pose an imminent endangerment to public health and the environment." Fate modeling used to support EPA's position utilized the air-to-beef model described in the draft Dioxin Exposure document (i.e., based on the principles included in the MPE framework) and assumed a subsistence farming family scenario. Exposure pathways considered beef, milk and vegetable ingestion; soil dermal contact and childhood soil ingestion; and breast milk ingestion. The exposure duration for adults was assumed to be seventy years. Air concentrations used were the average from nine dairy farms located between five and twelve miles from the incinerator. Overall exposure and cancer risk were estimated for each of the exposure pathways, with cancer risk being highest for beef consumption (2×10^{-4}) and lowest for soil dermal contact (9×10^{-9}). Exposure from breast milk ingestion was determined to be higher by one order of magnitude than exposure from beef and milk consumption, and higher by two orders of magnitude than exposure from inhalation. Breast milk exposure near the incinerator site ranged between two and more than seven times the background dioxin levels. A TRIM.FaTE case study has been developed based on this analysis, including a direct model comparison component on the air-soil outputs, and will be available at: http://www.epa.gov/ttn/fera/trim_fate.html.

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