



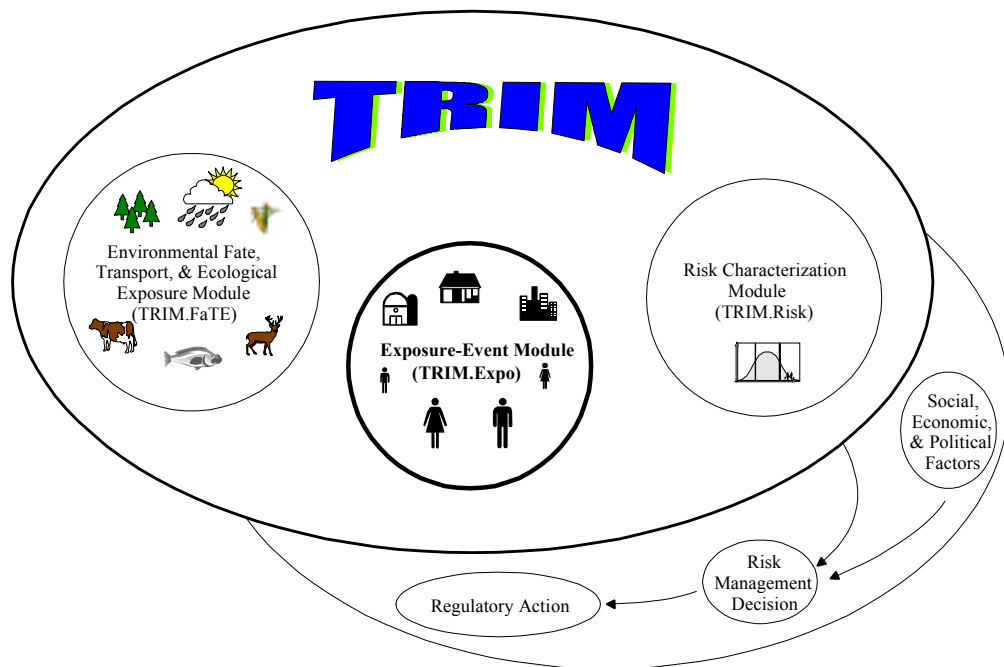
# TRIM

## Total Risk Integrated Methodology

### TRIM.Expo

# TECHNICAL SUPPORT DOCUMENT

### EXTERNAL REVIEW DRAFT



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TRIM

Total Risk Integrated Methodology

TRIM.Expo TECHNICAL SUPPORT DOCUMENT

U.S. ENVIRONMENTAL PROTECTION AGENCY  
Office of Air and Radiation  
Office of Air Quality Planning and Standards  
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External Review Draft  
November 1999

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## Acknowledgments

As described in this report, the Office of Air Quality Planning and Standards (OAQPS) of the U.S. Environmental Protection Agency is developing the Total Risk Integrated Methodology. The principal individuals and organizations in the TRIM.Expo development effort and in the preparation of this report are listed below. Additionally, valuable technical support for report development was provided by ICF Consulting.

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## PREFACE

This draft document, the *TRIM.Expo Technical Support Document*, is part of a series of documentation for the overall Total Risk Integrated Methodology (TRIM) modeling system. The detailed documentation of TRIM's logic, assumptions, algorithms, equations, and input parameters is provided in comprehensive Technical Support Documents (TSDs) for each of the TRIM modules. The purpose of the TSDs is to provide full documentation of how TRIM works and of the rationale for key development decisions that were made. This report documents the Exposure-Event module of TRIM (TRIM. Expo).

To date, EPA has issued draft TSDs for the Environmental Fate, Transport, and Ecological Exposure module (*TRIM.FaTE TSD*, U.S. EPA 1999a,b) and the TRIM. Expo (this report). When the Risk Characterization module (TRIM.Risk) is developed, EPA plans to issue a TSD for it. The TSDs will be updated as needed to reflect future changes to the TRIM modules.

The EPA has also issued the 1999 *Total Risk Integrated Methodology (TRIM) Status Report* (U.S. EPA 1999c). The purpose of that report is to provide a summary of the status of TRIM and all of its major components, with particular focus on the progress in TRIM development since the 1998 *TRIM Status Report* (U.S. EPA 1998a). The EPA plans to issue status reports on an annual basis while TRIM is under development.

In addition to status reports and TSDs, EPA intends to develop detailed user guidance for the TRIM computer system. The purpose of such guidance will be to define appropriate (and inappropriate) uses of TRIM and to assist users in applying TRIM to assess exposures and risks in a variety of air quality situations.

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## ACRONYMS

ACH	Air Exchange Rates
ADD	Average Daily Dose
AirPEX	Air Pollution Exposure Model
AIRS	Aerometric Information Retrieval System
AMEM	ADL Migration Exposure Model
APEX	Air Pollutant Exposure Model
ARB	Air Resources Board
ASPEN	Assessment System for Population Exposure Nationwide
BEADS	Benzene Exposure and Absorbed Dose Simulation
BEAM	Benzene Exposure Assessment Model
BM	Body mass
BOC	Bureau of Census
BW	Body weight
CAA	Clean Air Act
CAAA	Clean Air Act Amendments
CalTOX	California Total Exposure Model for Hazardous Waste Sites
CHAD	Comprehensive Human Activity Data
CMAQ	Community Multi-scale Air Quality
CO	Carbon monoxide
CONSEXPO	Consumer Product Exposure Model
CPIEM	California Population Indoor Exposure Model
DEPM	Dietary Exposure Potential Model
DERM	Dermal Exposure Reduction Model
DOE	U.S. Department of Energy
ECF	Energy conversion factor
EDMAS	Exposure and Dose Modeling and Analysis System
EE	Energy expenditure
EML	Exposure Models Library
EPA	U.S. Environmental Protection Agency
ETS	Environmental tobacco smoke
GEMS	Graphical Exposure Modeling System
GIS	Geographic information system
GUI	Graphical User Interface
HAP	Hazardous air pollutant
HAPEM4	Hazardous Air Pollutant Exposure Model, Version 4
HEM	Human Exposure Model
HPI	Hazard Potential Index
HVAC	Heating, ventilation, and air conditioning
IAQM	Indoor Air Quality Model
IEM	Indirect Exposure Methodology Model
IMES	Integrated Exposure Models Evaluation System
INTOXX	Integrated Toxic Expected Exceedance
ISC	Industrial Source Complex
ISCLT	Industrial Source Complex, Long-term
ISCST	Industrial Source Complex, Short-term

ISMCM	Integrated Spatial Multimedia Compartmental Model
LADD	Lifetime Average Daily Dose
LSODE	Livermore Solver for Ordinary Differential Equations
MAVRIQ	Model for Analysis of Volatiles and Residential Indoor Air Quality
MCCEM	Multi-Chamber Concentration and Exposure Model
MENTOR	Modeling Environment for Total Risk Studies
MEPAS	Multimedia Environmental Pollutant Assessment System
MET	Metabolic equivalent of work
MIMS	Multimedia Integrated Modeling System
MMSOILS	Multimedia Contaminant Fate, Transport, and Exposure Model
MPE	Multiple Pathways of Exposure
MSA	Metropolitan Statistical Area
NAAQS	National Ambient Air Quality Standard
NAMS	National Air Monitoring Station
NAS	National Academy of Sciences
NASQAN	National Stream Quality Accounting Network
NATA	National Air Toxics Assessment
NCC	National Computing Center
NCEA	National Center for Environmental Assessment
NCHS	National Center for Health Statistics
NEM	NAAQS Exposure Model
NHAPS	National Human Activity Pattern Survey
NHIS	National Health Interview Survey
NIST	National Institute of Standards and Technology
NOPEs	Non-occupational Pesticides Exposure Study
NRC	National Research Council
OAQPS	EPA Office of Air Quality Planning and Standards
OMS	EPA Office of Mobile Sources
ORD	EPA Office of Research and Development
OW	EPA Office of Water
PBPK	Physiologically-based pharmacokinetic
PC	Personal computer
PDF	Probability density function
PEC	Predicted environmental concentration
PEM	Personal exposure monitor
pHAP	Probabilistic Hazardous Air Pollutant Exposure Model
PM <sub>2.5</sub>	Particulate matter with aerodynamic size diameter of 2.5 $\mu$ m or less
PM <sub>10</sub>	Particulate matter with aerodynamic size diameter of 10 $\mu$ m or less
pNEM	Probabilistic National Ambient Air Quality Standards Exposure Models.
PNL	Pacific Northwest Laboratory
PTEAM	Particle Total Exposure Assessment Methodology
RESRAD	Residual Radiation
RIA	Regulatory impact analysis
RMR	Resting metabolic rate
SAB	EPA's Science Advisory Board
SCIES	Screening Consumer Inhalation Exposure Software
SCREAM2	South Coast Risk and Exposure Assessment Model, Version 2

SHAPE	Simulation of Human Activities and Pollutant Exposure
SHEDS	Stochastic Human Exposure and Dose Simulation
SLAMS	State and Local Air Monitoring Stations
STAR	STability ARray
STORET	Storage and Retrieval
TAP	Time Activity Patterns
TEAM	Total Exposure Assessment Methodology
THERdbASE	Total Human Exposure Risk database and Advance Simulation Environment
TOXLT	Toxic Modeling System, Long-term
TRIM	Total Risk Integrated Methodology
TRIM.Expo	TRIM Exposure-Event module
TRIM.FaTe	TRIM Environmental Fate, Transport, and Ecological Exposure module
TSD	Technical Support Document
USES	Unified System for the Evaluation of Substances
USGS	U.S. Geological Survey
VOC	Volatile organic compound

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# 1. INTRODUCTION

The Office of Air Quality Planning and Standards (OAQPS) of the U.S. Environmental Protection Agency (EPA, or the Agency) has the responsibility for the hazardous and criteria air pollutant programs described by sections 112 and 108 of the Clean Air Act (CAA). Several aspects of these programs require evaluation of the health risks and environmental effects associated with exposure to these pollutants.<sup>1</sup> In response to these risk-related mandates of the CAA, and the scientific recommendations of the National Academy of Sciences (NAS) (NRC 1994), the Presidential/Congressional Commission on Risk Assessment and Risk Management (CRARM) (CRARM 1997), as well as EPA guidelines and policies, OAQPS recognized the need for improved fate and transport, exposure, and risk modeling tools that:

- Have multimedia assessment capabilities;
- Have human health and ecological exposure and risk assessment capabilities;
- Can perform multiple pollutant assessments (*e.g.*, ability to assess mixtures of pollutants, ability to track chemical transformations);
- Can explicitly address uncertainty and variability;
- Have the ability to easily perform analyses iteratively, moving from the use of simpler assumptions and scenarios to more detailed assessments; and
- Are readily available and user-friendly, so that they can be used by EPA, as well as by a variety of Agency stakeholders.

In 1996, OAQPS embarked on a multi-year effort to develop the Total Risk Integrated Methodology (TRIM), a time series modeling system with multimedia capabilities for assessing human health and ecological risks from hazardous and criteria air pollutants.

The main purpose of the TRIM Status Report (U.S. EPA 1999c) is to summarize the work performed during the second developmental phase of TRIM. The first phase, which included the conceptualization of TRIM and implementation of the TRIM conceptual approach through development of a prototype of the first TRIM module, TRIM.FaTE (U.S. EPA 1998a), was reviewed by EPA's Science Advisory Board (SAB) in May 1998 (U.S. EPA 1998b). The second developmental phase has included refining TRIM.FaTE and developing a model evaluation plan, initiating development of the second module (TRIM.Expo), and conceptualizing the third module (TRIM.Risk). In addition, progress has been made on developing overarching aspects, such as the computer framework and an approach to uncertainty and variability. Consistent with the integral role of peer review in the TRIM development plan, the current Status Report and

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<sup>1</sup> Hazardous air pollutants (HAPs) include any air pollutant listed under CAA section 112(b); currently, there are 188 air pollutants designated as HAPs. Criteria air pollutants are air pollutants for which national ambient air quality standards (NAAQS) have been established under the CAA; at present, the six criteria air pollutants are particulate matter, ozone, carbon monoxide, nitrogen oxides, sulfur dioxide, and lead.

Technical Support Documents (TSDs) were subjected to review by representatives from the major program offices at EPA and an EPA Models 2000<sup>2</sup> review team prior to this SAB advisory.

This TSD describes the development of TRIM.Expo, detailing the work completed to date toward developing the first TRIM.Expo prototypes. More specifically, the report addresses the following areas:

- OAQPS' modeling needs and the intended goals for TRIM;
- Design of the TRIM modeling system;
- TRIM.Expo's relation to the TRIM modeling system;
- Purpose and ongoing development of TRIM.Expo;
- Conceptual framework of TRIM.Expo, in the context of the general approach to exposure assessment and modeling;
- Approach used in TRIM.Expo for calculating inhalation and ingestion exposures;
- Comparative overview of existing exposure models and modeling approaches, addressing the strengths and limitations of some of the more commonly used exposure models;
- Plans for developing and evaluating the TRIM.Expo prototypes;
- Glossary of terms and definitions; and
- Listing of examples of input parameters for TRIM.Expo.

## **1.1 GOALS AND OBJECTIVES FOR TRIM**

The TRIM modeling system is intended to represent the next generation of human and environmental exposure and risk models for OAQPS. For example, TRIM is expected to be a useful tool for performing exposure and/or risk assessments for the following CAA programs: the Residual Risk Program (CAA section 112[f]); the Integrated Urban Air Toxics Strategy (CAA section 112[k]); studies of deposition to water bodies and mercury emissions from utilities (CAA

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<sup>2</sup> Following the report of the Agency Task Force on Environmental Regulatory Modeling (U.S. EPA 1994a), the Agency conducted the Models 2000 Conference in December 1997. This conference has led to renewed emphasis on Agency-wide coordination of model development and the proposal for the implementation of a Council on Regulatory Environmental Modeling (CREM) to facilitate and promote scientifically-based, defensible regulatory computer models. The charter for CREM has been reviewed by SAB and is being updated for implementation by the Agency.

sections 112[m] and 112[n]); petitions to delist individual HAPs and/or source categories (CAA sections 112[b][3] and 112[c][9]); review and setting of the national ambient air quality standards (NAAQS) (CAA section 109); and regulatory impact analyses (RIA).

The goal in developing TRIM is to create a modeling system, and the components of that system, for use in characterizing human health and ecological exposure and risk in support of hazardous and criteria air pollutant programs under the CAA. The goal in designing TRIM is to develop a modeling system that is: (1) scientifically defensible, (2) flexible, and (3) user-friendly.

(1) Characteristics of the TRIM components important to their scientific defensibility include the following.

- **Conservation of pollutant mass.** The modeled pollutant(s)' mass will be conserved within the system being assessed, wherever appropriate and feasible, including during intermedia transfers. For pollutants where transformation is modeled, the mass of the core substance (*e.g.*, mercury for methylmercury as well as divalent mercury) within the modeling simulation will be preserved.
- **Ability to characterize parameter uncertainty and variability.** For critical parameters, the impacts of parameter uncertainty and variability on model outputs will be tracked and, where feasible, differentiated.
- **Capability for multiple pollutant, multiple media, multiple exposure pathway assessment.** The TRIM modeling system is being designed to facilitate assessment of risks posed by aggregate exposures to single or multiple chemicals from multiple sources and via multiple exposure pathways.

(2) To ensure flexibility, the features of TRIM include the following.

- **Modular design.** Major components of TRIM will be independent and can be used individually, with outside information or models, or in combination. Only those model components necessary for evaluating the particular pollutants, pathways, and/or effect endpoints of interest need be employed in an assessment.
- **Flexibility in temporal and spatial scale.** Exposure and risk assessments will be possible for a wide range of temporal and spatial scales, including hourly to daily or yearly time steps, and from local (10 kilometers (km) or less) to greater spatial scales (depending on the module).
- **Ability to assess human and ecological endpoints.** Impacts to humans and/or biota can be assessed.

(3) To ensure that TRIM will be user-friendly for a variety of groups, including EPA, state and local agencies, and other stakeholders, TRIM will have the following characteristics.

- **Easily accessible.** The TRIM modeling system will be accessible for use with a personal computer (PC). The system may be available for download from the Internet and accessible through an Agency model system framework (*e.g.*, Models-3 (U.S. EPA 1999d)).
- **Well-documented.** Guidance materials for use of the TRIM modeling system will be provided through a user's guide, with a focus on the modular aspects of the modeling system, limitations of the modeling system, and appropriate uses, user responsibilities, and user options.
- **Clear and transparent.** The graphical user interface of the TRIM computer framework will provide transparency and clarity in the functioning of the TRIM modules, and output from the risk characterization module will document modeling assumptions, limitations, and uncertainties.

## 1.2 TRIM DESIGN

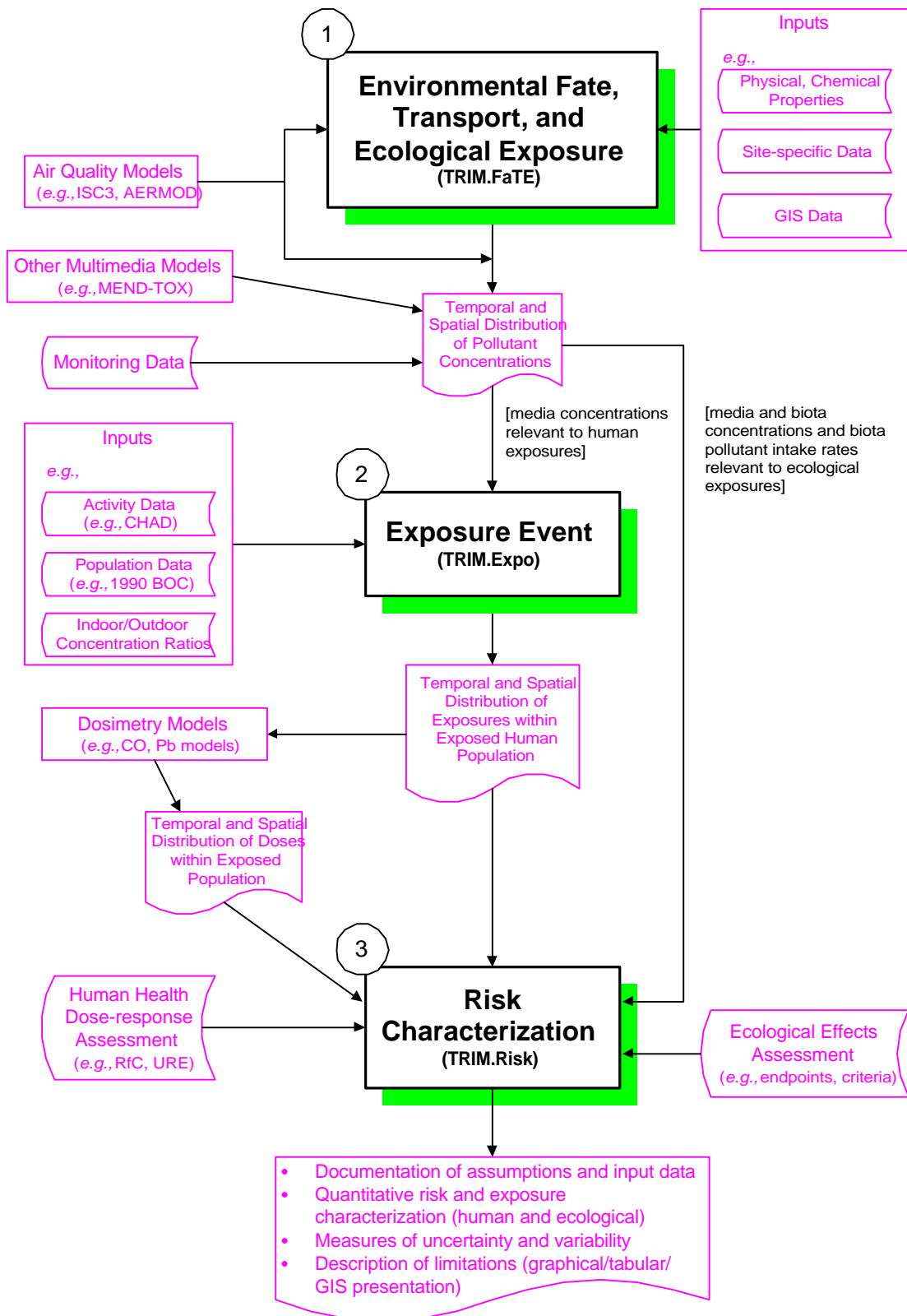
The current TRIM design (Figure 1-1) includes three individual modules. The Environmental Fate, Transport, and Ecological Exposure module, **TRIM.FaTE**, accounts for movement of a chemical through a comprehensive system of discrete compartments (*e.g.*, media, biota) that represent possible locations of the chemical in the physical and biological environments of the modeled ecosystem and provides an inventory, over time, of a chemical throughout the entire system. In addition to providing exposure estimates relevant to ecological risk assessment, TRIM.FaTE generates media concentrations relevant to human pollutant exposures that can be used as input to the Exposure-Event module, **TRIM.Expo**. In TRIM.Expo, human exposures are evaluated by tracking population groups referred to as "cohorts" and their inhalation and ingestion through time and space. In the Risk Characterization module, **TRIM.Risk**, estimates of human exposures or doses are characterized with regard to potential risk using the corresponding exposure- or dose-response relationships. The TRIM.Risk module is also being designed to characterize ecological risks from multimedia exposures. The output from TRIM.Risk will include documentation of the input data, assumptions in the analysis, and measures of uncertainty, as well as the results of risk calculations and exposure analysis.

An overarching feature of the TRIM design is the analysis of uncertainty and variability. A two-stage approach for providing this feature to the user is being developed<sup>3</sup>. The first stage includes sensitivity analyses that are useful in identifying critical parameters, while more detailed uncertainty and variability analyses using Monte Carlo methods (*e.g.*, for refined assessment of the impact of the critical parameters) are available in the second stage. The uncertainty and variability feature augments the TRIM capability for performing iterative analyses. For example, the user may perform assessments varying from simple deterministic screening analyses using conservative default parameters to refined and complex risk assessments where the impacts of parameter uncertainty and variability are assessed for critical parameters.

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<sup>3</sup> This approach is being developed for the overall TRIM system. However, it has only been implemented to date for the TRIM.FaTE module.

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



Additionally, the modular design of TRIM allows for flexibility in both its development and application. Modules can be developed in a phased approach, with refinements being made as scientific information and tools become available. Furthermore, the user may select any one or more of these modules for an assessment depending on the user's needs. For example, when performing a human health risk assessment for an air pollutant for which multimedia distribution is not significant, TRIM.Expo may be applied using ambient concentration data or the output from an air quality model external to TRIM; the output from TRIM.Expo may then be used as input to TRIM.Risk to perform the desired risk analyses. In the case of a multimedia air pollutant, such as mercury, the user may choose to run all three TRIM modules to assess both human and ecological risks posed by multipathway exposures from multiple media.

Overview descriptions of the TRIM modules are provided in Sections 1.2.1 through 1.2.3, the status and plans for development are presented in Section 1.3, and plans for application appear in Section 1.4. A summary of the previous SAB comments and OAQPS responses is presented in Chapter 2 of the TRIM Status Report. The approach for handling uncertainty and variability in TRIM is described in Chapter 3 of the TRIM Status Report. Certain aspects of the TRIM.FaTE module are addressed in greater detail in Chapters 4 through 7, and additional details on TRIM.Expo and TRIM.Risk are provided in Chapters 8 and 9, respectively, of the TRIM Status Report. Chapter 10 of the TRIM Status Report discusses the computer framework that is being implemented for the TRIM system. In addition, the TRIM.FaTE TSD (U.S. EPA 1999a,b) provides more detail on TRIM.FaTE.

### **1.2.1 DESCRIPTION OF TRIM.FaTE**

The first TRIM module to be developed, TRIM.FaTE, is a spatial compartmental mass balance model that describes the movement and transformation of pollutants over time, through a user-defined, bounded system that includes both biotic and abiotic components (compartments). The TRIM.FaTE module predicts pollutant concentrations in multiple environmental media and in biota and pollutant intakes for biota, all of which provide both temporal and spatial exposure estimates for ecological receptors (*i.e.*, plants and animals). The output concentrations from TRIM.FaTE also can be used as inputs to a human exposure model, such as TRIM.Expo, to estimate human exposures.

Significant features of TRIM.FaTE include: (1) the implementation of a truly coupled multimedia model; (2) the flexibility to define a variety of scenarios, in terms of the links among compartments as well as the number and types of compartments, as appropriate for the desired spatial and temporal scale of assessment; (3) the use of a transparent approach to chemical mass transfer and transformation based on an algorithm library that allows the user to change how environmental processes are modeled; (4) an accounting for all of the pollutant as it moves among the environmental compartments; (5) an embedded procedure to characterize uncertainty and variability; and (6) the capability to provide exposure estimates for ecological receptors. The TRIM.FaTE module is the most fully developed of the TRIM modules at this time, and this development has produced a library of algorithms that account for transfer of chemical mass throughout an environmental system, a database of the information needed to initialize these algorithms for a test site, and a working computer model.



## 1.2.2 DESCRIPTION OF TRIM.Expo

The TRIM.Expo module, similar to most human exposure assessment models, provides an analysis of the relationships between various chemical concentrations in the environment and exposure levels of humans. Because multiple sources of environmental contamination can lead to multiple contaminated media, including air, water, soil, food, and indoor air, it is useful to focus on the contaminated environmental media with which a human population will come into contact. These media typically include the envelope of air surrounding an individual, the water and food ingested by an individual, and the layer of soil and/or water that contacts the surface of an individual. The magnitude and relative contribution of each exposure pathway must be considered to assess total exposure to a particular chemical. Currently, the focus of TRIM.Expo development is on inhalation and ingestion exposure; however, dermal exposure will be added later.

The exposure analysis process consists of relating chemical concentrations in environmental media (*e.g.*, air, surface soil, root zone soil, surface water) to chemical concentrations in the exposure media with which a human or population has contact (*e.g.*, air, tap water, foods, household dusts, and soils). The initial prototype for TRIM.Expo will predict exposure by tracking the movement of a population cohort through locations where chemical exposure can occur according to a specific activity pattern. In a typical application, TRIM.FaTE could be used to provide an inventory of chemical concentrations across the ecosystem at selected time intervals (*e.g.*, days, hours). For chemicals that are not persistent and/or bioaccumulative, processed air monitoring data or air dispersion modeling results can be substituted for TRIM.FaTE output data. The TRIM.Expo module would then use these chemical concentration data, combined with the activity patterns of the cohorts, to estimate exposures. The movements are defined as an exposure-event sequence that can be related to time periods for which exposure media concentrations are available (*e.g.*, from TRIM.FaTE, ambient data, and/or dispersion modeling results). Each exposure event places the population cohort in contact with one or more environmental media within a specified microenvironment (*e.g.*, inside a home, along a road, inside a vehicle) in an exposure district for a specified time interval. In addition to the location assignments, the

### TRIM.Expo KEY TERMS

**Cohort** - A group of people within a population with the same demographic variables who are assumed to have similar exposures.

**Activity pattern** - A series of discrete events of varying time intervals describing information about an individual's lifestyle and routine. The information contained in an activity pattern typically includes the locations that the individual visited (usually described in terms of microenvironments), the amount of time spent in those locations, and a description of what the individual was doing in each location (*e.g.*, sleeping, eating, exercising).

**Microenvironment** - A defined space in which human contact with an environmental pollutant takes place and which can be treated as a well-characterized, relatively homogeneous location with respect to pollutant concentrations for a specified time period.

**Exposure district** - A geographic location within a defined physical or political region where there is potential contact between an organism and a pollutant and for which environmental media concentrations have been estimated either through modeling or measurement.

exposure event would provide information relating to the potential for pollutant uptake, such as respiration rate and quantity of water consumed. The TRIM.Expo module is intended to contribute to a number of health-related assessments, including risk assessments and status and trends analyses.

### 1.2.3 DESCRIPTION OF TRIM.Risk

Risk characterization is the final step in risk assessment and is primarily used to integrate the information from the other three key steps (*i.e.*, hazard identification, dose-response assessment, exposure assessment). Within the TRIM framework, TRIM.Risk, the risk characterization module, will be used to integrate the information on exposure (human or ecological receptor) with that on dose-response or hazard and for providing quantitative descriptions of risk and some of the attendant uncertainties. The TRIM.Risk module will provide decision makers and the public with information for use in developing, evaluating, and selecting appropriate air quality standards and risk management strategies. The purpose of TRIM.Risk is to integrate information from other TRIM modules and to facilitate the preparation of a risk characterization. The TRIM.Risk module will, therefore, be able to summarize or highlight the major points from each of the analyses conducted in the other TRIM modules. Where possible, the TRIM.Risk module will do so in an automated manner. In general, TRIM.Risk will (1) document assumptions and input data, (2) conduct risk calculations and data analysis, and (3) present results and supporting information.

Current and proposed EPA guidance on risk characterization will guide the development of TRIM.Risk. The TRIM.Risk module will be developed in a phased approach similar to other TRIM modules. Ideally, TRIM.Risk will provide all of the information required to prepare a full risk characterization. However, the type and variability of information needed for this purpose are vast. Therefore, the type of information generated by TRIM.Risk will evolve over time as the Agency gains experience and has the resources to implement more flexibility. For example, early versions of TRIM.Risk will be limited to preparing summaries of input data and results, without supporting text. However, as the Agency gains experience, it may be possible to incorporate generic language to more fully describe the information required for a full risk characterization. Many EPA risk assessments will be expected to address or provide descriptions of (1) individual risk,<sup>4</sup> including the central tendency and high-end portions of the risk distribution, (2) population risk, and (3) risk to important subgroups of the population such as highly exposed or highly susceptible groups or individuals, if known. Some form of these three types of descriptors will be developed within TRIM.Risk and presented to support risk characterization. Because people process information differently, it is appropriate to provide more than one format for presenting the same information. Therefore, TRIM.Risk will be designed so that the output can be presented in various ways in an automated manner (*e.g.*, Chart Wizard in Microsoft<sup>®</sup> Excel), allowing the user to select a preferred format.

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<sup>4</sup> The phrase individual risk as used here does not refer to a risk estimate developed specifically for a single member of a population. Rather, it refers to the estimate of risk for a subgroup of a population that is presented as an estimate of the risk faced by a person rather than by the population as a whole.

## 1.3 TRIM DEVELOPMENT

In the development of TRIM, existing models and tools are being relied upon where possible. Adopting or incorporating existing models or model components into a tool that meets OAQPS' needs is preferable as it is usually the most cost-effective approach. Consequently, review of existing models and consideration of other current modeling efforts is an important part of TRIM development activities. Reviews of relevant models existing at the initiation of development activities for each module are described in this document and in the TRIM.FaTE TSD. Additionally, OAQPS is closely following several current activities as they relate to TRIM.

Current Agency model development activities relevant to TRIM development include the recently published updated guidance on assessing health risks associated with indirect exposure to combustor emissions (U.S. EPA 1999h). This guidance, previously referred to as the Indirect Exposure Methodology (IEM), is now called the Multiple Pathways of Exposure (MPE) method. In addition, the multimedia model, FRAMES-HWIR, has recently been developed by the Agency to support a specific risk assessment need regarding hazardous chemicals released from land-based waste management units. The FRAMES-HWIR model has been developed as part of a focused fast-track (two-year) effort to support a risk-based regulation regarding disposal of hazardous waste (HWIR99).<sup>5</sup> Another model of interest for multimedia pollutants is the Stochastic Human Exposure and Dose Simulation (SHEDS) model (*e.g.*, Özkaynak et al. 1999). The OAQPS will be carefully considering the various aspects of MPE, FRAMES-HWIR, and SHEDS with regard to OAQPS needs, as well as compatibility with or future improvements or evaluations of TRIM. As TRIM is intended to be a dynamic method, developmental activities will consider and respond as appropriate to newly available methods and scientific information.

A current major Agency research project involves the design and development of a flexible software system to simplify the development and use of air quality models and other environmental decision support tools. This system, called Models-3, is designed for applications ranging from regulatory and policy analysis to understanding the complex interactions of atmospheric chemistry and physics (U.S. EPA 1999d). The June 1999 release of Models-3 contains a Community Multi-Scale Air Quality (CMAQ) modeling system for urban- to regional-scale air quality simulation of tropospheric ozone, acid deposition, visibility, and fine particles. The long-term goal is to extend the system to handle integrated cross-media assessments and serve as a platform for community development of complex environmental models. In recognition of the availability of Models-3 over the longer term, OAQPS has designed and is developing the TRIM computer framework to be compatible with the Models-3 system.

### 1.3.1 INITIAL DEVELOPMENT ACTIVITIES

The first phase of TRIM development included the conceptualization of TRIM and the implementation of the TRIM conceptual approach through the development of a prototype of the first TRIM module, TRIM.FaTE (U.S. EPA 1998a). The progress on TRIM.FaTE included the development of (1) a conceptual design for the module; (2) a library of algorithms that account

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<sup>5</sup> The FRAMES-HWIR documentation is scheduled for public release in fall 1999.

for chemical mass transfer throughout the ecosystem; (3) a database to initialize the algorithms for a test site; and (4) a working prototype in spreadsheet format.

Consistent with Agency peer review policy (U.S. EPA 1998c) and the 1994 Agency Task Force on Environmental Regulatory Modeling (U.S. EPA 1994a), internal and external peer review are an integral part of the TRIM development plan. Following the first phase of TRIM development, OAQPS submitted TRIM to SAB under their advisory method of review (U.S. EPA 1998b). In May 1998 in Washington, DC, the Environmental Models Subcommittee (Subcommittee) of the Executive Committee of SAB reviewed the TRIM project. The SAB Subcommittee was charged with assessing the overall conceptual approach of TRIM and the specific approach of TRIM.FaTE.

The SAB Subcommittee reported that the development of TRIM and the TRIM.FaTE module was conceptually sound and scientifically based (U.S. EPA 1998b). The SAB Subcommittee provided specific recommendations related to six specific charge questions. The SAB recommendations are detailed in Chapter 2 of the TRIM Status Report along with brief responses, and changes to TRIM.FaTE based in part on the SAB recommendations are highlighted in Chapter 4 of the TRIM Status Report.

### **1.3.2 RECENT ACTIVITIES**

During the most recent developmental phase of TRIM, progress has been made in many areas, including a change to the overall modular design of TRIM. As shown in Figure 1-1, the TRIM design now includes three modules: TRIM.FaTE, TRIM.Expo, and TRIM.Risk. The design presented to SAB in May 1998 included three other modules (Pollutant Uptake, Biokinetics, and Dose/Response). In recognition of the flexibility of the TRIM design, which provides an ability to rely on a variety of input data and outside models, OAQPS decided not to include the development of these modules in the TRIM design at this time.

In consideration of SAB comments, TRIM.FaTE was refined, including the development of new and updated capabilities, as well as the development and limited testing of methodologies for model set-up, uncertainty and variability analysis, and evaluation. In addition, OAQPS developed a conceptual plan for TRIM.Expo, initiated work on a prototype of TRIM.Expo (initially focusing on inhalation), and developed a conceptual design for TRIM.Risk. Furthermore, the overall computer framework for TRIM was designed and implemented in a PC-based platform, and substantial progress was made in installing TRIM.FaTE into this framework. Changes and additions to TRIM.FaTE are discussed in more detail in Chapter 4 of the TRIM Status Report. The development of TRIM.Expo is discussed in Chapter 8, and the conceptual plan for TRIM.Risk is described in Chapter 9 of the TRIM Status Report. In addition, the TRIM.FaTE TSD provides more details on TRIM.FaTE.

The current TRIM documentation has gone through internal Agency peer review, which involved reviewers across the Agency, including the major program offices, the Office of Research and Development, and staff involved in the Agency's Models 2000 efforts. The current SAB advisory will be the second on TRIM development activities.

### 1.3.3 FUTURE ACTIVITIES

Following the 1999 SAB advisory, improvements will be made to the uncertainty and variability approach, TRIM.Expo prototype, and TRIM.Risk conceptual plan. These revisions are scheduled to be completed in 2000. As needed, refinements will be made to the TRIM.FaTE evaluation plan, and completion of the bulk of those activities are also scheduled for 2000. The Agency has planned for a substantial amount of progress on each of the TRIM modules for 2000 and 2001, as described below.

- **TRIM.FaTE.** Future work on TRIM.FaTE will include model evaluation activities and additional development of the module to accommodate additional chemicals. The TRIM.FaTE module is expected to be available for limited external use late in 2000 and to be publicly released in 2001.
- **TRIM.Expo.** Future work on TRIM.Expo in 2000 will include the further development of ingestion algorithms, incorporation of EPA's Air Pollutant Exposure Model (APEX) coding into the TRIM platform followed by adjustments to APEX to include ingestion algorithms, a test case of the inhalation pathway, and a test case of inhalation and ingestion pathways. Over the longer term, addition of the dermal pathway to the module will be initiated.
- **TRIM.Risk.** Development of TRIM.Risk will begin after SAB comments are received on the conceptual design. Module development will include identification of data needs and formatting of data outputs. Programming for a TRIM.Risk prototype is expected to be completed in 2000.
- **TRIM computer framework.** Further development of the TRIM computer framework, including incorporation of the TRIM.Expo (inhalation) module, will take place during 2000. Features to be refined during this time frame include limited geographic information system (GIS) or mapping capabilities. Additionally, long-range comprehensive GIS planning will occur. Development of user guidance materials is planned for 2000 (see text box).

In addition to consulting with Agency scientists during future TRIM development (*i.e.*, peer involvement), in late 2000 or early 2001, OAQPS will seek both internal and external peer review of new aspects following the next phase of TRIM development. In addition to the SAB, which provides the Agency with reviews, advisories, and consultations, other external peer review mechanisms consistent with Agency policy (U.S. EPA 1998c) include the use of a group of independent experts from outside the Agency (*e.g.*, a letter review by outside scientists), an *ad hoc* panel of independent experts, and peer review workshops. The OAQPS intends to seek the peer review mechanism appropriate to the importance, nature, and complexity of the material for review.

### USER GUIDANCE

Development of the TRIM user's guide is scheduled to begin in 2000, along with a plan for training activities. The OAQPS recognizes the importance of developing detailed user guidance that will assist users in defining, for a particular modeling application, the spatial and temporal resolution, compartments and linkages, and parameters and initial conditions. For example, the TRIM.FaTE guidance will likely emphasize the value of performing several different preliminary simulations in verifying the adequacy of the parcel and compartment specifications for the desired application. Similarly, detailed user guidance will be developed for TRIM.Expo to assist users in defining cohorts, study areas, exposure districts, and microenvironments, as well as various parameters and exposure factors.

It also will be important for the guidance to note the responsibility of the user in defining the simulation as appropriate to the application. For example, in TRIM.FaTE, default values will likely be made available with the model for a variety of parameters ranging from physiological characteristics of various biota to physical characteristics of abiotic media; the user will need to consider appropriateness of these values or others (*e.g.*, site-specific data) for their application. While the TRIM modules are intended to provide valuable tools for risk assessment, and their documentation and guidance will identify, as feasible, uncertainties and limitations associated with their application, the guidance will emphasize that their appropriate use and the characterization of uncertainties and limitations surrounding the results are the responsibility of the user.

## 1.4 PHASING TRIM INTO OAQPS' SET OF MODELING TOOLS

As mentioned earlier, TRIM is intended to support assessment activities for both the criteria and hazardous air pollutant programs of OAQPS. As a result of the greater level of effort expended by the Agency on assessment activities for criteria air pollutants, these activities are generally more widely known. To improve the public understanding of the hazardous air pollutant (or air toxics) program, the Agency published an overview of the air toxics program in July 1999 (U.S. EPA 1999e). Air toxics assessment activities (National Air Toxics Assessment,

or NATA) are described as one of the program's key components.<sup>6</sup> The NATA includes both national- and local-scale activities. The TRIM system is intended to provide tools in support of local-scale assessment activities, including multimedia analyses.

One of the Agency's most immediate needs for TRIM comes in the Residual Risk Program, in which there are statutory deadlines within the next two to nine years for risk-based emissions standards decisions. As described in the *Residual Risk Report to Congress* (U.S. EPA 1999f), TRIM is intended to improve upon the Agency's ability to perform multipathway human health risk assessments and ecological risk assessments for HAPs with the potential for multimedia environmental distribution. Another important upcoming use for TRIM is in exposure assessment in support of the review of the ozone NAAQS. The TRIM.Expo and TRIM.Risk modules augmented with external air quality monitoring data and models are intended to support this type of criteria pollutant assessment as well as risk assessments for non-multimedia HAPs.

#### EXAMPLES OF TRIM APPLICATIONS

- A human health or ecological assessment of multimedia, multipathway risks associated with mercury emissions from one or several local sources could be performed using all three modules in the TRIM system.
- An assessment of human health risks associated with air emissions of a criteria air pollutant (e.g., ozone) or one or several volatile HAPs in a metropolitan area could be developed using an external air model or ambient concentration data from fixed-site monitors coupled with TRIM.Expo and TRIM.Risk.

Consistent with the phased plan of TRIM development, the application of TRIM will also be initiated in a phased approach. With the further development of the TRIM modules in 2000 and 2001, EPA will begin to use the modules to contribute to or support CAA exposure and risk assessments. These initial applications also will contribute to model evaluation. The earliest TRIM activities are expected to include the use of TRIM.FaTE side-by-side (at a comparable level of detail) with the existing multimedia methodology<sup>7</sup> in risk assessments of certain multimedia HAPs (e.g., mercury) under the Residual Risk Program. As TRIM.Expo is developed to accommodate inhalation modeling of HAPs and after it has undergone testing, OAQPS plans to initially run it side-by-side (at a comparable level of detail) with EPA's existing inhalation

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<sup>6</sup> Within the air toxics program, these activities are intended to help EPA identify areas of concern (e.g., pollutants, locations, or sources), characterize risks, and track progress toward meeting the Agency's overall air toxics program goals, as well as the risk-based goals of the various activities and initiatives within the program, such as residual risk assessments and the Integrated Urban Air Toxics Strategy. More specifically, NATA activities include expansion of air toxics monitoring, improvements and periodic updates to emissions inventories, national- and local-scale air quality modeling, multimedia and exposure modeling (including modeling that considers stationary and mobile sources), continued research on health effects of and exposures to both ambient and indoor air, and use and improvement of exposure and assessment tools. These activities are intended to provide the Agency with improved characterizations of air toxics risk and of risk reductions resulting from emissions control standards and initiatives for both stationary and mobile source programs.

<sup>7</sup> In support of the *Mercury Report to Congress* (U.S. EPA 1997a) and the *Study of Hazardous Air Pollutant Emissions from Electric Utility Steam Generating Units -- Final Report to Congress* (U.S. EPA 1998d), the Agency relied upon the Indirect Exposure Methodology, which has recently been updated and is now termed the Multiple Pathways of Exposure methodology (U.S. EPA 1999h). This methodology is being used in initial assessment activities for the Residual Risk Program (U.S. EPA 1999f).

exposure model, HEM (Human Exposure Model (U.S. EPA 1986)). When TRIM.Risk has been completed, it will be used, as appropriate, in both criteria and hazardous air pollutant risk assessments.

In later years, OAQPS intends to use TRIM and the TRIM modules in a variety of activities including (1) residual risk assessments using TRIM.FaTE, TRIM.Expo, and TRIM.Risk, in combinations appropriate to the environmental distribution characteristics of the HAPs being assessed; (2) urban scale assessments on case study cities as part of the Integrated Urban Air Toxics Strategy; and (3) exposure and risk assessments of criteria air pollutants (*e.g.*, ozone, carbon monoxide) in support of NAAQS reviews.



## 2. TRIM.Expo: GENERAL OVERVIEW AND BACKGROUND

Human exposures to pollutants can result from contact with contaminated air, water, soils, and food, as well as with drugs and consumer products. Exposures may be dominated by contact with a single medium, or concurrent contacts with multiple media may be significant. The nature and extent of such exposures depend largely on two things: (1) human factors and (2) the concentrations of a pollutant in the exposure media. Human factors include all behavioral, sociological, and physiological characteristics of an individual or cohort (*i.e.*, a group of people within a population that can be aggregated because the variation in exposure within the group is much less than the group-to-group variation across the population) that directly or indirectly affect a person's contact with the substances of concern. Important behavioral factors are contact rates with food, air, water, and soils. Activity patterns, which are defined by an individual's or cohort's allocation of time spent in different activities at various locations, are also significant because they directly affect the magnitude of exposures to substances present in different indoor and outdoor environments. Information on activity patterns are taken from measured data collected during field and telephone surveys of individuals' daily activities, the amount of time spent engaged in those activities, and the locations where the activities occur.

**EXPOSURE**

The contact between a target organism and a pollutant at the outer boundary of the organism. Exposure may be quantified as the amount of pollutant available at the boundary of the receptor organism per specified time period.

From an exposure assessment standpoint, the principal goal is to estimate or measure exposure as a function of both the relevant human factors and the measured or estimated pollutant concentrations in the contact, or exposure, media.

### 2.1 RATIONALE AND NEED FOR TRIM.Expo

The models currently being used by OAQPS for estimating human exposure to criteria air pollutants and HAPs do not include multimedia exposures. Furthermore, the models that estimate exposures to HAPs do not adequately estimate the spatial and temporal patterns of exposures for all of the HAPs listed in section 112(b) of the CAA. In addition, a review of currently available exposure models and modeling systems revealed that no single model or modeling framework meets the needs of OAQPS, or could function effectively by itself as part of the TRIM modeling system for estimating multimedia exposures for a population. Most models are constrained by the types of media and environmental processes that can be addressed. Furthermore, no model was identified that addresses the broad range of pollutants and environmental fate and transport processes that are anticipated to exist for HAPs and criteria air pollutants. Therefore, OAQPS concluded that the currently available exposure models and modeling frameworks are not sufficiently integrated multimedia systems that can provide the temporal and spatial resolution needed for estimating human exposures.

The TRIM exposure assessment process relates pollutant concentrations in the larger environmental media to pollutant concentrations in the immediate exposure media with which a human population has direct

contact. TRIM.Expo simulates the movement of an individual and/or cohorts according to activity patterns through locations (called microenvironments) in a defined physical or political region (*i.e.*, exposure districts). The movement of individuals or cohorts coincides with pollutants at varying concentrations. This creates the potential for contact between individuals or cohorts and pollutants, thus allowing the estimation of exposures of various individuals and cohorts within the population to the pollutants of interest.

#### EXPOSURE ASSESSMENT

Measurement or estimation of the magnitude, frequency, duration, and route of exposure of biological organisms to pollutants in the environment for a specified time period. An exposure assessment also describes the nature of exposure and the size and nature of the exposed populations.

While OAQPS supports and recognizes the value of collecting pollutant monitoring data for a variety of tasks (*e.g.*, assessment of trends, determination of attainment of standards for criteria pollutants, evaluation

of exposure models), exposure modeling is clearly needed for several reasons. First, it is very difficult to monitor the exposure of humans to low concentration mixtures of a large number of environmental pollutants. Direct monitoring of exposure (*i.e.*, personal monitoring) has been carried out for a number of airborne pollutants, but only limited direct monitoring studies have been used to assess ingestion and dermal exposures. Furthermore, direct monitoring is a resource intensive process. This is especially true for large populations, where the planning, conduct, and evaluation of such direct monitoring studies can be a lengthy and costly process.

#### TRIM'S EXPOSURE ASSESSMENT PROCESS

TRIM.Expo relates pollutant concentrations in the larger environmental media to pollutant concentrations in the immediate exposure media with which a human population has direct contact.

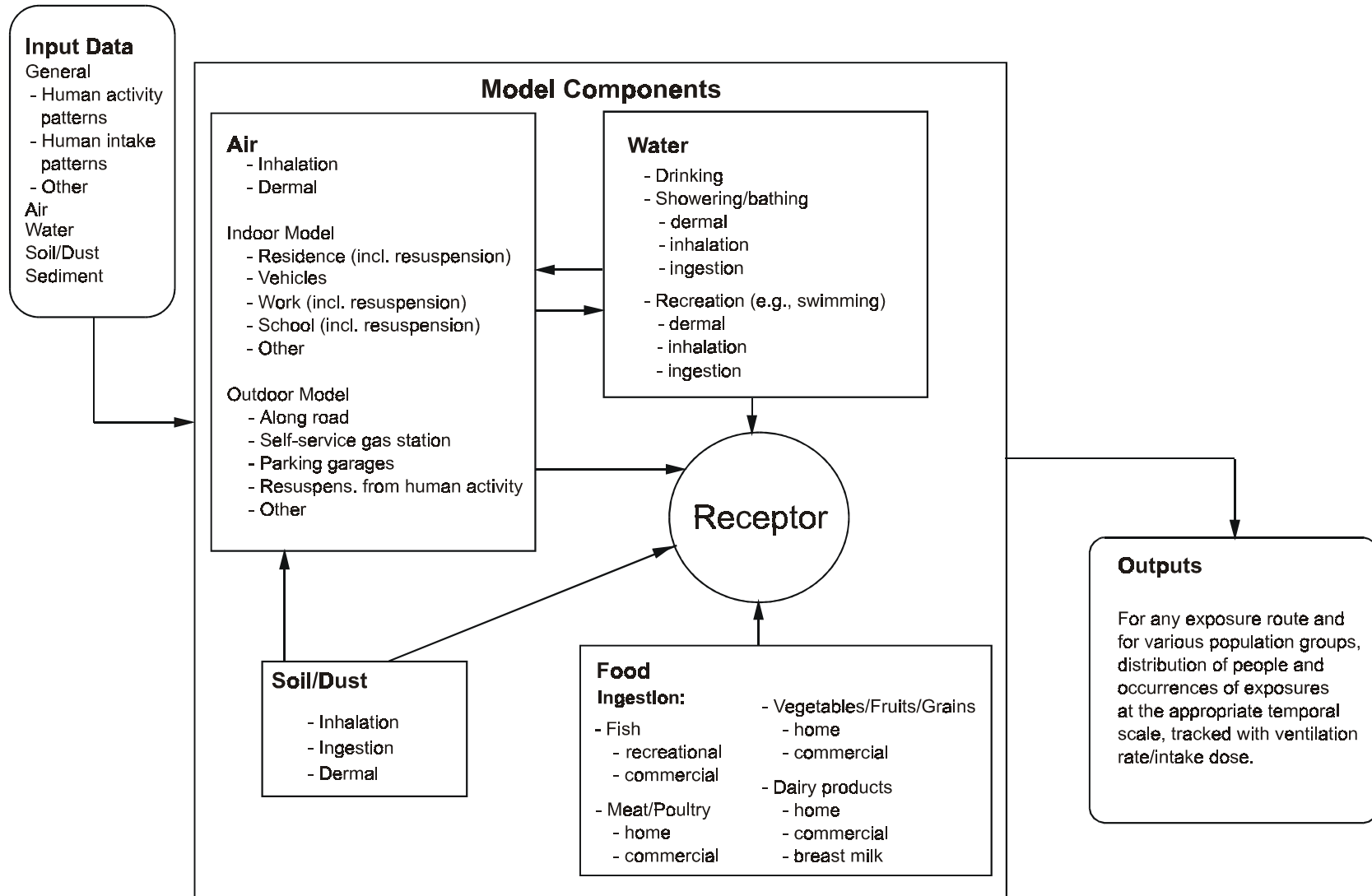
In addition, the use of modeling is required or preferred to address the following regulatory assessment needs.

- **Consideration of hypothetical situations.** Modeling can address situations such as impacts of planned facilities, proposed controls on existing facilities, exposure upon attainment of ambient standards, and accidental releases.
- **Temporal flexibility.** Modeling can be performed for a future time period.
- **Source attribution.** Individual sources and/or source categories can be tracked throughout the modeling process to yield estimates of the relative contribution or importance of each source or source category to overall exposures.

- **Inclusion of more chemical species.** Personal monitoring techniques do not exist for all pollutants at the present time.
- **Representation of long-term conditions.** Modeling can address long-term time scales needed for assessment of chronic exposures. Personal monitoring studies are generally short-term studies, since wearing the monitoring equipment is too burdensome for long-term studies to be practical.

The extent to which modeled exposure estimates would differ between the currently available models and a truly coupled source-to-dose, multimedia modeling system, such as TRIM, is unknown. However, models that are not fully coupled have long been considered to lack scientific credibility. Therefore, OAQPS has determined that it is necessary to undertake efforts to develop a truly coupled multimedia exposure modeling framework. Figure 2-1 illustrates the selected modeling features of TRIM.Expo. Because TRIM.Expo will be developed using a phased approach, future development of the model may include model components in addition to those shown in Figure 2-1.

**Figure 2-1**  
**Conceptual Diagram of TRIM.Expo**



## 2.2 IMPORTANT DEFINITIONS

To enhance understanding throughout this document, the following discussions define various terms relevant to exposure modeling. These definitions are based primarily on the guidelines published by EPA (U.S. EPA 1992a).

### 2.2.1 BASIC DEFINITIONS RELATED TO EXPOSURE

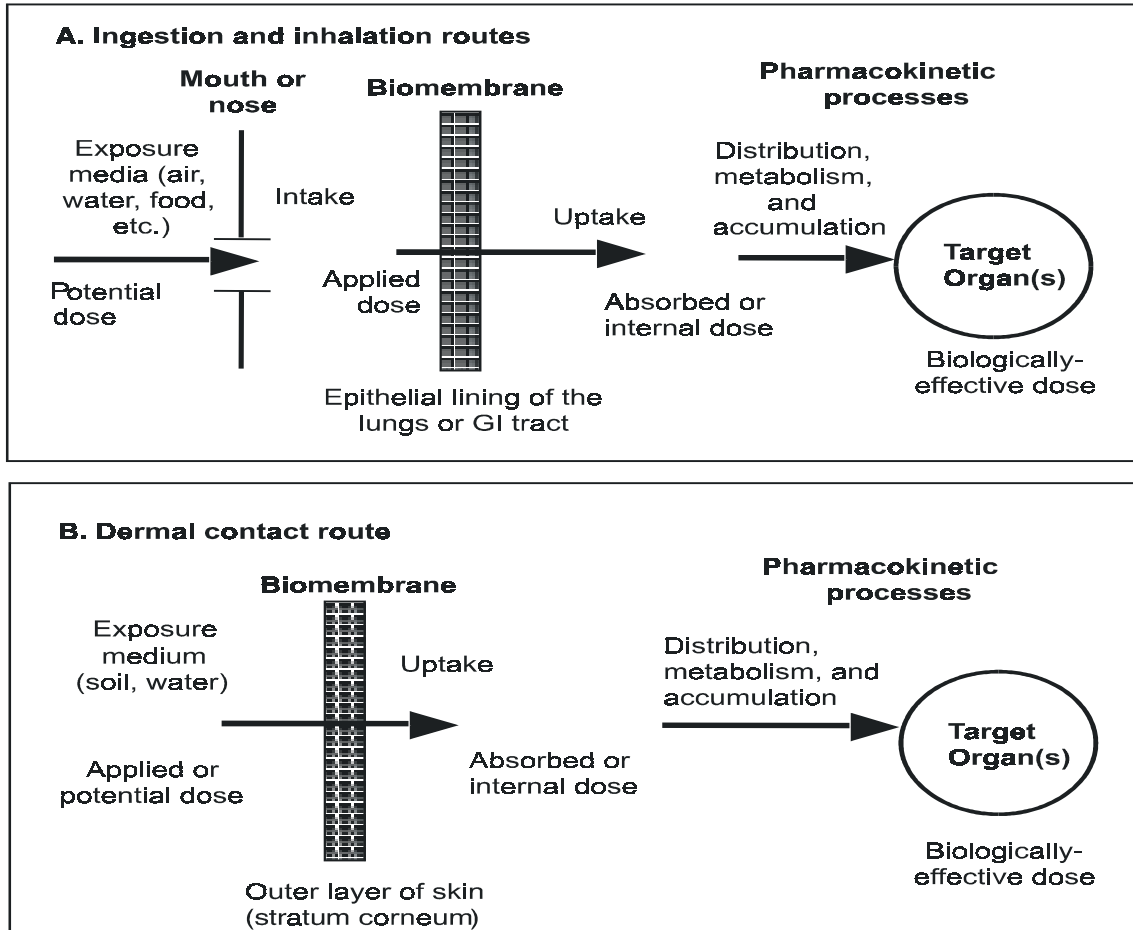
<b>BASIC DEFINITIONS RELATED TO EXPOSURE</b>	
<b>Environmental media</b>	Components of the physical environment that carry a pollutant, and through which pollutants can move and reach organisms (e.g., ambient air, ground water, surface water, surface soil, root zone soil, vadose zone soil, and several classes of vegetation).
<b>Exposure</b>	The contact between a target organism and a substance at the outer boundary of an organism. Exposure may be quantified as the amount of substance available at the boundary of the receptor organism per specified time period. For inhalation, exposure over a period of time can be represented by a time-dependent profile of the exposure concentration.
<b>Exposure district</b>	A geographic location within a defined physical or political region, where there is potential contact between an organism and a pollutant, and for which environmental media concentrations have been estimated either through modeling or measurement.
<b>Exposure factor</b>	A normalizing or standardizing factor used in an exposure assessment as a surrogate for specific information that is not available for a particular subject, cohort, or demographic group. These factors often are drawn from a distribution or range of data; see, for example, EPA's <i>Exposure Factors Handbook</i> (U.S. EPA 1997b).
<b>Exposure medium</b>	The part of the physical environment that surrounds or contacts organisms at the time of an exposure. The exposure media in TRIM.Expo include: outdoor air, indoor air (multiple microenvironments), tap water, home-grown food, locally-produced food, prepared food, breast milk, house dust, soil, swimming pools, and other recreational surface water.
<b>Exposure pathway</b>	The physical course a pollutant takes from the source to the organism exposed. An exposure pathway describes a unique mechanism by which an individual or population is exposed to pollutants or physical agents at, or originating from, a site. Each exposure pathway includes a source, or release from a source, an exposure point, and an exposure route. If the exposure point differs from the source, a transport/exposure medium (such as air) or media (in cases of intermedia transport, such as water to air) is also included.
<b>Exposure route</b>	The way a pollutant or physical agent comes in contact with an organism (e.g., inhalation, ingestion, dermal contact).

## 2.2.2 BASIC DEFINITIONS RELATED TO DOSE

TRIM.Expo will focus on the estimation of exposure only; estimation of dose, where appropriate, will need to be addressed by dosimetry modeling. Nevertheless, it is useful to review some concepts related to dose to create a context for understanding how the outputs of TRIM.Expo are likely to be used. This section contains definitions for several of these terms and clarifies the terminology used in this document. Figure 2-2 illustrates the relationships among many of these terms for the inhalation, ingestion, and dermal contact routes.

<b>BASIC DEFINITIONS RELATED TO DOSE</b>	
<b>Absorbed dose</b>	The amount of a pollutant crossing the exchange boundaries of an organism after contact, usually expressed as the mass of pollutant absorbed into the body per unit body mass per unit time, such as mg/kg/d. Absorbed dose is calculated from the intake and absorption efficiency. For inhalation exposure, absorbed dose is the amount of material that passes from the gas volume of the lung into the blood. For ingestion exposure, absorbed dose is the quantity of pollutant that passes from the gastrointestinal tract across the gut wall and into the blood stream. For dermal exposure, absorbed dose is the quantity of material that passes through the stratum corneum into the living cells of the epidermis and dermis and then into the blood stream. In some cases, the absorbed dose is referred to as the internal dose.
<b>Applied dose</b>	The amount of a pollutant given in mg/kg/d that comes in contact with the living tissue of an organism by entering into the lungs, by entering the gastrointestinal tract, and/or by crossing the stratum corneum into the living cells of the epidermis. In some experimental designs, the applied dose is referred to as the administered dose.
<b>Average Daily Dose (ADD)</b>	Dose rate within a population averaged over body weight and an averaging time and typically expressed in terms of mg/kg/d.
<b>Intake</b>	The process by which a pollutant is physically moved through an opening in the outer boundary (usually the mouth or nose) of the human body, typically via ingestion or inhalation.
<b>Lifetime Average Daily Dose (LADD)</b>	The average daily dose within a population when the averaging time is the expected individual lifetime. The LADD is usually expressed in terms of mg/kg/d. The LADD is used for compounds with carcinogenic or chronic effects.
<b>Potential dose</b>	An approximation of applied dose that is simply the amount of pollutant in the food or water ingested, air inhaled, or material applied to skin. The potential dose for ingestion and inhalation is analogous to the administered dose in a dose-response experiment. For the dermal route, the potential dose is the amount of pollutant applied or the amount of pollutant in the medium applied to skin.
<b>Uptake</b>	The process by which a substance crosses an absorption barrier and is absorbed into the body. Although the chemical is often contained in a carrier medium, the medium itself is typically not absorbed at the same rate as the chemical.

**Figure 2-2**  
**Illustration of the Relationships among Exposure and Dose**  
**for the Inhalation, Ingestion, and Dermal Contact Routes**



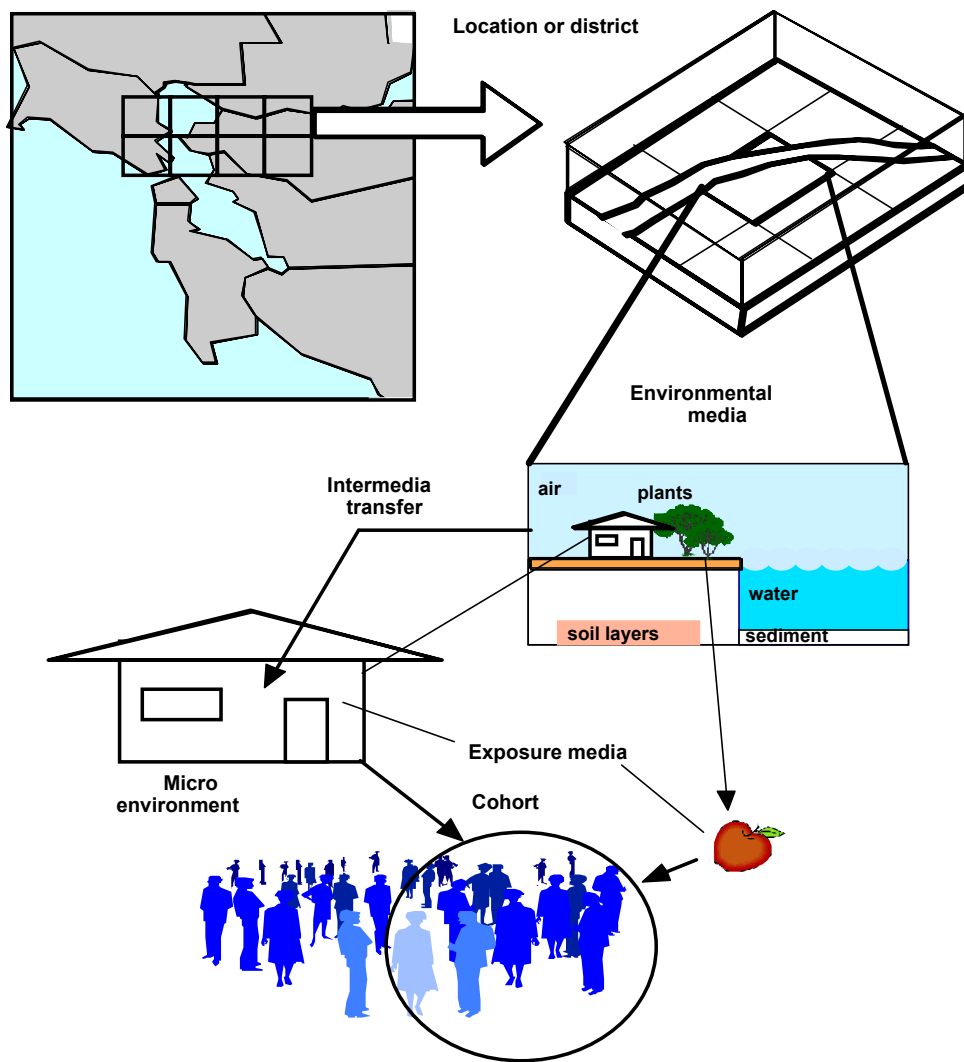
### 2.2.3 OTHER IMPORTANT TRIM.Expo DEFINITIONS

Figure 2-3 illustrates the interconnected nature of the relationships among location (districts), environmental media, microenvironments, intermedia transfers, exposure media, and cohorts as defined in this section.

<b>OTHER IMPORTANT TRIM.Expo DEFINITIONS</b>	
<b>Cohort</b>	A group of people within a population with the same demographic variables who are assumed to have similar exposures. Individuals within a cohort can be aggregated for exposure assessment purposes because the variation in exposure within the cohort is much less than the cohort-to-cohort variation across the broader population.
<b>Intermedia transfer</b>	An algorithm for “linking” the environmental media with the microenvironmental media that exposed individuals occupy (e.g., air compartments) or the exposure media with which they come in contact (e.g., air, water, food, soil). An intermedia transfer algorithm relates the pollutant concentration in a microenvironmental medium to the concentration in an ambient environmental medium that provides pollutant inputs to that microenvironment.
<b>Microenvironment</b>	A defined space in which human contact with an environmental pollutant takes place and which can be treated as a well-characterized, relatively homogeneous location with respect to pollutant concentrations for a specified time period. Microenvironments include spaces within buildings (e.g., rooms, household volumes, restaurants, schools), spaces inside vehicles (e.g., cars, buses, trains), and other spaces within which humans have contact with environmental pollutants (e.g., swimming pools, bathtubs, lakes, rivers).



**Figure 2-3**  
**Relationships among Districts, Environmental Media, Microenvironments, Intermedia Transfers, Exposure Media, and Cohorts**



### 2.3 APPROACH USED IN DEVELOPING TRIM.Expo

Based on a review of currently available exposure models and modeling systems (discussed in Chapter 3 of this report), no single model was identified that would exclusively satisfy all of the modeling features and requirements that TRIM.Expo will satisfy. However, several components of existing models were found to meet certain requirements of TRIM.Expo, and these components will be adapted for use in TRIM.Expo. For example, EPA is developing the Air Pollutant Exposure Model (APEX), which is based on EPA's human exposure models, probabilistic NAAQS Exposure Models (pNEM), and Hazardous Air Pollutant Exposure Model (HAPEM4). The APEX framework will be adapted to address both short- and long-term

exposures for the inhalation pathways modeled by TRIM.Expo. It also includes the incorporation of activity patterns to track cohorts and individuals as they move among exposure media. The pNEM model also includes a mass balance treatment of the relationship between environmental medium (*i.e.*, outdoor air) and exposure medium (*i.e.*, indoor air), as well as the characterization of uncertainty and variability.

For the ingestion pathways, exposure algorithms from the California Total Exposure Model for Hazardous Waste Sites (CalTOX) will be incorporated into TRIM. Expo. The CalTOX framework is capable of modeling multimedia transport and transformation of pollutants, and multipathway exposure for humans.

For the first prototype of TRIM.Expo, the exposure routes will be limited to inhalation and ingestion. However, TRIM.Expo will eventually be capable of modeling exposures from all three main routes of environmental exposure: inhalation, ingestion, and dermal contact.

## **2.4 TAXONOMY OF EXPOSURE ATTRIBUTES FOR MULTIMEDIA POLLUTANTS**

Despite the large amount of data and the numerous variables used in an exposure assessment, a relatively small subset of these variables actually significantly influences the estimated exposures (Morgan and Henrion 1990). However, little is known about how to isolate this defining set of variables and data. One potential method of sorting and organizing the complex web of exposure information that is collected during a modeling study is to develop a taxonomy of exposure-related questions that an exposure model is expected to answer. The purpose of this taxonomy is to first identify the relevant characteristics or properties as *building blocks*, and then rank the attributes of exposure that are important to both analysts and decision-makers. The taxonomy of exposure-related questions derived during TRIM.Expo's development is presented in the following sections.

### **2.4.1 EXPOSURE CHARACTERIZATION PROCESS AND EXPOSURE ATTRIBUTES**

Most of the inhalation pollutant exposures addressed by TRIM.Expo are location-specific and the individual's or cohort's locations and activities need to be tracked over time and space. Accounting for time and space is an important factor in determining exposure because of the spatial and temporal differences in pollutant concentrations among different exposure media. A log of the time- and activity-specific locations of individuals or cohorts and the time-specific concentrations of pollutants in the relevant exposure media is needed to create such an *exposure characterization process*. A critical issue in the exposure characterization process is to identify appropriate and transparent methods to combine pollutant concentration data with activity tracking information to assess both short- and long-term exposures. To develop the exposure characterization process for TRIM.Expo, the following attributes that define an exposure event (*i.e.*, human activities that bring people in contact with one or more pollutants in a microenvironment) were identified:

- Route of exposure;

- Temporal and spatial scale of the pollutant concentration;
- The seasonality of human activities and pollutant concentrations;
- Time scale of the health effects;
- Duration of the exposure event;
- Contributing environmental media;
- Exposure media; and
- Demographic characteristics of the exposed individual/cohort (*e.g.*, age, gender).

As shown in Figure 2-2, the route of exposure refers to the way the pollutant can enter the receptor during the exposure event (*i.e.*, inhalation, ingestion, dermal contact) and lead to actual absorption of the pollutant into the body (referred to as the route of potential uptake, *i.e.*, the process by which a pollutant crosses an absorption barrier and is absorbed into the body). The health effects resulting from an exposure may vary significantly among these three routes of exposure. Moreover, both the exposure media and exposure activity tend to be strongly associated with the route of potential uptake. For example, air is associated with the inhalation route, and the inhalation rate varies significantly with the type of activity. Water, food, and soil are associated with the ingestion route and with eating and hand-to-mouth related activities.

Pollutant concentrations over time and space are needed to construct an exposure event. If a pollutant shows little spatial variation in concentration over a large region, even if there is time variation in that region, there is little need for large numbers of separate geographic regions in an assessment. Similarly, for pollutant concentrations that do not vary significantly in time, even if they show large spatial variation, using longer time steps may be possible than that needed for a pollutant whose concentrations vary more greatly with time. TRIM.Expo will be flexible with regard to level of spatial resolution.

The interplay between the periodicity of human activities and pollutant levels is an important attribute for tracking by the exposure-event model. The often cyclic nature of human activities and pollutant levels is typically expressed in terms of seasonality in exposure modeling. Seasonality also affects people's habits such as whether they leave windows open or closed. This has a strong influence on the ability of outdoor pollutants to penetrate indoors. Another important attribute related to time that can affect exposure levels is the difference in activity patterns generally observed between weekdays and weekends. A person's activities, particularly those who work, are usually significantly different on weekends than they are on weekdays. It is important for an exposure model to distinguish between weekdays and weekends when constructing exposure-event sequences. TRIM.Expo will retain this information so that it is available to an analyst performing an exposure assessment. It should also be noted that in addition to a weekday/weekend effect in activity patterns, the emissions of many pollutants have a discernable weekday/weekend difference. The combination of effects caused by the day of the week, particularly weekdays versus weekends, makes this an important factor in exposure assessments.

The time scale of exposure associated with health effects for a particular pollutant also strongly affects the temporal resolution required of the exposure event-model. For some pollutants, including most of the criteria air pollutants and those HAPs associated with health effects due to short-term exposures, exposures may need to be assessed for periods as short as one hour or less. For many HAPs, only long-term cumulative exposure may need to be

characterized. TRIM.Expo will have the capability of aggregating exposures up from small time increments so that the subsequent time profile of exposure can match the time pattern or period of concern from a health perspective.

The durations of the exposure events and human activities are also important considerations in the structure of the exposure-event model. Other factors that affect the structure of the exposure-event model are the demographic characteristics of an exposed individual or cohort, such as age or gender, that may influence both the activity pattern and the health response to exposure. Proximity to particular emission sources, or health status, may also be important factors that affect the structure of the exposure event.

Cohorts are subsets of a population grouped so that the variation of exposure within a cohort is much lower than the variation between/among cohorts. The reason for using this approach is because the available data are not adequate to estimate the exposure of each individual in a population. Therefore, information about people who are expected to have similar exposures is aggregated together to make more efficient use of the limited data. The cohorts are assumed to contain people with exposures that can be characterized by the same probability distributions for key characteristics. The demographic variables used to describe a cohort are selected to minimize the differences between individuals within the cohort. The model selects an individual from the appropriate cohort and uses that individual's activity pattern data to create an exposure-event sequence for that day. The exposure event sequence represents the exposure pattern for the entire cohort. TRIM.Expo account for within cohort variability through multiple runs of the model for the exposure duration under study. As new statistical techniques are developed, future versions of TRIM.Expo will be modified to use the best available approaches for characterizing time/activity data. At the present time, however, the current method of using cohorts is a useful technique for modeling the exposures of a large population in the absence of complete time/activity pattern data.

TRIM.Expo is being designed to allow flexibility in the user's ability to select a cohort's characteristics. The demographic variables (*e.g.*, age, gender, work status) that characterize a cohort can be modified by a user of TRIM.Expo providing that the appropriate data are available. The level of stratification in the identification of the cohorts' characteristics depends on the particular problem being addressed and on the availability of data. Typically, input data for the demographic variables of a cohort are taken from census data. However, TRIM.Expo can be run using data supplied by the analyst as long as it is formatted correctly and provides sufficient information to execute the model. Hence, the cohorts' characteristics can be chosen for individualized studies on a site-specific or case-specific basis.

## **2.4.2 DIMENSIONS OF THE EXPOSURE ASSESSMENT PROBLEM**

The exposure attributes noted above were organized into a set of *key* exposure dimensions. The three most important dimensions of the exposure assessment problem were determined to be the (1) route of exposure, (2) time scale of an exposure event relevant to the pollutant's associated effects, and (3) degree of location dependence (*i.e.*, dependence of exposure on the location of the exposed subject). Addressing these three dimensions has a significant impact on the structure of the exposure model (*e.g.*, on the exposure media included, the degree of spatial resolution, and the level of temporal and spatial aggregation).

For example, consider a model used to assess inhalation exposures to pollutants with health effects that depend on the number and duration of contacts above some threshold concentration versus an exposure model used to assess ingestion contact with a pollutant that has health effects that depend primarily on a lifetime cumulative intake. The former model requires a compilation of short-term exposure events and must provide relatively detailed information on the location of the exposed individual. For the latter model, different temporal and spatial detail is required about the exposed individuals or cohorts (*i.e.*, a detailed time/location profile of the exposed cohort or individual is not as crucial as information on the location of the exposed cohort's/individual's food or water supply and the cumulative intake of food or water from a specific supply).

The primary time scales for exposure assessment models vary from short-term resolution (*e.g.*, minutes to hours and days) to long-term resolution (*e.g.*, days to months and years). Short-term resolution allows one to assess both cumulative intake as well as the number and duration of peak exposure events. Long-term resolution allows primarily for the assessment of cumulative intake. The quantitative distinction between short-term and long-term depends to some extent on the pharmacokinetics (*i.e.*, uptake and distribution) and toxicokinetics of the pollutants being considered.

Location-dependence specifies the level of detail required for the time-activity budget of an exposed individual. For example, to address inhalation exposures where pollutant concentrations vary significantly among several districts in which the exposed cohort or individual lives and differ strongly between indoor and outdoor microenvironments, location-dependence is high. However, if the properties of the pollutant are such that concentrations are similar in almost all microenvironments, then location-dependence is lower. For instance, for ingestion exposures to a pollutant in ground water that is distributed throughout a region, the location of the exposed cohort or individual is much less important than the source of the cohort's drinking water.

The above set of attributes gives rise to a broad range of exposure situations, such as short-term inhalation exposure with strong location dependence, long-term ingestion exposure with weak location-dependence, and short-term dermal contact exposure. The general exposure-event function used in TRIM.Expo can be adapted across the broad range of problems defined by these attributes. In some situations, combining two or more sets of exposure model attributes may be necessary (*i.e.*, combining long-term ingestion exposures that are weakly location-dependent with short-term inhalation exposures that are strongly location-dependent). TRIM.Expo will be designed to combine exposure model attributes, where possible.

## 2.5 TRIM EXPOSURE-EVENT CONCEPT

As stated previously, human exposures to pollutants may be dominated by contacts with a single medium, or concurrent contacts with multiple exposure media may be significant. The nature and extent of such exposures is mainly influenced by the pollutant concentrations in the exposure media and human factors (*i.e.*, behavioral, sociological, and physiological characteristics of an individual or cohort that directly or indirectly affect contact with pollutants). Therefore, from an exposure assessment standpoint the principal challenge is to estimate or

measure the individual or cohort exposure as a function of both the relevant human factors and the pollutant concentrations (measured and/or estimated) in the exposure media.

TRIM.Expo is built around the concept of simulating a series of exposure events. Exposure events are human activities that bring people in contact with a contaminated exposure medium within a specified microenvironment at a given geographic location for a specified period of time. In TRIM.Expo, exposure of each individual or cohort is determined by a sequence of exposure events specific to the individual or cohort. The exposure-event sequence is a chronologically ordered series of events that identifies the locations and amount of time spent in those locations. Each exposure-event sequence consists of a series of events with durations ranging from one to 60 minutes. Each exposure event assigns the individual or cohort to a particular combination of exposure district, microenvironment, and activity. To construct exposure events, an individual or cohort is linked with a series of time-specific activities and the exposure districts and microenvironments associated with those activities. The following important attributes of an exposure event are used to estimate the corresponding exposure concentrations and potential doses:

- Pollutant concentration in an environmental medium (*e.g.*, ambient air, surface water);
- Any significant intermedia transfer from environmental media to the exposure medium, (*e.g.*, from soil to house dust to air in an indoor microenvironment);
- Pollutant concentration in an exposure medium (*e.g.*, personal air, tap water);
- Duration of contact with the exposure medium; and
- Time scale of interest.

### **3. SUMMARY REVIEW OF EXISTING EXPOSURE MODELS AND RATIONALE FOR DEVELOPING TRIM.Expo**

This chapter provides a review of current exposure modeling approaches and an overview of several existing and emerging exposure assessment models. The exposure models and modeling frameworks described in this chapter are critically compared and their respective strengths and weaknesses are assessed. A more detailed comparison of the features for each of the different exposure models identified is provided in Appendix B.

This review revealed that none of the models described here adequately meets the exposure modeling needs of OAQPS (see Section 1.1 for a discussion of the needs of OAQPS). The review in this chapter highlights the unique features included in TRIM.Expo for meeting OAQPS' modeling needs.

#### **3.1 RATIONALE FOR DEVELOPING TRIM.Expo**

Current models used by OAQPS for estimating human exposure to criteria and hazardous air pollutants do not include multimedia exposures. Furthermore, the models currently in use for estimating exposures to HAPs do not adequately estimate the spatial and temporal patterns of exposures for all of the HAPs listed in section 112(b) of the CAA. Adopting or integrating existing models into a framework that meets OAQPS' needs represents the most cost-effective means for developing the tools needed to support the regulatory decision-making activities related to hazardous and criteria air pollutants.

Based on the review of currently available exposure models and modeling systems, there is no single model or modeling framework that meets the needs of OAQPS, nor any that could function effectively by itself as part of the TRIM modeling system for estimating multimedia exposures for a population. Most models are limited in the type of media and environmental processes that they are capable of addressing. No model currently exists that addresses the broad range of pollutants and environmental fate and transport processes that are anticipated to be encountered by OAQPS and other stakeholders when evaluating the risks from the multitude of hazardous and criteria air pollutants.

To summarize, none of the currently available exposure models is a sufficiently integrated multimedia model that provides the temporal and spatial resolution needed for estimating human exposures. It is not known to what extent modeled exposure estimates would differ between the currently available models and a truly integrated multimedia exposure model, such as TRIM.Expo. However, models that are not fully coupled have long been considered to lack scientific credibility. Therefore, OAQPS has determined that it is necessary to undertake efforts to develop a truly coupled multimedia exposure modeling framework.

#### **3.2 REQUIRED ATTRIBUTES OF THE TRIM.Expo MODULE**

In addition to the five features that are required of the TRIM Exposure-Event module (listed in Section 2.1), OAQPS determined that the module must also (1) address varying time-steps (*i.e.*, one hour or greater) and provide sufficient spatial detail at varying scales; (2) have the

“transparency” needed to be practical for a large and diverse group of users; (3) be modular in design; and (4) be easily accessible.

A key element in the development of TRIM.Expo is the need for the exposure model system or framework to be modular in design. A modular design is one that partitions the various algorithms necessary for evaluating the different aspects of an exposure assessment into generally discrete packages, or modules, which are able to interact with each other. By creating an exposure framework that is modular, only those model components necessary for evaluating particular aspects of the exposure assessment and/or endpoints of interest need to be used for a particular application.

OAQPS has decided to separately characterize uncertainty and variability on a selective basis. In concordance with EPA’s probabilistic modeling guidance (U.S. EPA 1997c), a staged approach (as described in Section 4.2.9.3) will be used in characterizing uncertainty and variability (*i.e.*, rather than attempting to characterize uncertainty and variability for all parameters, sensitivity analyses will be used to identify a limited number of critical parameters that most influence the exposure outcomes and, thus, will be subjected to further analysis). These parameters will be examined in more detail to determine whether it is appropriate to separately characterize uncertainty and variability based on available information. For some parameters, such as body weight, there are sufficient data to support the explicit characterization of variability. However, for other parameters where data may be insufficient to support the separate characterization of uncertainty and variability, a distribution will be defined to reflect overall parameter uncertainty, including inherent variability.

### **3.3 OVERVIEW OF CURRENT MODELS AND MODELING APPROACHES**

Exposure modeling approaches have long been based on physical principles. They were developed using a concise physical interpretation of the factors affecting exposures, which were determined prior to the development of a particular model. Examples of this type of modeling approach are the NAAQS Exposure Model (NEM) (U.S. EPA 1983) and several different indoor air quality mass balance models (Nazaroff and Cass 1986, Ryan et al. 1983, Özkaynak et al. 1982). A major limitation of these models is that they do not capture the full variability of people’s activities as part of the exposure simulation. In addition, uncertainty in the values of the parameters used to make the estimates is not included.

To overcome these limitations, subsequent exposure models were developed that used a stochastic approach. This made it possible for estimates of population exposure to be characterized as distributions rather than point estimates. One of the first models developed to use this “probabilistic” approach was the Simulation of Human Activities and Pollutant Exposure, or SHAPE, model (Ott 1982, Ott 1984, Ott et al. 1988). Shortly afterward, a probabilistic version of NEM was developed. The model (there were actually several pollutant-specific versions) was referred to as the probabilistic NAAQS Exposure Model, or pNEM (McCurdy and Johnson 1989). While it would be difficult to accurately represent the activities of an individual due to day-to-day variation, the general behavior of groups or subsets of the population can be



well represented using stochastic processes. By explicitly including variability and uncertainty in the models, the effects of the uncertainty on the modeled exposure values can be evaluated.

Many of the early models stressed exposures to industrial and mobile sources and attempted to account for the variability in those exposures. Some of the earliest work in exposure modeling attempted to simulate human exposures to lead and carbon monoxide. With the periodic review and revision of the NAAQS, models were developed to assess the exposures of the population to the air pollutants for which ambient standards had been established.

Over time, it has become clear that there are important outdoor sources other than large industrial facilities and mobile sources, that exposures can occur both indoors and outdoors, and that the sources of the pollutants can likewise be found both indoors and outdoors. Over the past decade, increasingly sophisticated methodologies have been developed for modeling and evaluating exposures. However, there is currently no single exposure model that can estimate all pollutants, all sources, and all routes of exposure. The models that have emerged are largely still restricted to single-medium exposure assessments. In recent years, emphasis has been placed on developing modeling frameworks that can assess multimedia, multipollutant human exposures within a unified framework. This type of approach is relatively new, and a usable framework for conducting multipathway exposure assessments has yet to emerge. This chapter provides a general overview of modeling approaches used to date to estimate exposures.

Table 3-1 identifies numerous air quality and exposure models and modeling systems. More detailed information is given in Appendix B. that are currently publicly available along with the agency or group who was its major developer. Some exposure models are proprietary (*i.e.*, they are not “public domain”) and therefore must be purchased from the developer. To facilitate public access, EPA has decided that no proprietary models will be considered in the development of TRIM.Expo. Examples of proprietary models include RISK\*ASSISTANT® and LifeLine®.

The EPA’s Office of Research and Development (ORD) is currently developing a number of exposure models and modeling systems. The development is on-going and therefore is not included in Table 3-1 at this time. However, since these models represent a major effort by ORD, a description of each has been included in Appendix B. Examples of new and continuing exposure modeling efforts at ORD include the development of the Stochastic Human Exposure and Dose Simulation (SHEDS) Model (see Section B.7.7). The SHEDS Model is a probabilistic, physically-based model that simulates aggregate exposure and dose for population cohorts and multimedia pollutants of interest. Initial applications of the model have assessed children’s exposures to pesticides (SHEDS-Pesticides) and population exposures to PM (SHEDS-PM). Another effort within ORD is the development of the Modeling ENvironment for TOtal Risk (MENTOR) project. The objective of the on-going MENTOR project is to develop, apply through case studies, and evaluate state-of-the-art computational tools, that will support multipathway, multiscale source-to-dose studies and exposure assessments for a wide range of environmental pollutants. More detail about MENTOR can be found in Appendix B. The EPA’s ORD is also engaged in the development of the MODELS-3/Multimedia Integrated Modeling System (MIMS). The MIMS will have capabilities to represent the transport and fate of nutrients and pollutants over multiple scales. The system will provide a computer-based problem solving environment for testing our understanding of multimedia (atmosphere, land, water) environmental

problems, such as the movement of pollutants through the hydrologic cycle, or the response of aquatic ecological systems to land-use change.

**Table 3-1  
 Air Quality and Exposure Models and Modeling Systems and Their Developers**

<b>Model</b>	<b>Developer</b>
<b>INDOOR AIR EXPOSURE MODELS</b>	
INDOOR, EXPOSURE, and RISK	EPA/Office of Research and Development (ORD)
MAVRIQ (Model for Analysis of Volatiles and Residential Indoor Air Quality)	EPA/ORD
AMEM (ADL Migration Exposure Model)	EPA/Office of Pollution Prevention and Toxics (OPPT)
CPIEM (California Population Indoor Exposure Model)	California Air Resources Board (CARB)/Indoor Program
<b>INDOOR / OUTDOOR AIR EXPOSURE MODELS</b>	
pNEM (probabilistic NAAQS)	EPA/OAQPS
HAPEM4 (Hazardous Air Pollutant Exposure Model)	EPA/OAQPS
AirPEX (Air Pollution Exposure Model)	National Institute of Public Health and the Environment (RIVM) [Netherlands]
HEM (Human Exposure Model)	EPA/OAQPS
SHAPE (Simulation of Human Activities and Pollutant Exposure)	EPA/ORD
BEAM (Benzene Exposure Assessment Model)	EPA/ORD
pHAP (probabilistic HAP Exposure Model)	EPA/OAQPS
<b>CONSUMER PRODUCT EXPOSURE MODELS</b>	
CONSEXPO (CONSUMER EXPOSURE Model)	National Institute of Public Health and the Environment (RIVM) [Netherlands]
SCIES (Screening Consumer Inhalation Exposure Software)	EPA/ OPPT/Economics, Exposure, and Technology Division (EETD)
DERMAL	EPA/OPPT/EETD
MCCEM (Multi-Chamber Concentration and Exposure Model)	EPA/OPPT; updated by EPA/ORD
<b>DIETARY EXPOSURE MODELS</b>	
DEPM (Dietary Exposure Potential Model)	EPA/ORD
<b>MULTIMEDIA EXPOSURE MODELS</b>	
The Exposure Commitment Method	National Radiological Protection Board (NRPB) [United Kingdom]
Layton et al. (1992) Indoor/Outdoor Air/Soil Transport Model	U.S. Department of Energy (DOE)
CalTOX (California Total Exposure Model for Hazardous Waste Sites)	California Environmental Protection Agency/Department of Toxic Substances Control (DTSC)

Model	Developer
MMSOILS (Multimedia Contaminant Fate, Transport, and Exposure Model)	EPA/ORD
RESRAD (RESidual RADiation)	DOE and Argonne National Laboratory
USES (Unified System for the Evaluation of Substances)	National Institute of Public Health and the Environment (RIVM) [Netherlands]
BEADS (The Benzene Exposure and Absorbed Dose Simulation)	EPA/ORD
DERM (Dermal Exposure Reduction Model)	Stanford University/Environmental Engineering and Science Group
SCREAM2 (South Coast Risk and Exposure Assessment Model, Version 2)	South Coast Air Quality Management District
Integrated Spatial Multimedia Compartmental Model (ISMCM)	University of California (Los Angeles)/School of Engineering and Applied Science
<b>EXPOSURE SIMULATION MODEL SYSTEMS</b>	
GEMS (Graphical Exposure Modeling System)	EPA/OPPT
THERdbASE (Total Human Exposure Risk database and Advanced Simulation Environment)	EPA/ORD
MEPAS (Multimedia Environmental Pollutant Assessment System)	DOE and Battelle Pacific Northwest Laboratory

In general, the models that most closely meet the design goals for TRIM development are the focus of this chapter. Generally, these include models that are able to calculate short-term exposures (*i.e.*, 1 hour or shorter in duration), because they can be adapted to evaluate long-term exposures as well. They may also be able to explicitly treat variability and uncertainty. Other desirable model attributes are the utilization of a mass balance approach for estimating indoor air concentrations and the ability to track potential intake rates concurrent with exposure. For inhalation, this means providing estimates of the respiration rate (also called ventilation or breathing rate) for various activities. Additional useful features include accounting for indoor air emission sources and the ability to include geographic mobility (*e.g.*, commuting) in the exposure simulation.

One model that has many of the desirable attributes is pNEM/CO (Johnson et al. 1992b, Johnson et al. 1999). Although this model is for a single medium only (air), it already incorporates nearly all of the features needed for the inhalation component of TRIM.Expo (see Appendix B, Table B-1). In addition to the criteria listed above, pNEM/CO is well documented and is already being used by OAQPS as an input to regulatory decision-making. Furthermore, the 1992 version of pNEM/CO has undergone review by the Clean Air Scientific Advisory Committee.

For modeling the non-inhalation routes of exposure, the CalTOX model (McKone 1993a, b, c), developed at the Lawrence Berkeley National Laboratory (LBL), already includes many of the features needed. CalTOX has the ability to calculate multipathway exposures for organic chemicals and some metals. In addition, the model is stochastic and can quantify the variability

and uncertainty in the exposure calculations. CalTOX, pNEM/CO, and several other models for estimating non-inhalation and inhalation exposures are discussed in the following sections.

### 3.3.1 INHALATION EXPOSURE MODELS

Perhaps the largest number of exposure models have been developed to assess the relationship between chemical releases to outdoor air and human exposure to these pollutants both indoors and outdoors. The early “indoor/outdoor” exposure models were the first to use newly collected information on activity patterns and microenvironmental concentrations. They simulated the microenvironmental concentrations based on empirical data derived from field measurements.

The EPA played a major role in developing exposure models that addressed the air pathway. The original purpose of these models was to assist in setting the ambient air quality standards by estimating the population exposure to air pollutants when alternative air quality standards were just met. One of the first models developed for this purpose was the NEM. The NEM was pollutant-specific and included versions for estimating exposures to ozone, carbon monoxide, and particulate matter. Later, a stochastic method for randomly selecting values for important variables was incorporated into the models. These models were referred to as “probabilistic” and hence are known as probabilistic NEM, or pNEM. Groups outside of EPA have used the NEM approach and developed variations of the NEM for specific applications. These models include SAI/NEM (Hayes et al. 1984, Hayes and Lundberg 1985), REHEX (Winer et al. 1989, Lurmann et al. 1990, Lurmann et al. 1992), and the Event Probability Exposure Model (EPEM) (Johnson et al. 1992a). All three of these models are related to the NEM approach, although significant variations now exist among the models (McCurdy 1994).

The EPA also developed exposure models for specific sources or types of sources. In 1985, EPA’s Office of Mobile Sources (OMS) in conjunction with EPA’s Office of Research and Development (ORD) developed a model for estimating human exposure to non-reactive pollutants emitted by motor vehicles. This model, named the Hazardous Air Pollutant Exposure Model for Mobile Sources, or HAPEM-MS, is similar in methodology to the pNEM models (Johnson 1995). However, it differs from pNEM in the averaging time for exposure concentrations. Instead of the hourly resolution of pNEM, HAPEM-MS aggregates the hourly exposure concentrations to 3-month averages, because HAPEM-MS is designed to address exposures to pollutants with carcinogenic and other long-term effects. Subsequently, HAPEM-MS has been enhanced and now is able to model exposures to numerous air toxics from different sources through the use of the air dispersion module of the Assessment System for Population Exposure Nationwide (ASPEN) model (SAI 1999). Given the model’s ability to estimate exposures from different types of sources (*i.e.*, not just mobile sources), the Mobile Sources, or “MS,” designation has been dropped from the model’s name. The latest version of the model is called HAPEM4.

Agencies in other countries have developed exposure models that are specific to their population. The Dutch, for example, have developed an inhalation exposure model based on the pNEM approach which is used for estimating exposures of people in the Netherlands (although the model may be adapted for any location). The model, called the Air Pollution Exposure Model, or AirPEX (Freijer et al. 1997), works on a personal computer (PC) using Windows®.

The PC platform enhances the accessibility of the model to various stakeholder groups that do not have extensive programming expertise. Several new exposure models are being designed to run on PCs, and some existing models, previously run on large machines, are being modified to run on PCs and via the Internet.

### 3.3.2 MULTIMEDIA EXPOSURE MODELS

Ingestion is another important route of exposure; however, modeling ingestion exposures presents a different set of requirements than does inhalation. For example, exposure to a particular pollutant from a certain food source can occur in a single location or in many places over time. The actual location where the exposure takes place may not be the same as where the contamination of the exposure medium occurred. Another difference is the time period for exposure due to ingestion. There may be long lags between the contamination of the exposure medium (*e.g.*, food, water, soil) and the time that exposure occurs. Much of the exposure modeling that has been done for ingestion pathways has been conducted as part of multimedia modeling efforts. Hence, ingestion exposures discussed in the context of multimedia exposure models.

Efforts to assess human exposure from multiple media date back to the 1950s when the need to assess human exposure to global fallout from nuclear testing led rapidly to a framework that included transport through and transfers among air, soil, surface water, vegetation, and various paths of the food chain. 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.

The CalTOX program was developed for the California EPA as a set of spreadsheet models and spreadsheet data sets to assist in assessing human exposures to toxic substances released in multiple media (McKone 1993a,b,c). CalTOX consists of two component models: a multimedia transport and transformations model that 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. It is a mass balancing model that also includes the ability to quantify uncertainty and variability. The exposure assessment process consists of relating pollutant concentrations in the multimedia model compartments to pollutant concentrations in the media with which a human population has contact (*e.g.*, personal air, tap water, foods, household dusts/soils).

The Integrated Spatial Multimedia Compartmental Model (ISMCM) has been under development for the past 15 years. The ISMCM considers all media, biological and non-biological, in one integrated system. The model includes both spatial and compartmental modules to account for complex transport of pollutants through the ecosystem. Assuming conservation of mass, ISMCM predicts transport by using estimates of intermedia transfer factors. A newer version of ISMCM, called MEND-TOX, is currently under evaluation by EPA.

The Indirect Exposure Methodology (IEM) is a significant current EPA methodology for multimedia, multipathway transport, fate, and exposure modeling. This methodology identifies procedures for estimating the indirect (*i.e.*, non-inhalation) human exposures that can result from

the transfer of emitted air pollutants to soil, vegetation, and water bodies. The IEM addresses exposures for a variety of receptor scenarios (*e.g.*, subsistence fisher) via inhalation, ingestion of food, water, and soil, and dermal contact. The most up-to-date version of the IEM methodology is scheduled to be published in late 1999 (U.S. 1999h). The updated documentation no longer refers to the methodology as IEM; it is now referred to as the Multiple Pathways of Exposure (MPE) methodology. Appendix B provides a more detailed discussion of the IEM model.

### 3.4 STRENGTHS AND LIMITATIONS OF EXISTING MODELS

TRIM development is designed to focus on the processes that have the greatest impact on pollutant fate and transport and on human exposure. In order to have the same scientific basis as the rest of the TRIM system, TRIM.Expo needs to incorporate the same attributes, including: (1) mass conservation to the extent feasible and appropriate; (2) ability to characterize uncertainty and variability; (3) capability to assess multiple pollutants, multiple media, and multiple exposure pathways; and (4) ability to perform iterative analyses. Hence, these four design attributes serve as the basis for critically comparing the strengths and limitations of existing exposure models.

By assessing the strengths and limitations of publicly available exposure models and modeling systems in regard to the needs defined for TRIM development, a determination can be made regarding the features of the various models that may be incorporated into TRIM. Table B-2 in Appendix B compares the strengths and weaknesses of some of the most commonly used EPA and non-EPA exposure models. The models in this table are included because they each have one or more of the desirable attributes identified above needed for TRIM.Expo.

The pNEM/CO and pNEM/O<sub>3</sub> (for ozone) models have been used extensively by OAQPS in its reviews of the CO and ozone NAAQS, respectively (see Table B-3 in Appendix B for a descriptive overview of many of the features of pNEM/CO). The pNEM/CO uses a stochastic approach for selecting input variables. This stochastic approach allows both sensitivity and uncertainty to be incorporated into the model operation. Many of the model's input variables come from measured data, thereby decreasing the uncertainty associated with the model's estimates. The pNEM/CO treats human exposure as a time series of the convergence of (1) human activities occurring in a particular microenvironment and (2) air quality in those microenvironments. The model is also designed to provide estimates of the intake dose associated with exposures. The focus on time series modeling and intake dose allows analysts to produce estimates of the "dose profile" of exposed people (McCurdy 1995). A disadvantage of the pNEM/CO model in its current form is that it is difficult to execute. The pNEM/CO model, as with all of the pNEM models, is a single pollutant, single media model.

The CalTOX model (see Table B-4, Appendix B) consists of two main components: a multimedia transport and transformation model and a multipathway human exposure model. The multimedia transport and transformation model is based on both the conservation of mass and chemical equilibrium. The multimedia transport model is a dynamic model that can be used to assess time-varying concentrations of pollutants introduced initially into the soil or released to the air, soil, or water. The exposure model has 23 exposure pathways encompassing all three environmental routes of exposure, which are used to estimate average daily doses within a human population in the vicinity of a hazardous air pollutant release site. The exposure assessment

process consists of relating pollutant concentrations in the multimedia model compartments to pollutant concentrations in the media with which a human population has contact (*e.g.*, personal air, tap water, foods, house dust). This explicitly differentiates the environmental media pollutant concentrations from the pollutant concentrations in the exposure media to which humans are exposed. In addition, all input variables are taken from distributions.

The CalTOX model is limited in the extent of the environmental settings for which it can be applied. For example, it has limited effectiveness for settings where there is a large ratio of land area to surface water area. In addition, it was developed for a limited range of pollutants (*i.e.*, non-ionic organic chemicals in a liquid or gaseous state). As a result, CalTOX does not provide adequate flexibility in the environmental settings or the chemical classes it models. Also, CalTOX does not allow spatial tracking of a pollutant, hence it is not directly applicable to the TRIM approach.

HAPEM has undergone many enhancements in recent years. The most recent of these is the ability of the model to use air quality concentration estimates from the ASPEN. This latest version of HAPEM is designated HAPEM4 (see Table B-5, Appendix B).. It allows exposure to population cohorts to be simulated at the census tract level. This is a much finer spatial resolution than was previously possible. It also means that calculation of population exposures no longer needs to rely solely on data from fixed-site monitors. This is important for estimating exposures to HAPs because widespread monitoring networks for these pollutants are not available.

The HAPEM4 calculates long-term average exposure concentrations in order to address exposures to pollutants with carcinogenic and other long-term effects. Thus, HAPEM4 does not preserve the time-sequence of exposure events when sampling from the time/activity database. This means that information to evaluate possible correlations in exposures to different pollutants due to activities that are related in time is not preserved. Also, the model does not include any measures of the ventilation rate associated with an activity, so that there is no ability to calculate the potential dose received when engaging in various activities.

The IEM has been used by EPA in a variety of applications and has undergone extensive scientific peer review. The methodology includes fate and transport algorithms, exposure pathways, receptor scenarios, and dose algorithms. It also includes procedures for estimating the indirect (*i.e.*, non-inhalation) human exposures and health risks that can result from the transfer of pollutants to soil, vegetation, and water bodies.

The IEM is limited, relative to OAQPS's needs, because the methodology, as currently implemented, can be applied only to pollutants that are emitted to air. While IEM is a significant current EPA methodology for multimedia, multipathway exposure modeling, it does not fully satisfy the needs of OAQPS. An important limitation of IEM, relative to the needs of OAQPS, is that it consists of a one-way process through a series of linked models, using as inputs the annual average air concentrations and wet and dry deposition values from external air dispersion modeling. As a result, it is not a truly coupled multimedia model and does not have the ability to maintain a full mass balance or model "feedback" loops between media or secondary emissions, nor can it provide a detailed time series estimation of media concentrations and resultant exposures. The methodology does not provide for the flexibility OAQPS needs in site-specific

applications or in estimating population exposures. Significant site-specific adjustments must be made to allow for spatially tracking the relationship between concentrations and exposures. Much of the focus of the methodology is on evaluating specific receptor scenarios (*e.g.*, recreational or subsistence fisher) that may be indicative of high-end or average exposures rather than on modeling the range of exposures within a population (*i.e.*, IEM cannot estimate population exposure distributions). Appendix B provides more detailed discussion of the IEM model.

The Integrated Spatial Multimedia Compartmental Model (ISMCM) has been undergoing development at the University of California's (Los Angeles) School of Engineering and Applied Science for the last 15 years. The latest version of ISMCM, called MEND-TOX, is currently under evaluation at EPA's Office of Research and Development. The ISMCM considers all media in a single integrated system. It includes both spatial and compartmental modules to account for complex transport of pollutants through the ecosystem. The model is mass conserving and is able to estimate intermedia transfer factors desirable for TRIM.

An important limitation of ISMCM for use in TRIM.Expo development is the lack of flexibility in the spatial configuration of the model. The links and compartments in ISMCM are predetermined, thus limiting its ability to be fully integrated into a system like TRIM. Another drawback to ISMCM is that it is not structured to incorporate uncertainty and variability directly into the model outputs.

The South Coast Risk and Exposure Assessment Model (SCREAM2) provides the ability to model both inhalation and multipathway non-inhalation exposures (see Appendix B, Table B-6) (Rosenbaum et al. 1994). The model can use both measured and modeled air quality data, thus increasing the spatial resolution and number of the pollutants being studied. The SCREAM2 also includes an indoor air model for calculating indoor air concentrations. An internal submodel, called MULTPATH, calculates population exposures from several non-inhalation pathways, including food ingestion, water ingestion, and dermal adsorption. The inhalation exposure module accounts for mobility patterns of the population, indoor-outdoor exposure concentration differences, and physical exercise levels.

The use of SCREAM2 in the TRIM.Expo framework is limited because it is a deterministic model, so that input and output data are represented as point estimates rather than ranges or distributions. This limitation also restricts the model's ability to explicitly characterize uncertainty. The SCREAM2 framework consists of a one-way process through a series of linked models, based on annual average air concentrations and wet and dry deposition values from air dispersion modeling. In contrast, TRIM.Expo will have the capability to report exposure results for both short-term and long-term averages and will allow for "feedback" loops and secondary emissions.

The California Population Indoor Exposure Model (CPIEM) was developed to evaluate indoor exposures for the general California population as well as certain subgroups such as individuals who may be highly sensitive to indoor pollutants (see Appendix B, Table B-7) (CARB 1998a). The CPIEM combines indoor-air concentration distributions with Californians' location and activity information to produce exposure and dose distributions for different types of indoor environments. This is achieved through a Monte Carlo simulation whereby a number of



location/activity profiles that were collected in Air Resources Board (ARB) studies are combined with airborne pollutant concentrations for specific types of microenvironments (*e.g.*, residences, office buildings).

Concentration distributions for many pollutants and microenvironments are included in the CPIEM database. However, for pollutants and microenvironments not included in the database, CPIEM presents two alternatives. The first option is to estimate indoor air concentration distributions based on distributional information for mass balance parameters such as indoor source emission rates, building volumes, and air exchange rates. The second option is for the user to directly specify concentration distributions. The concentration values for a particular environment are then sampled from the distributions and multiplied by time durations of the population groups in the environment, based on results from Californians' location/activity profiles, to calculate time-integrated exposure.

Model limitations for CPIEM include the assumption that concentrations in different environments on the same day are independent. For example, if outdoor concentrations have a significant impact on indoor concentrations they may be correlated, so that the assumption of independence may misrepresent the shape of the exposure/dose distribution. The impact could be significant, particularly at the upper end of the distribution where the calculated exposures could be underestimated. Also, since CPIEM uses activity profiles from a limited number of studies (*i.e.*, only those conducted in California), the results may not represent small subgroups of the population or population groups in other regions of the U.S.

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## 4. DESIGN FRAMEWORK AND CONCEPTUALIZATION OF TRIM.Expo

The TRIM.Expo module is expected to estimate past and future human exposure patterns by combining pollutant concentration data with population activity tracking information. The estimation procedure requires (1) the use of algorithms to organize and manipulate pollutant concentration data and activity pattern information and (2) a process to define the link between the multimedia “ambient” environment and the microenvironmental exposure media that individuals occupy (*e.g.*, air compartments) or contact (*e.g.*, water, food, soil). Pollution concentration data are required as input into TRIM.Expo and can be derived from monitoring data, a single media transport model, or a multimedia transport model (*e.g.*, TRIM.FaTE).

The TRIM.Expo module provides a model framework addressing features unique to each problem and providing a characterization of the uncertainty associated with exposure estimates for single and multiple media pollutants. This includes a process for predicting concentrations in exposure media based on both the transfer from the ambient environment and on sources internal to those microenvironments containing the exposure media. This chapter describes the TRIM.Expo modeling system and how it was conceptualized to meet the above goals.

In order to characterize aggregate human exposure to a pollutant, each exposure route and pathway must be considered. For example, a semi-volatile hazardous air pollutant (*e.g.*, aromatic hydrocarbon) that is released to ambient air can be transported to multiple locations where exposure may occur. The pollutant can be (1) transported to the indoor or outdoor air surrounding a human receptor who would then inhale the pollutant; (2) transferred by deposition and run-off to surface water that supports fish consumed by the human receptor or provides drinking water to the human receptor; or (3) transferred by deposition to vegetation that is consumed by the human receptor or to vegetation that is consumed by the animals that supply meat and milk that is consumed by the human receptor. Each scenario defines a pathway from the pollutant’s air emission to a receptor’s contact with it via an associated route of contact. Total exposure cannot be estimated until the pathways and routes that account for a substantial amount of the intake and uptake for a receptor population have been identified.

The TRIM.Expo module is designed to be used by analysts (*e.g.*, modelers) and decision-makers (*e.g.*, regulators). As part of the initial development of TRIM.Expo, questions and issues regarding pollutant exposure of concern to analysts and decision-makers were identified.

Some of the more significant questions pertinent to analysts include the following.

- Which input properties are the most critical for modeling the movement and persistence of chemicals in indoor and outdoor environments, and which are of lesser importance, for estimating human exposures?
- How reliable are the ambient and/or microenvironmental concentration data used as input to the model, and how does the reliability of these concentrations limit the reliability of the exposure estimate?

Some of the more significant questions pertinent to decision-makers include the following.

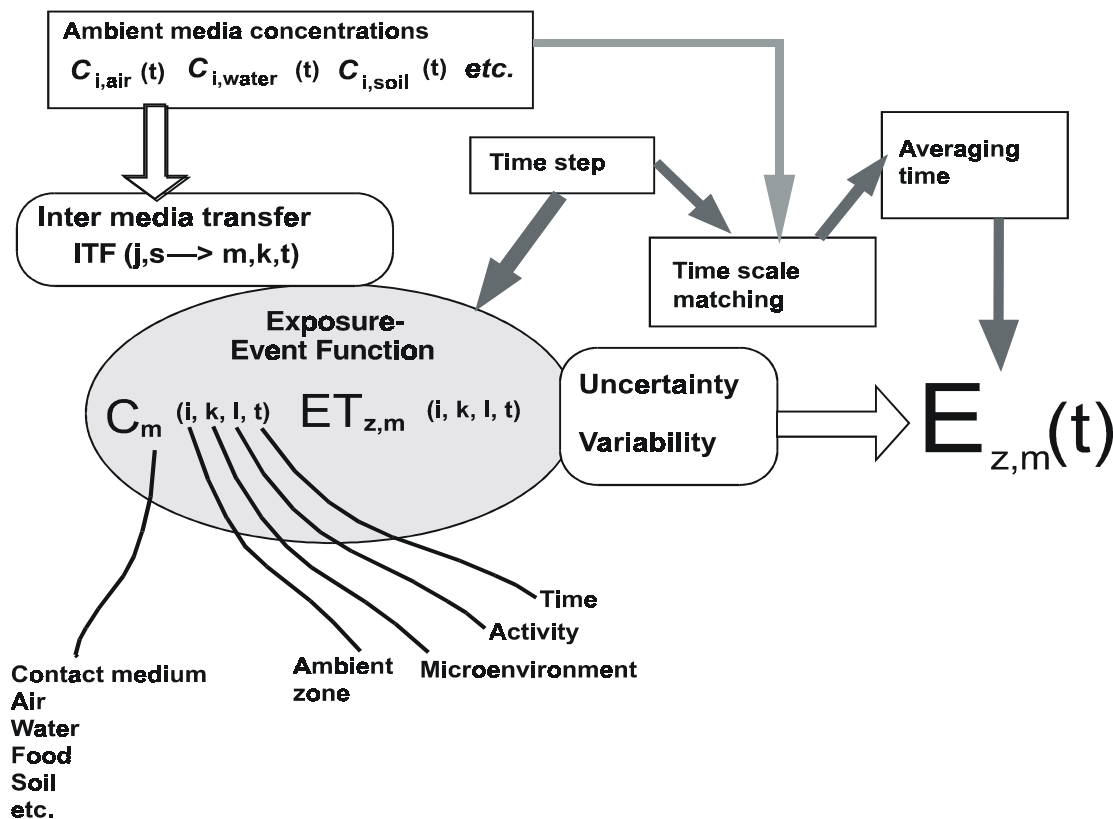
- For a given pollutant emission control measure or magnitude of reduction in ambient pollutant levels, how much reduction of exposure (and related health effects) can be expected?
- What is an indicator of exposure that can be estimated? How much of a change can be estimated in this indicator to provide evidence that a control measure might be effective?
- How long is the lag time between a change in pollutant emissions and the estimated change in the environment or exposure indicator?
- How likely are these estimates to be wrong? How uncertain are the quantitative estimates of exposure reduction and changes in environmental indicators of exposure?

To answer the questions identified above, a taxonomy of exposure questions was formulated (see Section 2.3). From this, a prioritized set of exposure-model attributes was selected, resulting in three primary model dimensions.

#### **4.1 EXPOSURE-EVENT MODULE STRUCTURE**

Exposure events are activities that bring people in contact with a contaminated exposure medium in a specified microenvironment within a given exposure district. To construct exposure events, an individual or a cohort must be linked with a series of time-specific activities and with the exposure districts and microenvironments associated with those activities. In addition, pollutant concentrations in each district-microenvironment combination must be defined through a combination of databases and stochastic process models. This process of constructing exposure events is illustrated in Figure 4-1. Exposure-event simulations must be able to provide a broad range of information, including (1) detailed information on the input distributions selected (*e.g.*, relative probability of values, fractiles and central tendency, confidence intervals, shape of the distribution); (2) detailed information on the output distribution (the information here would follow in a similar fashion to item 1, above); (3) information about the goodness-of-fit of the data; (4) information about interdependencies and correlations between variables; (5) the number of times the concentration exceeded specified concentration levels; (6) the average exposure concentration exceeding some specified level; and (7) the cumulative intake or uptake during a series of exposure events. The TRIM.Expo module will contain algorithms that determine all of these parameters. These algorithms will include the basic exposure-event function, the average exposure concentration, the intake-adjusted average exposure concentration, the intermedia transfer factor, and the average daily potential dose.

**Figure 4-1**  
**Illustration of an Exposure-Event Simulation**



### 4.1.1 BASIC EXPOSURE-EVENT FUNCTION

The basic exposure-event function determines the microenvironmental exposure to an individual or cohort from an exposure medium during time step,  $t$ . It defines exposure as the product of concentration and exposure duration, as illustrated in Figure 4-1 and shown in Equation 4-1. This equation can also be used to define an exposure concentration in other media, such as water and food, although it is less intuitive than an exposure of mg/kg-body-weight for food. For exposure media such as food and water, the potential dose rate is preferred as a basis for intake estimates (see Section 4.1.5).

$$E_{z,m}(t) = C_m(i,k,l,t)ET_{z,m}(i,k,l,t) \tag{4-1}$$

where

$E_{z,m}$  = Exposure experienced by person  $z$  from exposure medium  $m$  during time step  $t$ , given that person  $z$  is in exposure district  $i$  in microenvironment  $k$  conducting activity  $l$  during that time step  $t$ . For example, the exposure in air might be measured in units of mg-hr/m<sup>3</sup>. Note that the exposure time need not be a whole time step.

- $C_m$  = Concentration in exposure medium  $m$  (e.g., air, water, soil) in exposure district  $i$  in microenvironment  $k$  associated with activity  $l$  during time step  $t$ . Units of measurement for air might be  $\text{mg}/\text{m}^3$ , while units of measurement of food might be  $\text{mg}/\text{kg}$ .
- $ET_{z,m}$  = Exposure duration of individual or cohort  $z$  to exposure medium  $m$  in exposure district  $i$  in microenvironment  $k$  conducting activity  $l$  during time step  $t$ .
- $z$  = Individual or cohort.
- $m$  = Exposure medium contacted (i.e., air, water, food).
- $i$  = Exposure district.
- $k$  = Microenvironment in which the exposure occurs (e.g., indoors at home, in a vehicle, indoors at work).
- $l$  = Activity code that describes what the individual is doing at the time of exposure (e.g., resting, working, preparing food, cleaning, eating).

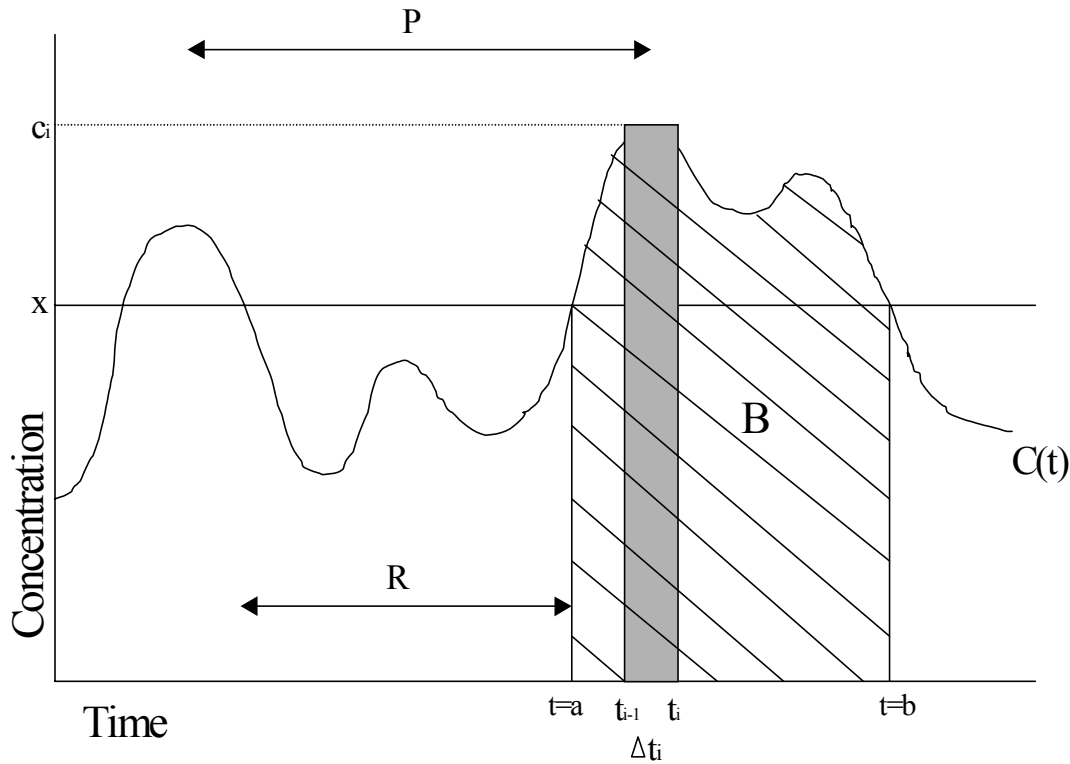
#### 4.1.2 EXPOSURE OR POTENTIAL DOSE PROFILES

The time series of concentrations that could potentially result in an exposure comprises a profile, as illustrated in Figure 4-2. As shown in Equation 4-1, exposure to a pollutant is calculated as the product of the concentration that a person contacts and the duration of the contact. This is shown graphically in Figure 4-2. The x-axis shows the time sequence, while the y-axis shows the concentration of a pollutant. Therefore, the concentration for each instant in time is given by the curve,  $C(t)$ . To simplify the discussion, suppose that a person was in a particular microenvironment from time  $t_{i-1}$  to  $t_i$  and that the concentration of the pollutant (given by  $c_i$ ) remained fairly constant during this time period (to make this example as simple as possible  $t_i - t_{i-1} = \Delta t_i$  is defined as one hour). The shaded rectangle in Figure 4-2 has height  $c_i$  and width  $\Delta t_i$ . The area given by this rectangle is, therefore,  $c_i (\Delta t_i)$  and as stated above and shown in Equation 4-1 the product of a concentration and a time interval is equal to exposure. Thus, the area given by the shaded rectangle approximates the person's exposure over the time interval from  $t_{i-1}$  to  $t_i$ . The sum of the areas of many such rectangles from time  $a$  to time  $b$  approximates the person's exposure for this interval of time and applies whether the person remains in a single microenvironment or visits many microenvironments. Therefore, the hatched area given by  $B$  in Figure 4-2 is the person's integrated exposure from time  $a$  to time  $b$ .

If a dose metric, such as breathing rate or ingestion rate, had been included with the information on concentration, then the profile in Figure 4-2 would approximate the potential dose. The dose profile combines information on pollutant concentrations, activity patterns, and intake rates. For many pollutants (e.g., ozone, carbon monoxide), the time series of exposure or potential dose may be more important for estimating the health impact than the overall average exposure or cumulative dose (McCurdy 1997). Figure 4-2 also shows some of the measures of

exposure or potential dose that may be derived from the profile. The output options for TRIM.Expo will include exposure and potential dose profiles.

**Figure 4-2**  
**Example of an Exposure or a Potential Dose Profile and Associated Measures**  
 (adapted from McCurdy 1997)



**KEY**

- B = integrated exposure from time  $t=a$  to  $t=b$
- P = time between peaks over  $x$
- R = respites between exceedances of  $x$

The method of combining the vital information that is used in a dose profile makes it possible to develop estimates for alternative exposure and dose metrics for different averaging times from one hour to a year or more. Examples of alternative metrics that OAQPS has needed to investigate recently include children exposed to 8-hour daily ozone values greater than 0.08 ppm while exercising at a breathing rate of 15 L/min/m<sup>2</sup> or higher, and cardiovascular-impaired persons with a daily carboxyhemoglobin level of 2 percent or higher due to CO exposures (McCurdy 1995). Indeed, by using this disaggregated approach, almost any combination of exposure and dose metrics is possible.

With respect to health effects, two important considerations are (1) the time-scale of the health effects that result from an exposure or repeated exposures and (2) whether there is

assumed to be a threshold concentration below which no health impacts are expected. Depending upon the health effects associated with the pollutant of interest, the exposure and potential dose profile may be used to derive several metrics. For example, if the time steps are one-hour, each concentration estimate represents a one-hour average. If the pollutant's health effect is associated with one-hour average exposures and has a lowest observed or a no observed adverse effect level (e.g.,  $x$ ), important metrics might include the following (refer to Figure 4-2).

1. The number of person-hours of exposure to concentrations above  $x$ :

$$= P(\text{cohort}) \times \sum_t [\partial(t) \times C(t)] \quad (4-2)$$

where:

$$\begin{aligned} P(\text{cohort}) &= \text{population of the cohort,} \\ \partial(t) &= 0 \text{ if } C(t) \leq x, 1 \text{ if } C(t) > x, \text{ and} \\ C(t) &= \text{exposure concentration for time step } t. \end{aligned}$$

2. The sum of the concentrations that exceed  $x$

$$= \sum_t [\partial(t) \times C(t)] \quad (4-3)$$

where:

$$t = a, t_1, t_2, \dots, t_{n-1}, t_n = b \text{ (refer to Figure 4-2).}$$

3. The average of the concentrations that exceed  $x$

$$= \frac{\sum_t [\partial(t) \times C(t)]}{\sum_t \partial(t)} \quad (4-4)$$

4. The sum of exceedances of  $x$ , when it is exceeded

$$= \sum_t [\partial(t) \times \{C(t) - x\}] \quad (4-5)$$

where:

$$t = a, t_1, t_2, \dots, t_{n-1}, t_n = b \text{ (refer to Figure 4-2).}$$



5. The average exceedance of  $x$ , when it is exceeded

$$= \frac{\sum_t [\delta(t) \times \{C(t) - x\}]}{\sum_t \delta(t)} \quad (4-6)$$

Other important metrics might include the average number of sequential hours exceeding  $x$ , or the average number of time steps between local concentration peaks (*i.e.*, average length of respites).

If the pollutant's health effect does not have a specific benchmark concentration (*i.e.*, lowest observed or no observed adverse effect level), but is associated with a certain averaging time (*e.g.*, 1-hour, 8-hour, 24-hour, annual), important metrics might include:

- The distribution of the maximum concentration corresponding to the averaging time of interest for the exposure period, typically one year (*e.g.*, distribution of the maximum 8-hour average concentration for any time during the year), or
- The average daily maximum concentration corresponding to the averaging time of interest for the exposure period (*e.g.*, the average of the maximum 8-hour average concentration for each day of the year).

The TRIM.Expo module was designed to address OAQPS' need for an integrated exposure model system that can evaluate the distribution of the population exposed to specified levels of air pollution and the number of times they are exposed for one-hour, eight-hour, monthly, quarterly, seasonal, and annual averaging periods (McCurdy 1995). As described above, TRIM.Expo will fulfill this need by producing population distributions of multiple exposure, dose, and dose-rate indicators.

### 4.1.3 AVERAGE EXPOSURE CONCENTRATION

During a relatively long time period (*e.g.*, day, week, year), individuals have different time/activity budgets and occupy different microenvironments with different pollutant concentrations. In such cases, exposure cannot be addressed by using the basic exposure-event function. Duan (1982) proposed a method to determine the average exposure concentration,  $EC_{z,m}$ , that has been used by others (Ott 1984, Ott et al. 1988, Ott et al. 1992a, Klepeis 1994, Lurmann and Korc 1994, MacIntosh et al. 1995):

$$EC_{z,m} = \frac{1}{T} \sum_t C_m(i,k,l,t) ET_{z,m}(i,k,l,t) \quad (4-7)$$

where:

$EC_{z,m}$  = average exposure concentration in exposure medium  $m$  of individual or cohort  $z$  over time period  $T$ , where  $T$  is used as the averaging time and is the sum of all time steps,  $t$

$T$  = sum of all time steps,  $t$ .

The algorithm would determine an exposure concentration averaged over the total potential exposure duration considered in a specific TRIM.Expo application. However, the averaging time may not correspond to the averaging time specified for a health benchmark. For example, the exposure averaging time for a particular application of TRIM.Expo may be a year, while the averaging time for the health benchmark for the pollutant may be specified for a lifetime. Such issues will need to be addressed in TRIM's Risk Characterization module, TRIM.Risk.

#### 4.1.4 INTAKE-ADJUSTED AVERAGE EXPOSURE CONCENTRATION

Cumulative exposure can also be determined using overall average concentration of the exposure medium that enters the body over time period  $T$ . The intake-adjusted average exposure concentration,  $IEC_z$ , is calculated using a weighting factor based on the intake rate, such as breathing or ingestion rate:

$$IEC_z = \frac{\sum_t C_m(i, k, l, t) ET_z(i, k, l, t) IU_{m,z}(t)}{\sum_t ET_z(i, k, l, t) IU_{mz}(t)} \quad (4-8)$$

where

$IU_{m,z}(t)$  = rate of intake/uptake in exposure medium  $m$  by individual or cohort  $z$  during an exposure time step  $t$ , and under other factors that are defined above. For food ingestion, the units of measurement for  $IU_{mz}$  might be kg-food/kg-body-weight during an exposure duration  $ET$ .

#### 4.1.5 INTERMEDIA TRANSFER FACTOR

In many situations, the concentration in the exposure medium,  $C_m$ , is not known directly and must be estimated from an intermedia transfer. For example, the outdoor air concentration of a particular pollutant may be known, but the pollutant concentration indoors and the exposure medium may be unknown. To differentiate the indoor air concentration contribution from that of the outdoor air requires an intermedia transfer factor, which converts the time history of concentrations that is known (*i.e.*, outdoor air) to an estimate of the time history of the unknown concentration (*i.e.*, indoor air). Other examples of intermedia transfers include soil to house dust, water to indoor air, water to fish, and soil to home-grown vegetables.

The intermedia transfer factor, *ITF*, is used as follows:

$$C_m(i, k, l, t) = \sum_j \sum_s C_n(j, s) ITF(j, s \Rightarrow m, k, t) \quad (4-9)$$

In this expression, for exposure medium *m* (e.g., air, water, soil) at location *i* in microenvironment *k* associated with activity *l* during time step *t*,  $C_m(i, k, l, t)$  is the concentration contributed by concentration  $C_n(j, s)$  from environmental medium *n* at location *j* and time *s*. *ITF* ( $j, s \rightarrow m, k, t$ ) is the intermedia transfer algorithm that maps concentration  $C_n(j, s)$  to concentration  $C_m(i, k, l, t)$ . Summation of the product  $C_n \times ITF$  time occurs over previous time steps that impact current time step *t* and over all locations *j* that impact current microenvironment *k*.

#### 4.1.6 AVERAGE DAILY POTENTIAL DOSE

The exposure-event function is frequently used to assess the potential dose to an exposed individual from his or her cumulative intake over some time period relative to an averaging time. The average daily potential dose,  $ADD_{pot}$ , is the potential dose per day (d). It is similar to the intake-adjusted average exposure concentration, but defines an average rate of intake in mg/kg/d or mg/d over the averaging time instead of a concentration.

$$ADD_{pot} = \frac{\sum (C_m(i, k, l, t) ET_{z, m}(i, k, l, t) IU_{z, m}(t))}{T} \quad (4-10)$$

where:

$T$  = averaging time used to assess the health effects of the intake,  
 $IU_{z, m}(t)$  = rate of intake/uptake.

## 4.2 DEFINING THE MODEL COMPONENTS FOR A TRIM.Expo APPLICATION

To set up a TRIM.Expo application, several steps must be performed.

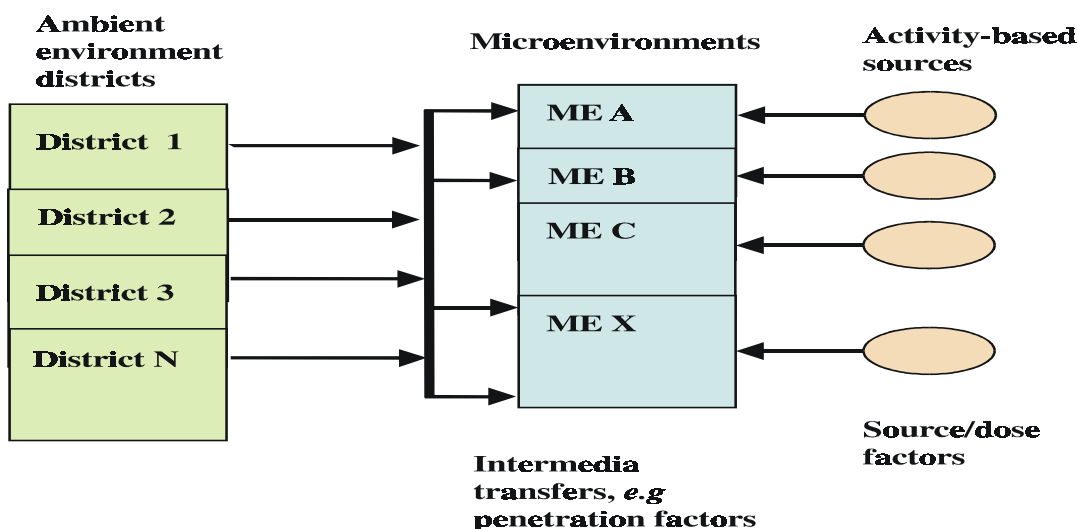
1. Identify the pollutant(s) of interest, the study area, the exposure districts, and the population(s) of interest.
2. Determine environmental media within each exposure district. Estimate ambient media and time-varying pollutant concentrations in the environmental media.
3. Identify exposure media for the population(s) of interest.
4. Construct and evaluate intermedia transfer factors relating time-varying exposure media concentrations to time-varying environmental media concentrations.

5. Divide the population(s) of interest into an appropriate set of cohorts.
6. Develop a sequence of exposure events linking the cohorts to exposure media.
7. Create a dose profile for each exposure route based on the intake of pollutant(s) in each exposure event for each cohort.

Figure 4-3 illustrates a typical TRIM.Expo application. Pollutants from environmental media contained in environmental districts are linked to microenvironments through the intermedia transfer factors. Cohort activities are linked to the microenvironments as well. This information is then used to assess an exposure profile and/or cumulative intake during a defined time period. These steps are described in more detail below.

**Figure 4-3**  
**Sequence of Exposure Events for a Set of Population Cohorts**

**Illustration of the Process by which Environmental Media Concentrations for Multiple Exposure Districts are linked using Intermedia Transfers to Exposure Media in a Set of Microenvironments**



**Examples**

**Residential zone**  
**Transit corridor**  
**Industrial area**  
**Business area**

**Indoors at home**  
**Outdoors at home**  
**Automobile**  
**Indoors at work**  
**Outdoors at work**  
**Indoors at school**  
**Outdoors at school**  
**Restaurant**

**Smoking**  
**Cooking**  
**Consumer products**

## 4.2.1 DEFINE STUDY AREA, EXPOSURE DISTRICTS, AND ENVIRONMENTAL MEDIA

A study area is an urban and/or local area for which environmental concentrations have been assembled for an exposure assessment. It is divided into one or more exposure districts. In order to perform multimedia exposure assessments, concentration data from multiple environmental media (*i.e.*, ambient air, vegetation, surface soil, root zone soil, deeper or vadose zone soil, ground water, surface water) are needed for each exposure district. The concentration information is gathered either from analysis of ambient monitoring data or from a simulation model such as TRIM.FaTE. Each ambient environmental medium is characterized in terms of one or more component phases – gas, water, liquid, and/or solids. Each environmental medium is described below.

### 4.2.1.1 Ambient Air

The ambient (*i.e.*, outdoor) air in an exposure district can be characterized in terms of its gas, particulate matter, and water composition. Its volume and mass are defined by the area of the exposure district and the depth of the lower troposphere. Pollutants in ambient air are dispersed by atmospheric advection and diffusion and are influenced greatly by meteorological parameters. Because particle size influences the particle's behavior in the atmosphere with respect to deposition and settling and its ability to penetrate the lung cavities and affect human health, it is important to consider particulate matter of various cut sizes, such as PM<sub>10</sub> and PM<sub>2.5</sub>. The TRIM.Expo module will consider other particle sizes, as the need arises, in the future. In addition, during precipitation (*e.g.*, rain, snow) and fog events, it is important to characterize the volume fraction of air that is water.

### 4.2.1.2 Vegetation

Vegetation is the dominant component of the terrestrial plants exposure district. Vegetation generally has contact with two other environmental media, air and soil. However, plant interactions with these media are not understood well enough to define an accurate method for predicting pollutant uptake. In order to assess potential vegetation-pathway exposures, vegetation can be further delineated into above-ground vegetation and root crops. Above-ground vegetation includes leafy vegetables (*e.g.*, cabbage, cauliflower, broccoli), exposed produce (*e.g.*, apples, berries, cucumber, squash), protected produce (*e.g.*, citrus fruits), and grains (*e.g.*, wheat, corn, rice). Root crops include, for example, carrots, beets, legumes, and melons.

### 4.2.1.3 Surface Soil

Surface soil consists of solid, liquid, and gas phases. Studies of radioactive fallout in agricultural land management units reveal that, in the absence of tilling, particles deposited from the atmosphere accumulate in and are resuspended from a thin ground or surface soil layer with a thickness in the range 0.1 to 1 cm (Whicker and Kirchner 1987). The ground-surface-soil layer, has a lower water content and higher gas content than underlying layers.

#### **4.2.1.4 Root Zone Soil**

Root zone soil consists of solid, liquid, and gas phases. Soil-water content in the root-zone is somewhat higher than that in surface soils because the presence of clay serves to retain water. The roots of most plants are confined within the first meter of soil depth. In agricultural lands, the depth of plowing is 15 to 25 cm. In addition, the diffusion depth, which is the depth below which a pollutant is unlikely to escape by diffusion, is on the order of 1 m or less for all but the most volatile pollutants.

#### **4.2.1.5 Vadose Zone Soil**

Vadose zone soil has solid, liquid, and gas phases. The soil in this layer typically has a lower organic carbon content and a lower porosity than the root zone soil. It is assumed that pollutants in this layer will move downward to the ground water zone primarily by capillary motion of water and leaching.

#### **4.2.1.6 Ground Water**

Ground water is defined as water that can be withdrawn from the saturated zone below the vadose zone of the soil layer. Ground water consists of both a liquid and a suspended particle phase.

#### **4.2.1.7 Surface Water**

Surface water is composed of two phases: pure water and suspended sediment material. The suspended sediment material phase contains sorbed pollutants. Surface water compartments are assumed to be well-mixed systems and include ponds, lakes, creeks, rivers, estuaries, seas, and oceans.

### **4.2.2 DEFINE EXPOSURE MEDIA AND MICROENVIRONMENTS**

The exposure assessment process consists of relating pollutant concentrations in the environmental media (*e.g.*, ambient air, surface soil, ground water) to pollutant concentrations in the exposure media with which a human population has contact (*e.g.*, personal air, tap water, foods, household dusts). The exposure media that have been identified for inclusion in TRIM.Expo include the following.

- Outdoor air;
- Indoor air;
- Tap water;
- Home-grown food (*i.e.*, produced by and consumed by a household);

- Locally-produced food (*i.e.*, produced by home gardens and commercial farms in contact with air, soil, and/or water in the study area);
- Prepared food;
- Breast milk;
- House dust;
- Soil;
- Swimming pools; and
- Recreational surface water.

Microenvironments are locations in which a population comes into contact with pollutants. They are well-characterized, relatively homogenous locations with respect to pollutant concentrations for a specified time period. Table 4-1 is an initial list of the microenvironments that will be included in TRIM.Expo., other microenvironments will be added during the course of module development.

**Table 4-1  
Microenvironments to be Included in TRIM.Expo**

Microenvironment #	Microenvironment	
	General	Specific
1	In vehicle	Car
2	In vehicle	Bus
3	In vehicle	Truck
4	In vehicle	Other
5	Indoors	Public garage
6	Outdoors	Parking lot/garage
7	Outdoors	Near road
8	Outdoors	Motorcycle
9	Indoors	Service station
10	Outdoors	Service station
11	Indoors	Residential garage
12	Indoors	Other repair shop
13	Indoors	Residence - no CO source
14	Indoors	Residence - gas stove
15	Indoors	Residence - attached garage

Microenvironment #	Microenvironment	
	General	Specific
16	Indoors	Residential - stove and garage
17	Indoors	Office
18	Indoors	Store
19	Indoors	Restaurant
20	Indoors	Manufacturing facility
21	Indoors	School
22	Indoors	Church
23	Indoors	Shopping mall
24	Indoors	Auditorium
25	Indoors	Health care facility
26	Indoors	Other public building
27	Indoors	Other location
28	Indoors	Not specified
29	Outdoors	Construction site
30	Outdoors	Residential grounds
31	Outdoors	School grounds
32	Outdoors	Sports arena
33	Outdoors	Park/golf course
34	Outdoors	Other location
35	Outdoors	Not specified
36	In vehicle	Train/subway
37	In vehicle	Airplane

### 4.2.3 DEFINE RELEVANT INTERMEDIA TRANSFERS

An intermedia transfer factor is an algorithm that expresses the transfer of a pollutant from an environmental medium to an exposure medium. The following tables summarize intermedia transfers which need to be considered in exposure modeling. Some of these intermedia transfers, where feasible and appropriate, will be included in TRIM.Expo, while others may be addressed within the TRIM.FaTE module. Each cell representing an interaction is shaded, and the exposure pathways (*i.e.*, inhalation, ingestion, dermal contact) that results from the intermedia transfer is indicated. The tables below show the matrix of links between the various exposure media noted above and ambient-air phases (Table 4-2), ambient soil media (Table 4-3), ambient water media (Table 4-4), and ambient vegetation (Table 4-5).



**Table 4-2**  
**Matrix of Links Between Ambient-Air Phases and Various Exposure Media**

EXPOSURE MEDIA	ENVIRONMENTAL MEDIUM = Ambient air			
	Gas Phase	PM <sub>2.5</sub>	PM <sub>10</sub>	Precipitation
<b>Outdoor Air</b>				
gases	Inhalation			
PM <sub>2.5</sub>		Inhalation		
PM <sub>10</sub>			Inhalation	
precipitation				
<b>Indoor Air</b>				
gases	Inhalation			
PM <sub>2.5</sub>		Inhalation		
PM <sub>10</sub>			Inhalation	
water vapor				
<b>House Dust</b>				
on floors		Ingestion/dermal	Ingestion/dermal	
on surfaces		Ingestion/dermal	Ingestion/dermal	
<b>Soil</b>				
<b>Water</b>				
<b>Food</b>				
home fruits				
protected				
unprotected	Ingestion	Ingestion	Ingestion	Ingestion
home vegetables				
above ground	Ingestion	Ingestion	Ingestion	Ingestion
root crops				
home grains	Ingestion	Ingestion	Ingestion	Ingestion
meat	Ingestion	Ingestion	Ingestion	
milk	Ingestion	Ingestion	Ingestion	
dairy products	Ingestion	Ingestion	Ingestion	
eggs	Ingestion	Ingestion	Ingestion	
breast milk	Ingestion	Ingestion	Ingestion	
prepared foods				

**Table 4-3  
 Matrix of Links Between Soil Media and Various Exposure Media**

EXPOSURE MEDIA	ENVIRONMENTAL MEDIUM = Soil		
	Surface Soil	Root Zone Soil	Vadose Zone Soil
<b>Outdoor Air</b>			
gases	Inhalation	Inhalation	
PM <sub>2.5</sub>	Inhalation		
PM <sub>10</sub>	Inhalation		
precipitation			
<b>Indoor Air</b>			
gases	Inhalation	Inhalation	Inhalation
PM <sub>2.5</sub>	Inhalation		
PM <sub>10</sub>	Inhalation		
water vapor			
<b>House Dust</b>			
on floors	Ingestion/dermal		
on surfaces	Ingestion/dermal		
<b>Soil</b>			
residential	Ingestion/dermal	Ingestion/dermal	
construction site	Ingestion/dermal	Ingestion/dermal	
industrial site	Ingestion/dermal		
agricultural site	Ingestion/dermal	Ingestion/dermal	
recreational site	Ingestion/dermal		
school	Ingestion/dermal		
<b>Tap Water</b>			
<b>Swimming Pool</b>			
<b>Surface Water used for Recreation</b>			
<b>Food</b>			
home fruits			
protected		Ingestion	
unprotected	Ingestion	Ingestion	
home vegetables			
above ground	Ingestion	Ingestion	
root crops			

EXPOSURE MEDIA	ENVIRONMENTAL MEDIUM = Soil		
	Surface Soil	Root Zone Soil	Vadose Zone Soil
home grains	Ingestion	Ingestion	
meat	Ingestion	Ingestion	
milk	Ingestion	Ingestion	
dairy products	Ingestion	Ingestion	
eggs	Ingestion	Ingestion	
breast milk	Ingestion	Ingestion	
prepared foods			

**Table 4-4**  
**Matrix of Links Between Water Media and Various Exposure Media**

EXPOSURE MEDIA	ENVIRONMENTAL MEDIUM = Water			
	Surface Water		Ground Water	
	Liquid Phase	Particle Phase	Liquid Phase	Particle Phase
<b>Outdoor Air</b>				
<b>Indoor Air</b>				
gases	Inhalation		Inhalation	
PM <sub>2.5</sub>				
PM <sub>10</sub>				
water vapor	Inhalation		Inhalation	
<b>House Dust</b>				
<b>Soil</b>				
residential	Ingestion/dermal		Ingestion/dermal	
construction site	Ingestion/dermal		Ingestion/dermal	
industrial site	Ingestion/dermal		Ingestion/dermal	
agricultural site	Ingestion/dermal		Ingestion/dermal	
recreational site	Ingestion/dermal		Ingestion/dermal	
school	Ingestion/dermal		Ingestion/dermal	
<b>Tap Water</b>	Ingestion/dermal	Ingestion	Ingestion/dermal	Ingestion
<b>Swimming Pool</b>	Ingestion/dermal		Ingestion/dermal	
<b>Surface Water used for Recreation</b>	Ingestion/dermal	Ingestion	Ingestion/dermal	Ingestion
<b>Food</b>				

EXPOSURE MEDIA	ENVIRONMENTAL MEDIUM = Water			
	Surface Water		Ground Water	
	Liquid Phase	Particle Phase	Liquid Phase	Particle Phase
home fruits				
protected	Ingestion		Ingestion	
unprotected	Ingestion		Ingestion	
home vegetables				
above ground	Ingestion		Ingestion	
root crops	Ingestion		Ingestion	
home grains	Ingestion		Ingestion	
meat	Ingestion		Ingestion	
milk	Ingestion		Ingestion	
dairy products	Ingestion		Ingestion	
eggs	Ingestion		Ingestion	
breast milk	Ingestion		Ingestion	
prepared foods	Ingestion	Ingestion	Ingestion	Ingestion

**Table 4-5  
 Matrix of Links Between Vegetation and Various Exposure Media**

EXPOSURE MEDIA	ENVIRONMENTAL MEDIUM = Vegetation			
	Above-Ground Plants			Root Crops
	Fruits	Vegetables	Grains	Crops
Outdoor Air				
Indoor Air				
House Dust				
Soil				
Water				
Food				
home fruits				
protected	Ingestion			
unprotected	Ingestion			
home vegetables				
above-ground		Ingestion		
root crops				Ingestion
home grains			Ingestion	
meat	Ingestion	Ingestion	Ingestion	Ingestion
milk	Ingestion	Ingestion	Ingestion	Ingestion
dairy products	Ingestion	Ingestion	Ingestion	Ingestion
eggs			Ingestion	Ingestion
breast milk	Ingestion	Ingestion	Ingestion	Ingestion
prepared foods	Ingestion	Ingestion	Ingestion	Ingestion

**4.2.4 DIVIDE POPULATION INTO APPROPRIATE SETS OF COHORTS**

The first step in selecting population(s) of interest is to define the total population associated with all of the exposure districts. This may be expanded to incorporate more than residents of the defined exposure districts. For example, people who do not reside within the exposure district but consume its agricultural products or fish may be included. Once the population(s) are identified, the second step is to decide whether to include all of the population members in a region or a subset of the population of concern due to a demographic factor, activity, or health characteristic (e.g., asthmatics, outdoor workers, pregnant women).

The population of interest is then divided into cohorts. In TRIM.Expo, each individual is exclusively assigned to a single cohort. Cohorts are distinguished from the overall population

based on attributes including age, gender, health status (*e.g.*, asthmatics), exposure district, and housing types (*e.g.*, gas stoves, HVAC systems). The number of cohorts selected depends largely on the level of resolution of the exposure factor data used to characterize the population and on the level of exposure resolution required. The type of pollutants and sources under consideration can affect the number and type of cohorts as well.

As previously stated, cohorts can be defined for a particular application or situation. For example, cohort exposure can be a function of demographic group, location of residence, location of work place, and type of home ventilation system. Cohort exposure can be linked to ambient pollutant concentrations in multiple districts (*e.g.*, home and work district). Specifying the demographic group allows cohort exposure to be linked to activity patterns that vary with age, work status, and other demographic variables. In some analyses, cohorts are further distinguished according to time spent in particular microenvironments. For example, in studies of ozone exposures, additional cohorts were created to account for children who spent significant amounts of time outdoors and also for adults who worked outdoors. These cohort designations helped analysts estimate exposures for subgroups in the population with the greatest potential for higher exposures.

#### **4.2.5 DEVELOP AN EXPOSURE-EVENT SEQUENCE FOR EACH COHORT**

Once a set of cohorts has been selected, a sequence of exposure events is defined for each cohort. An exposure-event sequence is a chronological set of events that define the activity/time allocation of each cohort. An exposure-event sequence defines a cohort by (1) exposure district, (2) microenvironment, and (3) activity at each time step of a calculation. Implicit in the definition of activities for the exposure-event sequence is information about the time of year or season, through the selection of activity patterns based on the outdoor air temperature that coincided with the collection of the activity pattern data. The following example in Table 4-6 shows simple eight-hour exposure-event sequence. Because an exposure-event sequence is developed from an individual's activity pattern data used to represent the cohort, concentrations in each of the microenvironments are the same for each member of the cohort. Multiple runs of the model results in variation of the activity patterns for a given cohort.

**Table 4-6**  
**Sample Eight-Hour Exposure-Event Sequence**

Time:	06:00	07:00	08:00	09:00	10:00	11:00	12:00
<b>Exposure District</b>							
	Zone 1		Zone 2				
<b>Microenvironment</b>							
	Indoors at home		Inside a vehicle	Indoors at work			
<b>Activity</b>							
	Sleeping	Dressing, eating	Comm-uting	Working at desk			Eating lunch

#### 4.2.6 DETERMINE EXPOSURE MEDIA CONCENTRATIONS AND CONTACT IN EACH MICROENVIRONMENT

Once a sequence of exposure events is established, the exposure medium concentration and the rate of contact between the cohort and the exposure medium in the various microenvironments must be estimated. The route of contact/intake can greatly influence the affected populations or the populations of interest that are studied in an exposure assessment. For example, hand-to-mouth contacts are more important for a population of children than for a population of adults. This information is then used to establish an exposure concentration profile, a cumulative intake, or an average exposure medium concentration over a defined averaging time.

#### 4.2.7 ESTIMATE AN INTAKE RATE FOR EACH DOSE EVENT

For each exposure event in the exposure-event sequence, TRIM.Expo estimates the intake rate of the pollutant for all relevant routes of exposure. Initially, TRIM.Expo will provide estimates for inhalation and ingestion only. To estimate the intake rate of a pollutant via inhalation, TRIM.Expo defines each exposure with a pollutant concentration and a ventilation rate indicator. The applied dose is a function of the pollutant concentration in contact with the individual or cohort, the activities that the individual or cohort are engaged in that affects breathing rate, and the ventilation rate value that is assigned to the exposure event. Section 5.1.5 describes in detail how pollutant concentrations and the ventilation rate associated with each exposure event will be estimated.

For ingestion, TRIM.Expo estimates the average daily potential dose (ADD) for many different ingestion pathways and media of exposure. The ADD represents the amount of

pollutant that enters the mouth of the exposed individual or cohort over a defined exposure event for a defined exposure duration. Data are provided on the rate of ingestion of the exposure medium (e.g., water, soil, food) during an exposure event and are used to calculate the ADD. Section 6.1 provides a summary of the general approach used to characterize the ADD for an exposure medium. Subsequent sections in Chapter 6 provide details on how the algorithm applies to specific exposure media.

#### 4.2.8 EXTRAPOLATE THE COHORT EXPOSURES TO THE POPULATIONS OF INTEREST

After the exposures to the cohorts have been calculated, they are extrapolated to the population at risk by estimating the population size for each cohort. Population estimates assigned to each cohort are calculated for both commuting (*i.e.* to work, to school) and non-commuting cohorts. The first step is to calculate the population of each demographic group that resides in a particular home district through data available from the Bureau of the Census. This information provides the population of all non-commuting cohorts by home district.

The population of non-commuting cohorts can be further divided to account for a particular attribute shared by the cohorts. The attribute should be one for which data about the size of the population can be obtained. The population size of each demographic group listed as having attribute *b* is calculated through the following equation:

$$pop(dg,ca,b) = f(ca,b) \times pop(dg,ca) \quad (4-11)$$

where:

- $pop(dg,ca,b)$  = The population of demographic group *d* in census area<sup>1</sup> *ca* having The attribute of interest *b*.
- $f(ca,b)$  = Fraction of people in census area *ca* that have attribute *b*.
- $pop(dg,ca)$  = Total number of people in demographic group *d* that reside in census area *ca*.

The values of  $pop(dg,ca,b)$  are summed over each home district to yield estimates of  $pop(dg,h,b)$ , the number of people in demographic group *dg* within home district *h* that share attribute *b*. Any number of attributes can be used to calculate  $pop(dg,h,b)$  if census area data are available.

The value of  $pop(dg,h,b)$  provides an estimate of the population in each non-commuting cohort associated with demographic group *dg* residing in home district *h* that shares the attribute of interest *b*. Next, the populations of the commuting cohorts in demographic group *dg* who share attribute *b* are calculated using the fraction of all commuters residing in home district *h* who travel to commute district *w* (including children who commute to school) using Equation 4-12:

---

<sup>1</sup> “Census area” can be any spatial area designated by the Bureau of the Census. For most exposure applications, the census tract designation is used.



$$com(dg,h,w,b) = pop(dg,h,b) \times com(h,w) / com(h) \tag{4-12}$$

where:

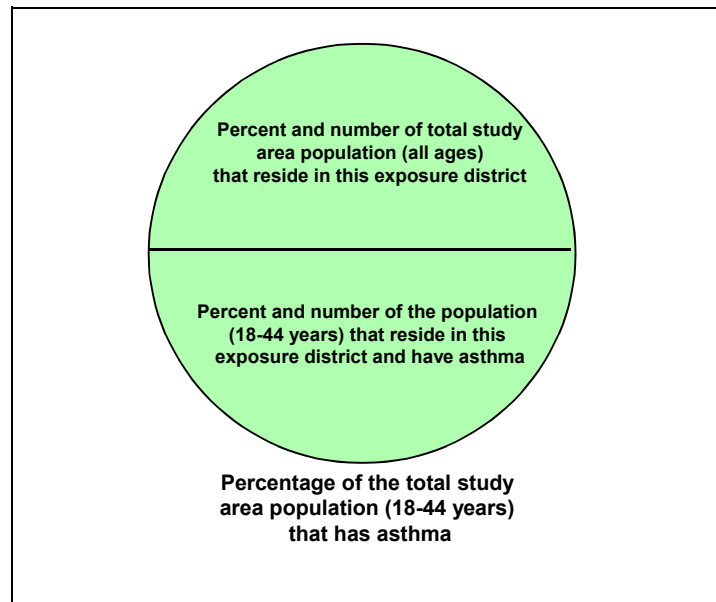
- $com(dg,h,w,b)$  = number of people in a commuting cohort associated with demographic group  $dg$  in home district  $h$  and commute district  $w$  having attribute  $b$ .
- $com(h,w)$  = number of commuters in all demographic groups that travel from home district  $h$  to commute district  $w$ .
- $com(h)$  = total number of commuters in home district  $h$ .

Estimates of  $com(h)$  can be obtained from census data specific to each district.

By defining cohorts according to attributes that are important to specific applications or situations, TRIM.Expo is able to extrapolate the cohort exposures to the general population while still retaining information about the incidence of exposure to the specific subset of the population under study. For example, suppose that the population of interest was individuals, ages 18 to 44, who experience asthma. For a particular study area, information for both of these attributes is available. Census data contains the breakdown of age information by location, while information on the incidence of asthma is available from various sources, including the National Center for Health Statistics and state and local health agencies. In this case, the TRIM.Expo analysis would be arranged to capture the demographic characterization of this subset of the population by selecting a demographic group that includes individuals from 18 to 44 years of age. The fraction of the demographic group with asthma can be determined from health data. When combined, this information provides an estimate of the exposures to this specific segment of the population for each exposure district, assuming that activity patterns for asthmatics do not differ significantly from those of the other members of the demographic group. Once the exposures of this sensitive subpopulation are known for each exposure district, the exposures can be readily extended to encompass the entire study area under investigation.

In the simple example given above, the fraction of the total population with the specified attribute in a particular exposure district can be quite different from the fraction of all people in the study area contained within that exposure district. Consider, for example, Figure 4-4 which presents a hypothetical illustration of the example above. In this figure, each circle represents an exposure district. The study area for this example is the sum of the three exposure districts. The total population of this hypothetical study area is 100,000 people. The fraction and number of the total study area population residing in each exposure district is indicated in the top half of each circle. The fraction and number of the 18 to 44 year olds in the study area population with asthma in each exposure district is indicated in the bottom half of each circle. As can be seen in this example, exposure district #3, which includes 50 percent of the total population of the study area, contains 2,500 people age 18 to 44 with asthma, only 2.5 percent of the total study area population (*i.e.*, all three exposure districts combined). However, exposure district #2, which includes only 20 percent of the total population of the study area, accounts for 7 percent (7,000) of the cases of asthma in the 18 to 44 year-olds in the study area. Finally, exposure district #1, which has one-third of the study area's total population, has 18,000 cases of asthma in people of age 18 to 44, 18 percent of the total study area population.

**Figure 4-4**  
**Hypothetical Spatial Distribution of the Incidence of Asthma**

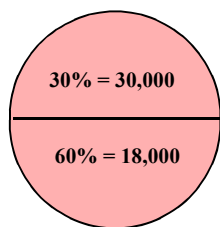


**SCENARIO:**

Study area population (all ages) = 100,000

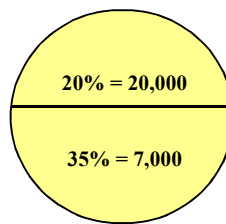
Study area population (18-44 years) that has asthma = 27,500 (27.5 percent)

**Exposure District 1**



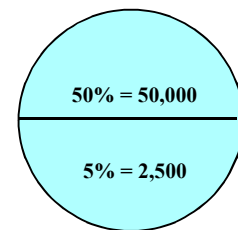
**18%**

**Exposure District 2**



**7%**

**Exposure District 3**



**2.5%**

The example above illustrates that the spatial distribution of a demographic variable, such as the incidence of a particular disease, is not necessarily the same as the spatial distribution of the general population. The illustration also points out that conducting exposure analyses on a smaller spatial scale is likely to lead to more accurate results. This is particularly true when investigating exposures related to factors that have a high degree of variability over small distances. Different exposure estimates for the sensitive subpopulation of individuals suffering from asthma would have been obtained if the exposures of the entire population were calculated and then adjusted for the incidence of asthma based on the percentage of reported cases for the study area as a whole without regard for the spatial variation of this disease.

## 4.2.9 FUNCTIONAL ATTRIBUTES

The TRIM.Expo module will include important attributes that are needed by analysts and decision-makers to investigate the complex nature of multipollutant and multipathway human exposures to hazardous and criteria air pollutants in the environment. This section briefly describes many of the functional attributes that will be included in TRIM.Expo. The attributes fall into two major categories: (1) important considerations related to the scientific defensibility of the exposure estimates, and (2) design features of TRIM.Expo that help ensure the needed flexibility and ease of use of the modeling system.

### 4.2.9.1 Inclusion of Indoor and Outdoor Environments and Their Emission Sources

Recent studies have shown the importance of including both indoor and outdoor environments when assessing human exposures to toxic pollutants (Ozkaynak et al. 1996, U.S. EPA 1987, Wallace et al. 1985, Wallace et al. 1991). These studies called the Total Exposure Assessment Methodology (TEAM) and Particle Total Exposure Assessment Methodology (PTEAM) studies, and other indoor/outdoor studies that have succeeded them, reported that indoor concentrations of many toxic air contaminants were often greater than concurrent outdoor concentrations. Other studies have reported that most people in the U.S. can spend as much as 90 percent of their time indoors or inside motor vehicles (Jenkins et al. 1992, U.S. EPA 1996a). Conversely, exposures to the NAAQS pollutants (*e.g.*, ozone, sulfur dioxide) are dominated by outdoor levels or by ambient air that infiltrates to indoor environments. Therefore, it is vital that a framework for assessing the total human exposure to pollutants include the indoor, in vehicle, and outdoor environments.

An important microenvironment for exposure to multiple airborne pollutants is inside a passenger vehicle. This microenvironment is treated similarly as the indoor environment, although a significant fraction of the concentration found indoors may come from penetration of ambient air. Nevertheless, exposures to many pollutants within a moving vehicle have been reported to be higher than either roadside or ambient (*i.e.*, away from a road) exposures (CARB 1998b). Lawryk et al. (1995) reported that commuting can account for a substantial amount of a person's daily exposure to select toxic pollutants. Furthermore, both studies reported that many factors can affect the levels of pollutants inside a vehicle, including the general condition and maintenance of the vehicle, the vehicle's age, the density of the surrounding traffic, and the resulting effect these factors have on the speed of the vehicle.

Besides traveling in a vehicle, other activities that can have a significant impact on exposures are cooking and smoking. Increased concentrations in close proximity to gas stoves have been reported for NO<sub>2</sub> (Sega and Fugas 1991), CO (U.S. EPA 1984), and PM<sub>2.5</sub> and PM<sub>10</sub> (Ozkaynak et al. 1996). The concentrations of other pollutants produced through incomplete combustion have also been found to be higher close to a cooking appliance. Ozkaynak et al. (1996) also reported that smoking was a significant source of particles in homes in the PTEAM study. They found that homes where smoking was reported averaged approximately 30 μg/m<sup>3</sup> higher levels of PM<sub>10</sub> than homes without smoking. Numerous other exposure studies have reported higher concentrations of CO, particles, and toxic pollutants in indoor environments (particularly the home) with environmental tobacco smoke (ETS) (Daisey et al. 1998, Jenkins et al. 1996, Miller et al. 1998, Phillips et al. 1998, Quackenboss et al. 1991, Thomas et al. 1993, Waldman et al. 1991).

The TRIM.Expo module has several indoor and in-vehicle microenvironments, including inside a home (several different locations); in transit (*e.g.*, automobiles, buses, trains), indoors at work or school; indoor recreational facilities (*e.g.*, movie theaters), shopping malls, and restaurants. In addition, TRIM.Expo has the flexibility to include other indoor microenvironments of importance as information becomes available.

While evidence continues to accumulate regarding the importance of indoor sources and environments on exposures, there remains important sources of exposure outdoors, too. In fact, studies show that in the absence of indoor sources, penetration of outdoor pollutants were responsible for elevated indoor concentrations (see, for example, Lioy et al. 1991). However, investigations into the sources of outdoor pollutants have found that, although human activities, such as motor vehicle use have a major impact on ambient levels of particles and toxic pollutants, relatively small, local sources of specific toxic pollutants such as repair shops can also have a significant impact on the exposures to a nearby population. Moreover, exposures to pollutants from certain outdoor sources can be affected by local climatology, thereby exhibiting seasonal variations in the exposure profile. An example are pollutants that are emitted by the burning of heating fuel in the winter months (Lioy and Daisey 1990).

The TRIM.Expo module currently has several outdoor environments included in its modeling system. There are outdoor microenvironments specified for at home, in transit (*e.g.*, walking, bicycling), at work, and recreational locations. The location where eating takes place may also be important for estimating ingestion exposures.

#### **4.2.9.2 Flexible, Modular, and Portable Algorithms**

The TRIM.Expo module is designed with features that will facilitate future expansion and integration of the framework in anticipation of new modeling techniques and data. Additionally, there is a need for TRIM.Expo to be compatible with other exposure modeling platforms developed both within and outside of EPA. The design features that will allow for these capabilities are portability, modularity, and flexibility. These three features are all interrelated in function and purpose. They follow the recommended guidance set forth by the National Research Council's *Committee on Advances in Assessing Human Exposure to Airborne Pollutants* (NRC 1991b). Flexibility means that the model algorithms are written using precise,

standard encoding practices. This approach will allow the model to be updated relatively easily as new data and new modeling techniques become available. The TRIM.Expo module algorithms are being designed to readily incorporate new information regarding both data and methods. As an example, comments will be included within the model's source code which will help future developers understand how the model was constructed and explain each of the functional components of the model. This seemingly minor point has important implications for the future development of TRIM.Expo because (1) model development and revisions may continue indefinitely, and (2) responsibility for future updates of the model may shift to different groups.

Another aspect of flexibility is the use of modular design in model development. Modular design, as its name implies, means that the components of the model involved in the computation of exposures are separated into discreet units, where each unit is responsible for a particular function. These discreet units, or modules, are called upon during the execution of a model run to perform a specific function or set of functions. If a particular application does not require the function(s) performed by a certain module, then the calculations or routines performed by the module are not called upon. In most of the early exposure models, all of the functions of a model were executed regardless of whether they were required for the particular application. Using only the modules that are needed for a specific application reduces the amount of computer resources required. Using a modular approach also aids in the development of the model because when specific model functions are in modules, they can be revised and tested without running the entire model. This makes isolating and correcting mistakes in the model's algorithms easier, as well.

The functional attribute of portability is important to the development of the TRIM.Expo modeling system. Portability refers to how easily the model can be integrated with other modeling systems such as Models-3 or MENTOR, in the case of TRIM. Expo. The overall goal of systems such as Models-3 and MENTOR is to simplify and integrate the development and use of complex environmental models. The developers of these systems seek to provide a set of ready-to-use methodological tools and linkages to relevant databases for performing assessments of exposure. Hence, it is important that TRIM.Expo can take full advantage of the designs and numerical analysis tools provided by these systems. Therefore, TRIM.Expo is based on an open, user-oriented implementation that is compatible with the components of other modeling systems. An open system design means that TRIM.Expo's development is not specific to a single computing platform. Finally, TRIM.Expo can be run without the use of proprietary software or model components, enhancing both the flexibility and portability of TRIM. Expo.

#### **4.2.9.3 Explicit Treatment of Uncertainty and Variability**

While the importance of characterizing uncertainty and variability explicitly and separately is well recognized (NAS 1994, CRARM 1997, U.S. EPA 1997c), OAQPS intends to *selectively* apply uncertainty and variability analyses on a case-specific basis, (*i.e.*, for critical parameters and, where appropriate, based on the underlying science and data).

The TRIM.Expo module explicitly treats the uncertainty in the model estimates of exposure. Uncertainty is the lack of knowledge of the actual values of physical variables

(parameter uncertainty) and of physical systems (model uncertainty). For example, parameter uncertainty results when non-representative sampling (to measure the distribution of parameter values) gives sampling errors. Model uncertainty also results from simplification of complex physical systems. Uncertainty can be reduced through improved measurements and improved model formulation.

As with uncertainty, the variability in model inputs will be explicitly characterized in TRIM.Expo, wherever feasible. Variability is not to be confused with uncertainty; they are two separate aspects inherent in data sampled from a population. Variability represents the diversity or heterogeneity in a population or parameter and is sometimes referred to as natural variability. An example is the variation in the heights of people. Variability cannot be reduced by using more measurements or measurements with increased precision (*i.e.*, more precise measurements of people's heights does not reduce the natural variation in their heights). However, it can often be reduced by a more detailed model formulation. For example, modeling people's heights in terms of their age will reduce some of the unexplained variability in the distribution of data on heights. Variability among the members of a population in factors such as food ingestion rates, exposure duration, and expected lifetime can be described by purely stochastic (*i.e.*, involving chance or probability) processes. These processes are random or variable and are not characterized by a single value but can be described by a distribution. Thus, estimation of the moments of the distribution (*e.g.*, mean, variance, skewness) is possible.

The TRIM framework includes an approach to estimate uncertainty and variability in a manner that allows for integration between the TRIM modules while tracking the uncertainty and variability through the modules. The remainder of this section briefly describes the approach for estimating uncertainty and variability. For a more rigorous explanation on uncertainty and variability and implementation in the TRIM framework, please refer to the 1999 TRIM Status Report (U.S. EPA 1999c).

The EPA chose a staged approach for analyzing uncertainty and variability since it has several advantages for models as complex as TRIM. The first stage, which is comparatively easy to implement, is known as a sensitivity and screening analysis. This stage involves identifying influential parameters and developing an importance-ranking of parameters to focus and reduce the number of parameters analyzed in the uncertainty and variability analysis. The sensitivity and screening analysis computes the importance of parameters by calculating the extent to which model results change when parameters are varied singly or in pairs. This process provides for a first-order determination of the most influential parameters and allows further analysis to focus on the key parameters. Furthermore, this screening approach narrows down the scope of the detailed analysis in the second stage and reduces the number of parameters by identifying influential parameters that should be retained for further analyses. This is a critical step toward the goal of producing an economical representation of uncertainty and variability by excluding unnecessary terms and parameters and still capturing all of the significant features of model uncertainty and variability.

The second stage of TRIM.Expo's uncertainty and variability analysis is more complex and involves a Monte Carlo approach. Monte Carlo methods analyze model uncertainty by using statistical sampling techniques to estimate statistics that characterize uncertainty. Essentially, a

Monte Carlo approach entails performing many model runs with model inputs that are randomly sampled from specified distributions for the model inputs. These can be set up to characterize the propagation of uncertainty and variability of the model input parameters, taking into account distributions of parameter uncertainty and variability and parameter dependencies. These simulations provide uncertainties of model outputs in terms of distributions of model outputs, joint distributions of model inputs and outputs, and summary scalar measures (*i.e.*, the core data from which information about uncertainty and variability can be extracted).

This two-stage analysis of uncertainty and variability will be performed for each of the TRIM modules to study the propagation of uncertainty. The Monte Carlo simulations for each TRIM module will be performed sequentially in the order that the TRIM modules are run. Sufficient information must be transmitted from one module to the next to be able to propagate distributional information to succeeding Monte Carlo simulations. Since the amount of data produced from Monte Carlo simulations is voluminous, the full results will be archived and a reduced set will be retained as input for the next module. The output values from each of the TRIM modules as well as the model inputs (*i.e.*, parameter values) for each Monte Carlo simulation will be saved and can be passed along to the next module for subsequent uncertainty analysis. However, the amount of data would increase drastically from one module to the next. Therefore, it is important to track the input parameters to each TRIM module.

To reduce the size and complexity of the transfer of uncertainty and variability information between TRIM modules, the results can be summarized in the form of non-parametric probability distributions that can be passed to the next module, where each distribution to be passed is characterized non-parametrically by its percentiles.

The screening stage described above involves a sensitivity ranking analysis to select the critical parameters to be tracked for the more detailed uncertainty analysis; all other parameters would be set at their central tendency value. This focus on critical parameters also decreases the amount of information to be tracked. To further reduce the volume of information, after summarizing the results from one module as probability distributions, the transmission of information to the next module is filtered to select the most critical parameters (*e.g.*, those that account for 95 percent of the variance of the uncertainty and variability).

It is important to note that since data for many of the input variables in TRIM.Expo (*e.g.*, time-activity patterns, ventilation rates, air exchange rates) are not available to cover the entire range of possible values, Monte Carlo simulations are used to better represent the distribution of exposures that occur among the people in an exposure assessment. While this method better captures the variability of the population's exposures, it underestimates the repetitive nature of certain high exposure situations (*e.g.*, long commutes in slow-moving traffic or preparing foods in a manner that increases the release of toxic pollutants) for certain segments of the population.

Furthermore, it should be noted that much of the data used to characterize variability related to exposure, such as time-activity patterns or other exposure factors are sometimes based on short-term (multiday) measurements (*e.g.*, diary studies, recall, monitoring). Despite the limitations and assumptions built into using such data to generate long-term factors, OAQPS believes that these data are the best available and extrapolating to generate long-term factors or

creating a longer term sequence of such data is the best approach. It should be reiterated that TRIM, due to its architecture, is a dynamic modeling system, not a static model, and will be able to undergo frequent updates that reflect new science and information. Therefore, once alternative and improved approaches (*e.g.*, correlated diaries for activity and consumption information at the individual level developed through statistical analysis of multiday diaries) become available, they will be evaluated and incorporated into TRIM where appropriate.

### 4.3 DATA INPUT REQUIREMENTS

Inputs to TRIM.Expo include environmental media concentrations, intermedia transfer factors, and/or the input needed to calculate intermedia transfers from algorithms, cohort activity data, and demographic and at-risk population data. The sections below summarize the principle sources of input data in these areas.

Although TRIM.Expo is primarily a stochastic model, distributions for many of the model's inputs are either not available or are incomplete. Through the use of a systematic sensitivity analysis, exposure pathways and parameters can be identified by the model that do not make a major contribution to the assessment endpoint nor to the overall uncertainty and variability. The use of point estimates can then be considered for these parameters (U.S. EPA 1997c). Conversely, TRIM.Expo will use Monte Carlo analysis for those parameters that are found to have a significant impact on exposure and that have data available. Hence, assessments in TRIM.Expo will be able to use a combination of distributional data for input parameters that are judged to be important by the analyst, and point estimates for those parameters that are either determined to contribute little to the exposure outcome or that have insufficient data available. Whichever distribution type is selected for a particular parameter, the analyst will be informed by the model of the choices made and the implications that may result.

A *probability density function* (PDF) will be developed for many of the input variables used in TRIM.Expo. For continuous random variables, the PDF expresses the probability that the random variable falls within some very small increment (U.S. EPA 1997c). It must be emphasized that distributions for many of the exposure factors in TRIM.Expo have not been developed to date, hence, a major effort is required to develop the PDFs for input to the model.

Probability density functions can be characterized by numerous distributional forms (Cullen and Frey 1999). For each TRIM.Expo application, the analyst needs to address several critical issues regarding data sorting and manipulation. These issues include, but are not limited to the following: (1) how to develop a PDF based on limited data; (2) how to set the confidence or uncertainty limit for a PDF; (3) how to truncate PDFs to eliminate unrealistic scenarios; and (4) how to use data that is below its detection limit. The EPA has convened workshops to address important issues regarding data distributions and their variability and uncertainty (U.S. EPA 1996b, U.S. EPA 1999g). The reader is urged to refer to these workshop reports for more in-depth information regarding these issues.

Another issue concerning the development and use of data inputs is that as studies provide new information on exposure factors, discrepancies may appear between the factors in



one study as compared to those from a different study. This complicates the selection of exposure factors for use in TRIM.Expo. Therefore, whenever possible, the developers of TRIM.Expo will use exposure factors that are consistent across EPA program offices. Furthermore, they will draw on the efforts of, and work cooperatively with, ORD and the other program offices to determine the most appropriate exposure factors and will update these periodically to reflect the most current knowledge in this field.

#### 4.3.1 ENVIRONMENTAL MEDIA CONCENTRATIONS

The required environmental media concentration data input for TRIM.Expo includes ambient pollution concentration estimates. For the exposure duration of interest in TRIM.Expo, a concentration profile for each of the principal environmental media (*i.e.*, air, soil, water, vegetation) included in the analysis for each exposure district is needed. Pollutant concentration data for TRIM.Expo is assumed to be available from analysis of monitoring data, from a dispersion model, or from a multimedia transport model such as TRIM.FaTE. The two environmental media for which monitoring data are most abundant are air and water.

The OAQPS is responsible for managing a monitoring network of ambient fixed-site monitors for air pollutants. The OAQPS uses this network of monitors to help ensure that the levels of the criteria pollutants (*i.e.*, carbon monoxide, nitrogen dioxide, sulfur dioxide, ozone, particulate matter, lead) do not exceed the NAAQS established to comply with the CAA. The air quality measurements are collected by monitors at thousands of sites across the nation operated by state and local environmental agencies. Each monitor measures the concentration of a particular pollutant in the air. Monitoring data indicate the average pollutant concentration during a time interval, usually one hour or 24 hours. The monitoring stations in this network are called the State and Local Air Monitoring Stations (SLAMS). To obtain more timely and detailed information about air quality in strategic locations across the nation, OAQPS established an additional network of monitors, called the National Air Monitoring Stations (NAMS). The NAMS sites, which are part of the SLAMS network, must meet more stringent monitor siting, equipment type, and quality assurance criteria.

The CAA also stipulates that each state include a comprehensive inventory of existing sources of air pollution and an accurate estimate of the total amount of pollutants (*e.g.*, VOCs) emitted to the air by each source during a calendar year. These pollutant emissions estimates are compiled by operators of industrial and commercial enterprises, state and local environmental agencies, and EPA. The amount of pollutant is calculated using EPA-approved methods and measurable factors such as the quantity of fuel used.

All of these emissions data are compiled in a single database called the Aerometric Information Retrieval System (AIRS). The AIRS contains all of the air quality, emissions, compliance, and enforcement information that OAQPS and state agencies collect to carry out their respective programs for improving and maintaining air quality.

The EPA's Office of Water (OW) manages information collected on pollutant concentrations measured in waterbodies. The data are collected from monitoring conducted at regular sites on a continuous basis, at selected sites on an as needed basis or to answer specific

questions, on a temporary or seasonal basis, or on an emergency basis. The responsibility to monitor water quality rests with many different agencies. State pollution control agencies have key monitoring responsibilities and conduct vigorous monitoring programs. Many local governments, such as city and county environmental offices, also conduct water quality monitoring. In addition, other Federal agencies are also involved in water quality monitoring. For example, the U.S. Geological Survey (USGS) conducts extensive chemical monitoring through its National Stream Quality Accounting Network (NASQAN) at fixed locations on large rivers around the country.

Many agencies and organizations maintain computerized data systems to store and manage the water quality data they or others collect. Perhaps the single largest such ambient water quality data system is EPA's STORET (STORage and RETrieval) system. Much of the data collected by state, local, and federal agencies and by some private entities such as universities and volunteer monitors are entered into STORET. Raw data in STORET can be accessed, analyzed, and summarized by many users and for many purposes.

The TRIM.Expo module will be capable of using data from multimedia transport models as input data for ambient pollutant concentrations, particularly for multimedia, multipathway pollutants. One such model is the TRIM.FaTE module. The TRIM.FaTE module can estimate pollutant concentrations in multiple environmental media and biota, and accounts for transfer of mass throughout an environmental system. It models the movement of pollutant mass over time through a bounded system, which includes both biotic and abiotic components. The boundaries of the system are defined by the user, and can easily conform to the exposure districts in a TRIM.Expo application.

### **4.3.2 CONCENTRATIONS OF POLLUTANTS IN MICROENVIRONMENTS**

Pollutant concentrations will need to be supplied to TRIM.Expo for all microenvironments in which significant contributions to exposures occur. When measured data are unavailable, there are various techniques for estimating these microenvironmental concentrations. These techniques are discussed below, with a focus on ways of estimating microenvironmental concentrations of pollutants in air.

#### **4.3.2.1 Indoor Versus Outdoor Concentrations**

Studies that simultaneously measure indoor and outdoor concentrations of various pollutants show that numerous factors affect a pollutant's ability to penetrate to the inside of a building from outdoors (Johnson et al. 1996c). One of the most comprehensive measurement studies of indoor/outdoor concentrations of air pollutants conducted to date is the Total Exposure Assessment Methodology (TEAM) (U.S. EPA 1987). This multi-year study was conducted in the early to mid 1980's. During the study, measurements of the exposures of 600 individuals to 20 target chemicals in both air and water were made. The 600 study participants were a representative sample of a total population of 700,000 residents of cities in New Jersey, North Carolina, North Dakota, and California. One of the most important findings of the TEAM study was that personal (air) and indoor exposures to VOCs are nearly always greater than outdoor levels (Wallace et al. 1991, U.S. EPA 1987). The TEAM studies answered a question of equal

importance for modeling exposures to air pollutants, that is: “Is there any indoor and outdoor relationship associated with the variation of one or more air pollutants measured simultaneously at a residence?” In the New Jersey TEAM study, results showed that (1) during times conducive to accumulation of high outdoor VOC concentrations, substantial contributions to indoor levels can be made, and (2) in homes where there are no indoor sources of a VOC compound, the indoor concentration variation can be driven by outdoor VOC levels (Liroy et al. 1991).

#### 4.3.2.2 Mass Balance Model Approach

For estimating air pollutant concentrations for indoor microenvironments, TRIM.Expo will include the option of using a mass balance modeling approach where sufficient data exist. In general terms, the mass balance model can be described as:

$$\begin{aligned}
 \textit{The change in indoor pollution concentration} = & \\
 \textit{the pollutant entering from outside} & \\
 + \textit{the indoor generation of pollutant} & \\
 - \textit{pollutant leaving the indoor microenvironment} & \\
 - \textit{removal of the pollutant by an air cleaning device} & \\
 - \textit{decay of the pollutant indoors.} &
 \end{aligned}$$

Each term in the above conceptual model requires data inputs. Implicit in the above terms are data needs for other variables such as infiltration, air exchange rate, surface reactivity, building volume, and recirculation. Additionally, air exchange removal can be separated into fractions removed for unfiltered and filtered air, and similarly penetration of outdoor air can be separated into fractions for penetration of filtered and unfiltered air. Another factor which has a great influence on several of these variables is the type and use of air conditioning. One of the most ubiquitous sources of indoor air pollutants is smoking. This source type (when present) is responsible for elevated indoor concentrations of numerous air pollutants. Section 5.2.1 of this report describes in more detail the mass balance model that will be included in the initial inhalation prototype of TRIM.Expo.

McCurdy (1994) discusses the “indoor data factors and parameters” that were required inputs to the mass balance model used in pNEM/O<sub>3</sub>. These factors, along with seasonal considerations, affect how much outdoor air pollution is estimated to come inside and how much indoor sources affect the indoor exposures. For the pNEM/O<sub>3</sub>, values for most of the variables in its mass balance model are obtained by Monte Carlo sampling from empirical distributions of measured data. The variables include (McCurdy 1994):

- Probability of having open windows, given the type of air conditioning system found in the home and the outdoor temperature;
- Air exchange rate, which is also affected by the “window status”;
- Residential surface-to-volume ratio, which is necessary to determine surface reactivity losses; and

- Emission rates from any indoor sources and the probability that the sources will be operating or not.

There is an ever increasing database for all of the factors mentioned above. For example, the Source Ranking Database provides data on indoor source emission factors (Johnston et al. 1996). In addition, the U.S. Census Bureau, as part of its American Housing Survey, routinely collects information on housing and building characteristics, including the use of air conditioning, methods of heating, square footage, and number of rooms. Researchers have become much more aware of the importance of seemingly minor factors such as whether a house's windows were open or shut when conducting studies of indoor and outdoor air pollutants. As a result, new studies are providing distributions for these important factors. Johnson et al. (1996a) provides a literature survey of recent studies for many of these factors. EPA will examine available databases such as the Source Ranking Database and American Housing Survey for relevant information on indoor sources and housing and building characteristics that can be used in TRIM.Expo.

### 4.3.2.3 Empirical Indoor/Outdoor Ratios Approach

The use of empirical indoor/outdoor relationships for estimating pollutant concentrations for indoor microenvironments is an approach that is often used when measured pollutant data or data needed for a mass balance model are lacking. This approach relies on observed relationships between outdoor concentrations and concurrent indoor or in-vehicle microenvironmental concentrations for selected pollutants. The Hazardous Air Pollutant Exposure Model (HAPEM4), a model similar to pNEM, uses this approach for estimating indoor and in-vehicle microenvironmental concentrations. The HAPEM4 uses a method of indoor/outdoor ratios called "microenvironmental (ME) factors" for determining the pollutant concentration in each indoor or in-vehicle microenvironment.

The EPA's OAQPS is currently collecting and analyzing data relevant to the development of ME factors for HAPs corresponding to those addressed in Section 112(k) of the Clean Air Act Amendments of 1990. Eventually, ME factors will be developed for all HAPs listed under Title III of the CAA. In addition to the traditional ME factor (also referred to as the penetration factor), data will be collected whenever possible for a separate factor relating the closeness of key sources to a microenvironment. Referred to as the proximity factor, this factor accounts for the higher concentrations usually expected when a receptor moves closer to a source. The resulting ME factors used in HAPEM4 are given by the expression:

$$C_{in}(i, k, t, cq) = \{[\gamma(k, cq)][C_{out}(i, t, cq)][\alpha(k, cq)]\} \quad (4-13)$$

where:

- $C_{in}(i, k, t, cq)$  = Average pollutant concentration in microenvironment  $k$  at exposure district  $i$  during time step  $t$  for calendar quarter  $cq$ .
- $\gamma(k, cq)$  = Penetration factor (relates outdoor concentration to indoor or in-vehicle microenvironmental concentration).

$C_{out}(i,t,cq)$	=	Ambient pollutant concentration taken at a fixed-site monitor or from a modeled value.
$\alpha(k,cq)$	=	Proximity factor (relates the closeness of key sources to a microenvironment).

Note that the ME factors typically do not vary by exposure district or from one time step to the next. However, they may be affected by calendar quarter (*i.e.*, by season).

### 4.3.3 ACTIVITY PATTERN DATA

Activity pattern data are used to determine the frequency and duration of exposure for specific groups within various microenvironments. As mentioned in Chapter 2, information on activity patterns are taken from measured data collected during demographic surveys of individuals' daily activities, the amount of time spent engaged in those activities, and the locations where the activities occur. Two common methods for collecting these data are through diary studies and activity recall studies. Diary studies involve a volunteer carrying a specially designed time-activity diary with them during their daily routine. They use the diary to record the start time of the activity, their location at the time, a description of the activity, the time the activity ended or changed to another one, and, sometimes, an estimate of their breathing rate. Diaries can be designed to obtain additional information for specific purposes or study requirements. In an activity recall study, respondents are asked to complete a questionnaire that details their activities from memory. The respondent is typically asked to recall his or her activities at the end of each day for the preceding 24-hour period. Data from this type of study are usually not as detailed as. However, activity recall studies can generally be conducted on larger populations than diary studies, since large numbers of respondents can be contacted by telephone.

In addition to recording the duration and location of a person's activities, important demographic information about the person is also then collected. The demographic information usually includes the person's age, gender, and ethnic group. Most activity pattern studies also try to collect information on other attributes of a respondent, such as highest level of education completed, number of people in their household, whether the person or anyone in their household is a smoker, employment status, and the number of hours spent outdoors. These are a sample of the possible items that might be requested on a questionnaire.

One of the largest databases for human activity pattern data is EPA's Comprehensive Human Activity Database (CHAD) (Glen et al. 1997). CHAD is comprised of nearly 17,000 person-days of activity pattern data. At present, 140 activities and 114 locations are included in CHAD. The data have been collected and organized from eight human activity pattern surveys. CHAD contains the sequential patterns of activities for each individual. Each activity has a corresponding location code so that the microenvironment of each activity is known. The activities in CHAD range from one minute to multiple hours in duration (activities longer than one hour are broken into segments and do not cross over from one clock hour to the next). The CHAD also provides an indicator of the rate of energy expenditure during a particular activity for each exposure event. This indicator is the metabolic equivalents or "METs" (see Section 6.1.5

for a description). In addition, CHAD includes an estimate of the body mass for each individual. This parameter is important for calculating uptake and dose (McCurdy 1999).

The TRIM.Expo module will have the ability to use the data in CHAD or, alternatively, use the data from a particular survey directly, providing the data are formatted properly. The CHAD will be updated periodically as additional data from new time/activity pattern surveys become available. In this way, a user has the two option mentioned above for using time/activity survey data in TRIM.Expo.

#### **4.3.4 DEMOGRAPHIC AND AT-RISK POPULATION DATA**

One of the purposes of TRIM.Expo is to perform analyses for subsets of the population that are particularly at risk to exposure to pollutants because of age or preexisting medical conditions. There are many sources of information detailing the demographic character of the population for the U.S. The originating source for most of this information is the Bureau of the Census (BOC), which compiles detailed demographic information about the U.S. population every ten years. The information is collected for the entire country at the census "tract" level or for the smaller census "block." Census tracts are small, relatively permanent statistical subdivisions of a county. Census tracts usually include between 2,500 and 8,000 persons. Census tracts do not cross county boundaries. The spatial size of census tracts varies widely depending on the population density of the area. Census blocks are smaller than census tracts in areal extent.

The BOC collects data on numerous aspects of the demographic character of U.S. citizens, including national and state population trends and projections; geographical mobility; school enrollment; educational attainment; households and families; marital status and living arrangements; fertility; child care arrangements; child support; disability; health insurance; labor force and occupation; income and poverty; and characteristics of various ethnic and elderly populations. Much of this information can be useful for understanding the demographic patterns that put segments of the population at risk from exposures to environmental pollutants.

Although the census is a good source of information about the geographic, housing, business related, and demographic characteristics of the U.S. population, it is limited in the amount of information available about the general health status of the population. However, there are other sources of information available about the incidence of diseases and illnesses in the U.S. For example, the National Center for Health Statistics (NCHS) publishes data from its National Health Interview Survey (NHIS). The households selected to be interviewed each week in the NHIS are a probability sample representative of the target population. Data are collected annually from approximately 43,000 households including about 106,000 persons. Data collected includes household composition, sociodemographic characteristics, basic indicators of health status, and utilization of health care services. Other information sources published by NCHS include the National Health and Nutrition Examination Survey, Ambulatory Health Care Data, and the National Maternal and Infant Health Survey. These databases can be used to estimate the size of various at-risk population groups.

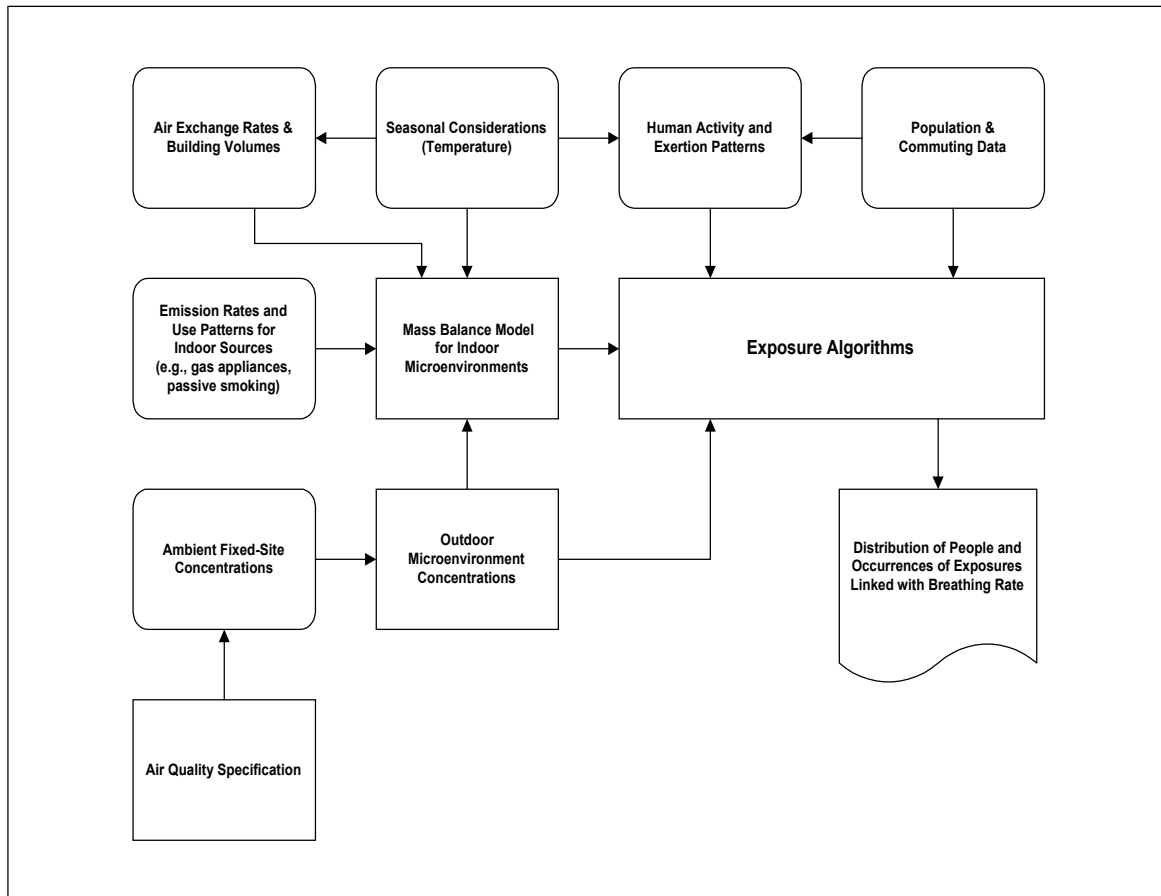
## 5. INHALATION

This chapter provides details of the inhalation component of TRIM.Expo. The structure of the inhalation component will be consistent with the conceptualized framework for TRIM.Expo described in Chapter 4. In addition, the initial development of the inhalation component will be based on the logic of pNEM. This will provide a firm scientific foundation for TRIM.Expo’s inhalation exposure algorithms, so that they are responsive to OAQPS’ need for a scientifically-sound, human exposure model for inhalation.

### 5.1 OVERVIEW OF THE APPROACH

Because of the flexible structure of TRIM.Expo, when performing an inhalation exposure assessment, the user must make a number of selections regarding the input parameters. The following six subsections provide the generalized approach for modeling inhalation exposures in TRIM.Expo. This approach is adopted from pNEM/CO (Johnson et al. 1999). Figure 5-1 is a schematic representation of the various input parameters and the resulting output of pNEM/CO.

**Figure 5-1**  
**Schematic Representation of the Input Parameters**  
**and Resulting Output of pNEM/CO**



### **5.1.1 SELECTION OF STUDY AREA**

The study area for inhalation exposures can be user-defined so long as estimates of outdoor air concentrations for the pollutant(s) of interest are available. The data on outdoor concentrations can be taken from ambient, fixed-site monitors or alternatively can be calculated using either an air quality dispersion model (*e.g.*, the Industrial Source Complex, or ISC, model), TRIM.FaTE, or other air quality models. In TRIM.FaTE, the ambient air compartment is characterized in terms of its gas phase, particulate matter, and water composition.

The study area is divided into exposure districts. The exposure districts are spatial areas with defined boundaries (either physical or political). If ambient monitoring data are used, then the exposure district may be defined as the area within a given distance of the monitor. If modeled air quality data are used, the exposure district can be defined according to the resolution of the modeled data. Modeled air quality data that are organized in a gridded pattern can have the exposure districts defined for each modeled grid-square or for aggregations of grid squares. Alternatively, a modeled grid-square value can be associated with a geopolitical area for which demographic information is available. For example, a modeled value could be assigned to the census-tract to which it belongs, thus relating calculated outdoor concentrations to the population information specified in census data.

### **5.1.2 SELECTION OF POPULATIONS OF INTEREST**

When conducting an exposure assessment using TRIM.Expo, the user may select a specific population group, or a set of groups, for which exposures will be estimated. Groups can be defined by any number of attributes including age, gender, family income, work status, health status (*e.g.*, heart disease patients), or proximity to particular emission sources (*e.g.*, natural gas cooking fuel). Since the movements and daily activities of the population of interest will determine which exposure media the individuals contact and in which exposure districts the contacts occur, data about the behavior of the population are required. Typically, the entire population for all of the exposure districts in the study area is included. Then, through the selection of cohorts, discussed below, exposure for subsets of the population are estimated. Characteristics for defining cohorts can be geographic factors, demographic factors, or both. Alternatively, the user may specify a set of individuals for an exposure assessment. In this case, the user supplies additional information about the individuals, as discussed below.

### **5.1.3 DEFINITION OF POPULATION COHORTS**

For an exposure analysis using groups, the population of interest, once chosen, is divided into groups with similar attributes; these groups are called cohorts. Each cohort is assumed to contain persons with similar exposures that are taken from the same probability distribution. Each person is associated with only one cohort. The use of cohorts is a useful technique when estimating the exposures of a large population with inadequate information about each individual's activity profile. Aggregating information about people who are expected to have similar exposures makes better use of the limited data that are available.



Cohort exposure is typically assumed to be a function of demographic group, location of residence, and location of work or school. A demographic group is comprised of all individuals that share one or more demographic features, such as a particular age (or age range), gender, ethnic background, or occupation. Specifying the home and commuting district of each cohort provides a means of linking cohort exposure to ambient concentrations. Specifying the demographic group provides a means of linking cohort exposure to activity patterns that vary with age, work or school status, and other demographic variables. In some analyses, cohorts are further distinguished according to factors relating to proximity to emission sources (*e.g.*, an indoor source such as a gas stove) or time spent in particular microenvironments.

#### 5.1.4 DEVELOP AN INHALATION EXPOSURE-EVENT SEQUENCE FOR EACH COHORT

When performing an inhalation exposure analysis using TRIM.Expo, information is needed about each “location” that each individual or cohort visits during their daily activities (*e.g.*, in the kitchen at home, outdoors at school, indoors at work). These locations are called microenvironments. An important feature of TRIM.Expo is the ability of the user to vary the scale of the microenvironments to individual model applications. This feature is important because it allows the user to relate the size of a microenvironment to the potential for exposure from different pollutants.

In TRIM.Expo, the inhalation exposure of each individual or cohort is determined by an exposure-event sequence specific to the individual or cohort. Furthermore, the exposure-event sequence for a particular cohort applies to all individuals in that cohort. The exposure-event sequence is a chronologically-ordered series of events which identifies locations and activities and the amount of time spent performing each activity in each location. In addition, the exposure-event sequence is specific to the day of the week. The information about the day of the week is obtained from the activity pattern database. Each exposure-event sequence consists of a series of events with durations ranging from 1 to 60 minutes. Once an exposure-event sequence is selected to represent the daily exposure of a cohort, it is followed through for an entire 24-hour period. A different exposure-event sequence is selected for each day in the study period. The TRIM.Expo module retains the information about the day of the week and season throughout the entire analysis because these variables can affect exposure results. Each exposure event assigns the cohort to a particular combination of exposure district, microenvironment, and activity (*e.g.*, cooking, playing, resting). Although no two individuals’ exposure will be *exactly* the same due to the myriad of factors that affect a person’s exposure; for the purposes of estimating a population’s exposure, especially considering the dearth of long-term time/activity information for a large enough cross section of the population, the model uses the simplifying assumption that all individuals within a particular cohort have the same exposure.

Information about the exposure-event sequences can be obtained by sampling from a human activity database. The human activity database is made up of diary and telephone survey records which identify a study participant’s daily activities and locations during a 24-hour period. Because each participant of most activity diary studies provides data for only a few days, the construction of a longer exposure-event sequence requires either the repetition of data from one participant or the use of data from multiple participants. The latter approach is being used in the

initial development of TRIM.Expo to better represent the variability of exposure that is expected to occur among the persons included in the cohort. The need to extrapolate short-term activity diary information to chronic exposure assessments is a recognized shortcoming in long-term exposure studies. There is a critical need for data on long-term activity patterns that can be used for constructing year-long exposure-event sequences. This issue, and discussion of an alternative statistical approach for augmenting short-term activity pattern diary data, are expanded upon in Section 5.4.2.

For the initial development of a TRIM.Expo Prototype, a compilation of time-activity surveys will be used for a cohort analysis. These surveys have been organized into a single database called the Consolidated Human Activity Database (CHAD) which was described previously in Section 4.3.3. The developers of CHAD have supplemented the activity pattern survey information with data showing the day of the week that a diary entry was made and also the maximum outdoor air temperature for that day. Knowledge of the day of the week is important when constructing exposure-event sequences since human activities are usually quite different for weekdays than they are on weekends (U.S. EPA 1996a). Providing information about the maximum outdoor air temperature that occurred on the day that a diary entry was made is a useful method for selecting activity data that account for seasonal variation when constructing year-long exposure-event sequences. For an individual analysis, the user must either provide demographic information about the individuals so that appropriate activity pattern data can be extracted from CHAD, or directly provide the time sequence of exposure district/microenvironment/activity pattern combinations, as well as the demographic data related to breathing rate (*i.e.*, age, gender, body weight).

### **5.1.5 ESTIMATE POLLUTANT CONCENTRATION AND VENTILATION RATE ASSOCIATED WITH EACH EXPOSURE EVENT**

The exposure-event sequence defined for each individual or cohort is used to determine a corresponding sequence of exposures, event-by-event. Each inhalation exposure is defined by a pollutant concentration and a ventilation rate indicator. The applied dose is a function of the pollutant concentration, the demographic characteristics of the individual or cohort affecting breathing rate, and the ventilation rate values assigned to the activity.

The first step in estimating the microenvironmental pollutant concentrations is to estimate the ambient pollutant concentrations. As discussed in Section 5.1.1, these are estimated from either fixed-site monitoring data, through the use of an air dispersion model, or from TRIM.FaTE. Next, microenvironmental concentrations are calculated from ambient concentrations and data on microenvironmental emission sources for indoor microenvironments (1) through the use of mass balance algorithms (described in Section 5.2.1), (2) with intermedia transfer factors, and/or (3) with measurements of concentration increments associated with indoor sources. Intermedia transfer factors are empirically derived and relate outdoor concentrations to the concentration contributions in the various indoor microenvironments used in TRIM.Expo. In addition, measurements of concentration increments associated with certain outdoor microenvironments (*e.g.*, gas stations, parking garages) may be used if they are not modeled or monitored explicitly. For other special outdoor microenvironments (*e.g.*, near

roadways), statistical analysis of ambient-to-microenvironment concentration relationships may be used to estimate microenvironmental concentrations based on fixed-site monitoring data.

Concentrations are determined for each microenvironment in each exposure district for each time step in the exposure-event sequence. These concentrations constitute the values for  $C_m(i,k,l,t)$  in Equation 4-1. For inhalation, the concentrations are calculated for air only; therefore, the only exposure medium  $m$  in Equation 4-1 is air.

In TRIM.Expo, an array of microenvironmental pollutant concentration values  $C_m$  are created for each individual or cohort. Each array consists of a set of year-long sequences of hourly-averaged  $C_m$  values; one for each combination of exposure district, microenvironment, and activity. In the initial development of TRIM.Expo, the district will be either the home, work, or school district specified for the individual or cohort. For an exposure event during time step  $t$ , an individual or cohort is assigned the value of  $C_m$  specified for that time step in the designated exposure-district/microenvironment/activity sequence.

In addition to the pollutant concentration, a ventilation rate ( $V_E$ ) value is estimated for each exposure event.  $V_E$  is expressed as liters of air respired per minute (liters  $\text{min}^{-1}$ ). The procedure for calculating  $V_E$  is summarized below. An approach to estimate the various values and relationships needed to model the ventilation rate using Equations 5-3, 5-4, and 5-5 (below) is described in Appendices C and D of Johnston et al. (1999).

The CHAD database provides an activity indicator for each exposure event. Each activity type is assigned a distribution of values for the metabolic equivalent of work ( $MET$ ). The  $MET$  is a dimensionless quantity defined by the ratio:

$$MET = EE/RMR \quad (5-1)$$

where  $EE$  is the rate of energy expenditure during a particular activity (expressed in kcal/min), and  $RMR$  is a person's typical resting metabolic rate (also expressed in kcal/min).

A probabilistic procedure is used to assign a  $RMR$  value to cohort for a typical 365-day exposure period. An  $EE$  value is calculated for each exposure event by the equation:

$$EE_a(r,p,z) = [MET(r,p,z)][RMR(z)] \quad (5-2)$$

in which  $EE_a(r,p,z)$  is the average energy expenditure rate (kcal  $\text{min}^{-1}$ ) for cohort  $z$  during exposure event  $r$  on day  $p$ ;  $MET(r,p,z)$  is a value randomly selected from the distribution of  $MET$  values associated with each activity type in CHAD; and  $RMR(z)$  is the  $RMR$  value randomly generated for cohort  $z$ .

Energy expenditure requires oxygen, which is supplied through ventilation (respiration). Let  $ECF(y)$  indicate an energy conversion factor defined as the volume of oxygen required to produce one kilocalorie of energy in person  $y$ . The oxygen uptake rate ( $VO_2$ ) associated with a particular activity can be expressed as:

$$VO_2(r,p,z) = [ECF(y)][EE_a(r,p,z)] \quad (5-3)$$

in which  $VO_2(r,p,z)$  has units of liters oxygen  $\text{min}^{-1}$ ,  $ECF(y)$  has units of liters oxygen  $\text{kcal}^{-1}$ , and  $EE_a(r,p,z)$  has units of  $\text{kcal min}^{-1}$ . The value of  $VO_2(r,p,z)$  is determined from  $MET(r,p,z)$  by substituting Equation 5-2 into Equation 5-3 to produce the relationship:

$$VO_2(r,p,z) = [ECF(y)][MET(r,p,z)][RMR(y)] \quad (5-4)$$

Ventilation rate ( $V_E$ ) tends to increase as  $VO_2$  increases up to the point of maximum oxygen uptake ( $VO_{2max}$ ). The relationship is known to be non-linear, with the slope of the relationship usually increasing at higher values of  $VO_2$ . The relationship between  $V_E(r,p,z)$  and  $VO_2(r,p,z)$  is modeled by the generic equation:

$$\ln[V_E(r,p,z)/BM(y)] = a + (b)\{\ln[VO_2(r,p,z)/BM(y)]\} + d(y) + e(r,p,z) \quad (5-5)$$

in which  $V_E(r,p,z)$  is the  $V_E$  value associated with the  $r^{\text{th}}$  event of day  $p$  for person  $y$ ,  $BM(y)$  is the body mass assigned to person  $y$ , and  $a$  and  $b$  are constants determined by the age and gender of person  $y$ . The term  $d(y)$  is a random variable selected for each person from a normal distribution with mean equal to zero and standard deviation equal to  $\sigma_d$ . The term  $e(r,p,z)$  is a random variable selected for each individual event from a normal distribution with mean equal to zero and standard deviation equal to  $\sigma_e$ .

### 5.1.6 EXTRAPOLATE THE COHORT INHALATION EXPOSURES TO THE POPULATIONS OF INTEREST

For a population analysis, the inhalation exposures calculated for the cohorts can be extrapolated to the larger general population by estimating the number of individuals in each cohort. First, the population of each demographic group that resides within a particular exposure district is extracted from census data specific to that district. This gives an estimate of the population of each non-commuting cohort residing within each exposure district. Then, as described in Equation 4-12 (shown below), the populations of the commuting cohorts (assumed to include all cohorts of working adults and school children) are determined by the expression:

$$com(dg,h,w,b) = pop(dg,h,b) \times com(h,w) / com(h)$$

where  $com(dg,h,w,b)$  is the number of persons in the commuting cohort associated with demographic group  $dg$ , residing in exposure district  $h$  (*i.e.*, the home district), commuting to exposure district  $w$  (*i.e.*, the commute district) and having attribute  $b$  (*e.g.*, the incidence of a particular disease or ailment). The  $pop(dg,h,b)$  is the population of demographic group  $dg$  residing in exposure district  $h$  that has attribute  $b$ . The  $com(h,w)$  is the number of commuters in all demographic groups that commute from their residence in exposure district  $h$  to work or school in exposure district  $w$ , and  $com(h)$  is the total number of commuters that reside in exposure district  $h$ .

## 5.2 PRESENTATION OF THE MODEL ALGORITHMS BY MICROENVIRONMENTAL LOCATION

The TRIM.Expo module will be able to model inhalation exposures for several indoor, in-vehicle, and outdoor microenvironments. As mentioned earlier in this chapter, a user will have the ability to specify additional microenvironments of various scales to fit individual modeling requirements. In this section, the general algorithms are presented for each of these locations. The methodology presented here for calculating indoor, in-vehicle, and outdoor microenvironmental concentrations conforms to the requirements specified earlier for TRIM framework development. One of the important goals for modeling microenvironmental concentrations is that the methodology conserve mass, where appropriate and feasible. Alternative methodologies will also be included as options when the information required for mass balance is not available.

### 5.2.1 MICROENVIRONMENTAL LOCATIONS SPECIFIC TO INDOOR AIR AND INSIDE VEHICLES

The TRIM.Expo module will include algorithms that can be used to estimate pollutant concentration for several indoor microenvironments, such as residences, residential garages, the work place, school, and other indoor locations such as restaurants and stores. In addition, the inside of passenger vehicles, such as automobiles and buses, will be treated similarly to the indoor microenvironment. In general, there are two types of contributions to the pollutant concentrations in these microenvironments: infiltration of air from outside the microenvironment's boundaries, and direct emission of a pollutant of concern from a source within the microenvironment. Infiltration will be modeled by TRIM.Expo using either a mass balance approach, described below, or an assumed transfer factors (ME factors).

For indoor emission sources, TRIM.Expo will provide two options. For the first option, information on the emission rate (in units of mass/time) for a source is used as an input to the mass balance model. For the second option, sample values are drawn stochastically from a distribution that relates the presence of an indoor source in a particular microenvironment to incremental increases in pollutant levels. For example, to estimate the contribution to pollutant concentrations in the home from tobacco smoking using the first option, the user may specify the frequency of smoking (*e.g.*, the number of cigarettes per hour), which TRIM.Expo will use to derive a pollutant emission rate for input to the mass balance equation. If smoking frequency information is unavailable, the user may simply indicate that smoking occurs in the home. In that case, TRIM.Expo will estimate the contribution to pollutant concentrations from smoking by sampling from a distribution of the measured increase in pollutant concentrations in homes of smokers. Alternatively, the user may supply his or her own distributional data.

The TRIM.Expo mass balance model and description are adapted from Johnson et al. (1996b). The mass balance model is based on the generalized mass balance model presented by Nagda et al. (1987) for a single indoor compartment. As originally proposed, this model uses the assumption that pollutant concentration decays indoors at a constant rate. However, Johnson et al. (1996b) reports that pollutant decay rate is a function of the indoor pollutant concentration.

Therefore, in TRIM.Expo, the model of Nagda and co-workers was revised to incorporate an alternative assumption that the indoor decay rate is proportional to the indoor concentration. The resulting model is expressed by the differential equation:

$$\frac{d}{dt}C_{in} = (1 - F_B) vC_{out} + \frac{S}{cV} - MvC_{in} - F_dC_{in} - \frac{qFC_{in}}{cV} \quad (5-6)$$

where:

$C_{in}$	=	indoor concentration (mass/volume)
$F_B$	=	fraction of the outdoor pollutant concentration intercepted by the building or structure (dimensionless fraction)
$v$	=	air exchange rate (1/time)
$F_d$	=	pollutant decay coefficient (1/time)
$C_{out}$	=	outdoor concentration (mass/volume)
$S$	=	indoor generation rate (mass/time)
$cV$	=	effective indoor volume where $c$ is a dimensionless fraction (volume)
$M$	=	mixing factor ( <i>i.e.</i> , the portion of the ventilation air flow that is completely mixed with room air) (dimensionless fraction)
$q$	=	flow rate through air-cleaning device (volume/time)
$F$	=	efficiency of the recirculation air-cleaning device (dimensionless fraction)

The model is further generalized to include a mixing factor for outdoor air infiltration and the possibility of infiltrated air from outside being filtered as follows:

$$\frac{d}{dt}C_{in} = (1 - F_B) Mv_uC_{out} + \frac{S}{cV} - Mv_uC_{in} - F_dC_{in} - \frac{qF_1C_{in}}{cV} + (1 - F_2) Mv_fC_{out} - Mv_fC_{in} \quad (5-7)$$

where:

$v_u$	=	air exchange rate, unfiltered (1/time)
$v_f$	=	air exchange rate, filtered (1/time)
$F_1$	=	efficiency of the recirculation air-cleaning device (dimensionless fraction)
$F_2$	=	efficiency of the outdoor makeup-air cleaning device (dimensionless fraction)

Equation 5-7 can be simplified by substituting a “penetration factor,”  $F_p$ , for the fraction of the outdoor concentration intercepted by the enclosure and an “effective volume,”  $V_e$ , for  $cV$ .  $F_p$  and  $V_e$  are given by Equations 5-8 and 5-9, respectively:

$$F_p = 1 - F_B \quad (5-8)$$

$$V_e = cV \quad (5-9)$$

Substituting Equations 5-8 and 5-9 into Equation 5-7 results in:

$$\frac{d}{dt}C_{in} = F_p Mv_u C_{out} + \frac{S}{V_e} - Mv_u C_{in} - F_d C_{in} - \frac{qF_1 C_{in}}{V_e} + (1 - F_2) Mv_f C_{out} - Mv_f C_{in} \quad (5-10)$$

Combining and rearranging terms yields:

$$\frac{d}{dt}C_{in} = M(F_p v_u + [1 - F_2]v_f)C_{out} + \frac{S}{V_e} - M(v_u + v_f)C_{in} - F_d C_{in} - \frac{qF_1 C_{in}}{V_e} \quad (5-11)$$

Equation 5-11 can be simplified by combining terms proportional to  $C_{in}$ :

$$\frac{d}{dt}C_{in} = M(F_p v_u + [1 - F_2]v_f)C_{out} + \frac{S}{V_e} - v' C_{in} \quad (5-12)$$

where:

$$v' = M(v_u + v_f) + F_d + \frac{qF_1}{V_e} \quad (5-13)$$

It can be shown that Equation 5-12 has the following approximate solution:

$$C_{in}(t) = k_1 C_{in}(t-\Delta t) + k_2 C'_{out} + k_3 \quad (5-14)$$

where:

$$k_1 = e^{-v'\Delta t} \quad (5-15)$$

$$k_2 = \frac{M(F_p v_u + [1 - F_2]v_f)}{v'} (1 - k_1) \quad (5-16)$$

$$k_3 = (S / v' V_e) (1 - k_1). \quad (5-17)$$

$C'_{out}$  is the average value of the outdoor concentration over the interval  $t$  to  $t + \Delta t$ .

The average indoor concentration for hour  $h$  is given by  $C'_{in}$  in the expression:

$$C'_{in}(h_0) = a_1 C_{in}(h-1) + a_2 C'_{out}(h_0) + a_3 \quad (5-18)$$

where  $C_{in}(h-1)$  is the instantaneous indoor concentration at the end of the preceding hour and  $C'_{out}(h)$  is the average outdoor concentration for hour  $h$ . Also,  $a_1$ ,  $a_2$ , and  $a_3$  are given by:

$$a_1 = z(h_0) \quad (5-19)$$

$$a_2 = \frac{M(F_p v_u + [1 - F_2] v_f)}{v'} (1 - z(h_0)) \quad (5-20)$$

$$a_3 = \frac{S}{v' V_e} (1 - z(h_0)) \quad (5-21)$$

$$z(h_0) = (1 - e^{-v'}) / v' \quad (5-22)$$

A steady-state version of the mass balance model (Equation 5-12) can be developed if it is assumed that the change in indoor concentration with time is zero.

When information about the indoor emission source strength is not available,  $a_3$  may be sampled from a distribution of measured incremental concentrations associated with the presence of the indoor source. Some of these distributions will be included in TRIM.Expo. The user will also have the option of supplying his or her own indoor source distribution.

## 5.2.2 MICROENVIRONMENTAL LOCATIONS SPECIFIC TO AMBIENT AIR

One of the options for obtaining pollutant concentration data for outdoor locations in TRIM.Expo is through the use of air dispersion modeling. The output files from TRIM.FaTE or another air model may be used if data are properly formatted. Regardless of the method for modeling the dispersion of pollutants, the ambient pollutant concentrations at receptors must be related to geopolitically defined exposure districts where people live, work, or attend school. For example, suppose the user wants to design an exposure analysis to cover a large city and the surrounding suburbs with an areal extent of 100 km within an urban area. For this example, a typical TRIM.Expo exposure analysis could be conducted using census tracts as the exposure districts. In that case, time sequences of hourly-averaged estimates of outdoor pollutant concentrations for each census tract in the study area are required. These concentration estimates could come directly from the air dispersion model, if census tract centroids were used as the model receptors, or they may be derived from concentration estimates made at other receptor points in the study area. There are several ways to do this.



If the spatial resolution of model receptors is finer than the spatial resolution of exposure districts, concentrations can be assigned to exposure districts from modeling receptors that fall within each exposure district according to the formula:

$$\bar{C}_i(v,t) = (1/v_i) \sum C(c,i,t) \quad (5-23)$$

where  $\bar{C}_i(v,t)$  is the average ambient pollutant concentration in exposure district  $i$  from the  $v$  modeled receptor points for time step  $t$ ,  $v_i$  is the number of receptor points in exposure district  $i$ , and  $C(c,i,t)$  is the ambient concentration at receptor point  $c$  within exposure district  $i$  during time step  $t$ . The values of  $C(c,i,t)$  are summed over the total number of receptor points in each exposure district (*i.e.*,  $v_i$ ).

If the spatial resolution of modeled receptor points is more coarse than the resolution of exposure districts, concentrations can be spatially interpolated to the exposure district centroids using the formula:

$$C(i,t) = \frac{\sum [C(c,t) / d^2(c,i)]}{\sum [1 / d^2(c,i)]} \quad (5-24)$$

where:  $C(c,t)$  = estimated concentration at receptor point  $c$  for time step  $t$   
 $d(c,i)$  = distance from a receptor point  $c$  and the centroid of exposure district  $i$ .

Alternatively, exposure districts could be redefined as aggregations of contiguous census tracts, with each tract assigned the concentration estimate at the nearest modeled receptor.

The second method for obtaining a time sequence of outdoor concentrations for each exposure district is through the use of monitored ambient data. There are several limitations to the use of monitoring data for air toxics. At present, the number of routine monitoring sites for air toxics is much smaller than for criteria air pollutants. Also, air toxics are often measured as 24-hour integrated samples taken every sixth or twelfth day. However, with increased concern about health effects from toxic air pollutants, EPA plans to increase the extent of its monitoring efforts. In addition, future development of TRIM.Expo will make it easier to use a variety of mathematical tools and spatial interpolation techniques such as kriging for estimating outdoor pollutant concentrations.

Because the spatial resolution of monitors, even for criteria air pollutants, is typically rather coarse, it is customary to specify exposure districts by assigning concentrations to census tracts according to the values measured at the nearest monitor. Using this method, an air pollutant's concentration is assumed to be the same for all census tracts within a particular exposure district. In making these assignments, attention should be paid to the spatial area of representation for the monitors. The EPA has four different monitor classifications as follows:

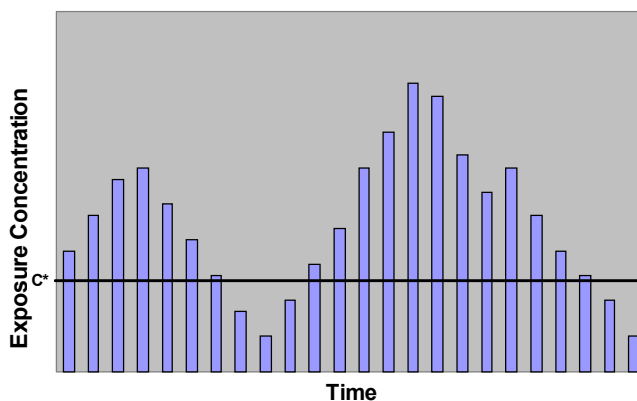
1. Micro-scale: representative of from a few to 100 m;
2. Middle-scale: representative from 100 to 500 m;
3. Neighborhood-scale: representative from 0.5 to 4 km; and
4. Urban-scale: representative from 4 to 50 km.

There are a number of outdoor locations that may have enhanced pollutant concentrations, such as gasoline stations, parking garages, and near roadways. As noted above, if these microenvironments are not modeled or monitored explicitly for the particular study area, it may be necessary to derive concentration estimates from measurements in those microenvironments from other locations. Alternatively, it may be necessary to derive the concentrations from the more generalized outdoor estimates and information about the relationship between the generalized outdoor concentration and the outdoor microenvironment (*e.g.*, the distribution of ratios of CO concentrations near roadways to concentrations at other outdoor locations). Some of this information will be provided in TRIM.Expo. The user will also have the option of providing his or her own distributions.

### 5.3 INTEGRATION OF EXPOSURE ACROSS MULTIPLE LOCATIONS AND TIMES

The TRIM.Expo module will have the ability to integrate exposures of varying durations across numerous microenvironments. This is accomplished by TRIM.Expo's exposure characterization process. The purpose of the exposure characterization process is to combine and simultaneously track all of the relevant information needed to assess exposures across several exposure media occurring with varying time-durations. In this chapter, the exposure media of concern are outdoor and indoor air. As noted above, for each individual or cohort, a sequence of exposure events is defined. Exposure-event sequences are chronological sets of events that define the time-activity allocation of the individual or cohort. A simple example of an exposure-event sequence is presented in Table 4-6 (Section 4.2.5). The exposure-event sequence tracks the individual or cohort by (1) exposure district, (2) microenvironment, and (3) activity at each time step. Each exposure event will be associated with an exposure concentration and a breathing rate. The TRIM.Expo algorithms will use the information on the exposure concentration at each time step to create an exposure time series or profile. Figure 5-2 shows an example of an exposure profile covering 24 time steps. By

**Figure 5-2**  
**Hypothetical Exposure Profile**  
**Covering 24 Time Steps**



combining the exposure concentration and the breathing rate at each time step, TRIM.Expo will also create a potential dose profile (see Section 4.1.2). McCurdy (1997) summarizes the definition of dose profile as the collection of the instantaneous intake doses over a time interval ( $t_0, t_1$ ), where the instantaneous intake dose is the rate at which the pollutant penetrates into the target at a given instant of time.

## 5.4 SUMMARY OF INPUTS AND VALUES

Because the types of data used in a TRIM.Expo exposure analysis are quite diverse, each one is described in a separate section below. These sections summarize these data inputs and provide values for them wherever possible.

### 5.4.1 DATA INPUTS FOR THE MASS BALANCE MODEL

The mass balance model (Equation 5-12) requires information on the air exchange rate, the building volume, the indoor generation of the pollutant, the fraction of the pollutant penetrating the building from outdoors, and the pollutant decay rate. Many of these parameters depend on several factors. For example, the fraction of pollutant mass in infiltration air that actually enters the building (*i.e.*, the penetration rate) depends upon the state of the pollutant (*i.e.*, whether it is a gas, a fine particle, or a coarse particle), the type of building construction, whether the building's windows are open, if windows are open, by how much, and the type of air conditioning and/or air handling system. Therefore, data are not available for every pollutant and every scenario.

Two factors that are important to the calculation of indoor concentrations which are not pollutant-specific are the air exchange rate and building volume. Data on these factors have been collected by numerous studies in different parts of the U.S. Some of these data were summarized in Johnson et al. (1999) for the pNEM/CO model and are shown in Tables 5-1 and 5-2. Table 5-1 shows the sources of information on the distributions for air exchange and building volumes. Table 5-2 shows the references for specific microenvironmental air exchange rate data. These microenvironments correspond to those currently used in pNEM/CO. Information on building volume and air exchange rate will need to be developed for additional microenvironments for TRIM.Expo system applications to other pollutants based on these and other databases.

**Table 5-1  
Distributions and References for Air Exchange and Building Volume Data**

Parameter	Distribution of Parameter	Reference
Air exchange rate, exchanges/h: residence - windows closed	Lognormal distributions by season	Murray and Burmaster 1995
Air exchange rate, exchanges/h: residence - windows open	Lognormal distribution	Johnson, Weaver, Mozier et al., 1998
Air exchange rate, exchanges/h: nonresidential, enclosed microenvironments, including motor vehicles	See Table 5-2	See Table 5-2
Residential volume, cubic meters	Lognormal distribution	Bureau of Census 1995

**Table 5-2  
Distributions and References for Specific Microenvironmental  
Air Exchange Rate Data**

Microenvironment		Activity Diary Locations Included in Microenvironment	Distribution of Air Exchange Rate	
			Distribution Type	Source of Data
General Location	Specific Location			
Indoors	Nonresidence A	Service station or auto repair	Lognormal	a
Indoors	Nonresidence B	Other repair shop Shopping mall	Lognormal	a
Indoors	Nonresidence C	Restaurant Other indoor location Auditorium	Lognormal	a
Indoors	Nonresidence D	Store Office Other public building	Lognormal	a
Indoors	Nonresidence E	Health care facility, School, Church, Manufacturing facility	Lognormal	b
Indoors	Residential garage	Residential garage	Lognormal	a
Vehicle	Automobile	Automobile	Lognormal	c
Vehicle	Other	Bus, Truck, Bicycle, Motorcycle, Train/subway, Other vehicle	Lognormal	c
Vehicle	Airplane	Airplane	NA	--

<sup>a</sup> Data set containing all non-school AER values provided by Turk et al. (1989) and CEC (Lagus Applied Technology, Inc. 1995).

<sup>b</sup> Data set containing all AER values provided by Turk et al. (1989) and CEC (Lagus Applied Technology, Inc. 1995).

<sup>c</sup> Ott, Switzer, and Willis (1994).

## 5.4.2 DATA INPUTS FOR TIME/ACTIVITY PATTERNS

The time/activity data for use in TRIM.Expo were obtained from CHAD. The CHAD is comprised of approximately 17,000 person-days of 24-hour time/activity data developed from eight surveys (Glen et al. 1997). The surveys include probability-based recall studies conducted by EPA and the California Air Resources Board, as well as real-time diary studies conducted in individual U.S. metropolitan cities using both probability-based and volunteer subject panels. All ages of both genders are represented in CHAD. The data for each subject consist of one or more days of sequential activities in which each activity is defined by start time, duration, activity type (140 categories), and microenvironment classification (110 categories). Activities vary from one minute to one hour in duration, with longer activities being subdivided into clock-hour durations to facilitate exposure modeling. Refer to Section 4.3.3 for a more detailed discussion of CHAD.

Extrapolating the information from short-term recall surveys to longer-term chronic exposure assessments is currently a potential source of uncertainty in exposure modeling. Additional research into longer term activity pattern data is needed to address this shortcoming. The EPA's Office of Research and Development is embarking on research to develop statistical methods to develop long-term exposure profiles from the activity pattern survey data that is currently available (Ozkaynak 1999). As part of this effort, careful analysis of multiday diaries from currently available surveys will be used to develop alternative statistical approaches for generating correlated diaries for activity and consumption information at the individual level. Once these statistical approaches are developed, they will be incorporated into TRIM.Expo as appropriate. Ultimately, year-long or greater measured exposure data will need to be collected to verify the validity of these statistical techniques.

A statistical technique developed to augment the activity pattern data for pNEM/CO will be used during the initial development of TRIM.Expo. Earlier versions of pNEM/CO defined cohorts solely according to home district, demographic group, work district (if applicable), and residential cooking fuel. The new feature installed in pNEM/CO (Version 2.0) permits the user to specify a "replication" value (n) such that the model will produce n cohorts for each combination of the above four indices. Because pNEM/CO uses a Monte Carlo process to construct an activity pattern for each cohort, each of the n cohorts associated with a particular combination of home district, demographic group, work district, and residential cooking fuel is associated with a distinct exposure sequence. The replication feature permits the analyst to divide the population of interest into a larger number of smaller cohorts; a process which pNEM/CO's developers report decreases the "lumpiness" of the exposure simulation. For example, if a replication value of five ( $n = 5$ ) is specified, the pNEM/CO model analyzes five times the number of cohorts it would have considered if the cohorts had been defined solely by home district, demographic group, work district, and residential cooking fuel. The use of replication values is a technique that is intended to enhance the utility of existing data while more robust statistical techniques are developed and additional data are collected on chronic or longitudinal exposures of individuals within the population.

### 5.4.3 DATA INPUTS FOR VENTILATION RATE

As described in Section 5.1.5, CHAD provides an activity indicator for each exposure event. In turn, a distribution of values for the ratio of oxygen uptake rate to body mass (referred to as metabolic equivalents or “METs”) is provided for each activity type listed in CHAD. The forms and parameters of these distributions were determined through an extensive review of the exercise and nutrition literature. The primary source of distributional data was a compendium developed specifically to facilitate the coding of physical activities and to promote comparability across studies by Ainsworth et al. (1993). Table 5-3 contains a list of the parameters used in pNEM/CO (Version 2.0) for estimating ventilation rates.

**Table 5-3**  
**Parameters Used to Estimate Ventilation Rates**

Parameter	Abbreviation	Functional Form	Source of Data
Body mass	BM	Lognormal distribution	Brainard and Burmaster 1992
Metabolic equivalence	MET	Distribution specified in CHAD Database	Johnson et al. 1999
Resting metabolic rate	RMR	Regression equations specific to age and gender	Schofield 1985, as compiled by Johnson et al. 1999
Normalized oxygen uptake rate	NVO <sub>2max</sub>	Normal distribution	Åstrand 1960, Mercier et. al. 1991, Katch and Park 1975, Heil et. al. 1995, Mermier et al. 1993, Rowland et al. 1987

## 6. INGESTION

For many pollutants, an understanding of the ingestion exposure pathway is critical to accurately assessing potential health risks. This chapter provides a detailed presentation of the algorithms used in TRIM.Expo to assess, compare, and combine different ingestion pathways of exposure. Ingestion exposures are characterized in TRIM.Expo using the potential average daily dose (ADD). The ingestion exposure ADD represents the amount of pollutant that enters the mouth of the exposed individual over a defined exposure event or during a defined exposure duration. This chapter begins by providing an overview of the general approach used in TRIM.Expo to characterize the equivalent daily intake from an exposure medium. Of particular importance here is how the attributes of ingestion exposure define the spatial, temporal, and cohort resolution of the ingestion exposure algorithms. This is followed by a description of the media-specific algorithms used to estimate these exposures in TRIM.Expo. The chapter concludes with a presentation of the inputs and default values necessary to assess the ingestion exposure pathway.

### 6.1 OVERVIEW OF THE APPROACH

In Section 2.3.2, all exposure attributes relevant to exposure routes and pathways were organized into a set of three *key* exposure dimensions that has a significant impact on the structure of the exposure model (*e.g.*, on the exposure media included, the degree of spatial resolution, and the level of temporal and spatial aggregation). These three important *key* exposure dimensions of the exposure assessment problem were determined to be the (1) route of exposure, (2) time scale of an exposure event relevant to the pollutant's associated effects, and (3) degree of location dependence (*i.e.*, dependence of exposure on the location of the exposed subject).

In addition to incorporating the above exposure dimensions, ingestion exposure-event functions must also account for some unique modeling constraints. For example, slower rates of temporal variation in pollutant concentrations are exhibited in soil, water, vegetation, and animals because of their larger mass and tendency to retain pollutants. Furthermore, the food and water consumption data available from sources, such as EPA's Exposure Factors Handbook (U.S. EPA 1997b), provide only seasonal resolution which limits the use of this data for shorter-term assessments. Thus, ingestion exposure algorithms for media such as water, soil, and home-grown or locally-produced foods cannot support as high a degree of time and spatial resolution as inhalation exposures.

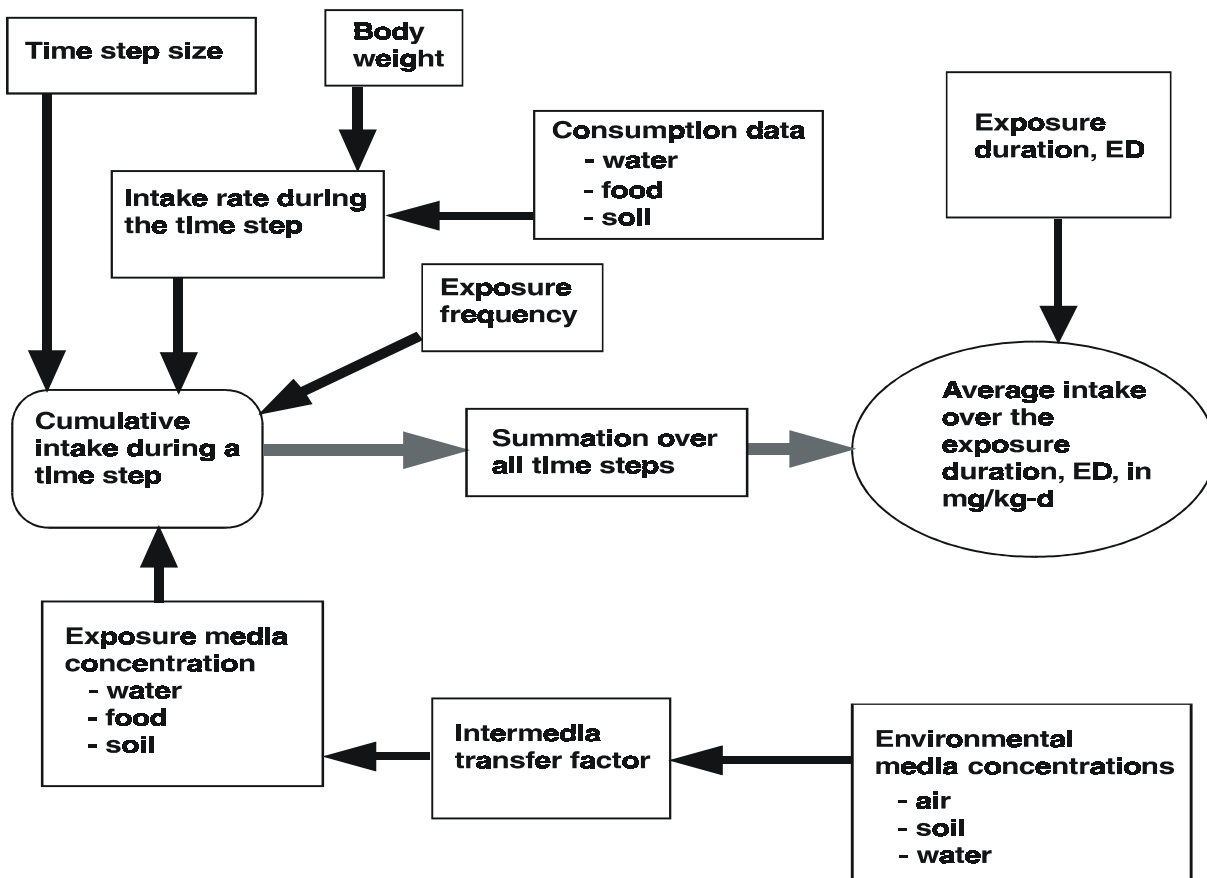
Based on the above constraints, the exposure-event functions for ingestion focus on pollutant concentration variations among exposure districts. Activities (*i.e.*, ingestion patterns) are characterized as daily equivalent intakes representative of each month. Concentrations are assessed at a time resolution of daily or greater and are then averaged for a representative exposure duration (*i.e.*, monthly).

To characterize an ingestion exposure, the ingestion intake algorithms require information on the following factors:

- The pollutant concentration in the exposure medium during an exposure event;
- The ingestion rate of the exposure medium during an exposure event;
- The body weight of the individual exposed or the body weight distribution of the exposed cohort;
- The fraction of the cohort's ingested water, soil, and food products that come from an exposure district with a specified pollutant concentration in the exposure medium; and
- The frequency of exposure events over the exposure duration.

Figure 6-1 below illustrates how this information is linked to characterize exposure and intake over an exposure duration.

**Figure 6-1**  
**An Illustration of How Information is Combined to Assess**  
**Ingestion Exposure over a Defined Exposure Duration**





In order to organize this information into a form that expresses population exposure, an algorithm of the following form is used for each exposure medium considered in TRIM.Expo:

$$ADD_{z,m}(T) = \frac{\sum_t \left( \frac{I_{z,m}(k,l)}{BW_z} \right) C_m(i,k,l,t) EF_{z,m}(i,t) ET(t)}{T} \quad (6-1)$$

where:

- $ADD_{z,m}(T)$  = for individual or cohort  $z$  the average daily dose or intake of a pollutant from exposure medium  $m$  averaged over the time period  $T$ , which is one day or greater
- $[I_{z,m}(k,l)/BW]$  = the equivalent rate of intake of exposure medium  $m$  (expressed kg/d, L/d) over the time step  $t$  by individual or cohort  $z$  divided by that individual's body weight ( $BW$ ). The microenvironment and activity codes  $k$  and  $l$  are not used in the ingestion calculations, but are included here to provide consistency with the general exposure model presented in Chapter 2. This parameter can be obtained from EPA's Exposure Factors Handbook (U.S. EPA 1997b) for most exposure media
- $C_m(i,k,l,t)$  = the pollutant concentration in mg/kg in exposure medium  $m$  (e.g., tap water, dairy products, meat, fish, vegetables) in exposure district  $i$  or location of the exposure media itself, averaged over the time step  $t$ . These concentrations are obtained from environmental samples or from a fate and transport model such as TRIM.FaTE
- $EF_{z,m}(i,t)$  = the frequency (fraction of days in the time step) that individual or cohort  $z$  from district  $i$  has contact with exposure medium  $m$  during time step  $t$ . This term is used to make adjustments for factors such as drinking water consumption that can be dispersed among several exposure districts. Typically, for food, the exposure frequency is set equal to the number of days in the time step because the exposure frequency is already implicitly incorporated into the daily intake rate.
- $ET(t)$  = the duration of time step  $t$  in months or days depending on the time resolution required
- $m$  = the exposure medium contacted (e.g., air, water, food)

- $i$  = the geographical location in which the exposure takes place (*i.e.*, the exposure district) or the location of origin of the exposure media of concern (*e.g.*, drinking water).
- $k$  = microenvironment in which the exposure occurs, [*e.g.*, indoors at home; in a vehicle; indoors at work (not an important attribute for ingestion exposures)]
- $l$  = activity code that describes what the individual is doing at the time of exposure (*e.g.*, resting, working, preparing food, cleaning, eating)

The summation of pollutant exposures from all exposure media is over all time steps,  $t$ , that comprise the time period,  $T$ .

### 6.1.1 SELECTION OF POPULATION COHORTS

For ingestion exposures, important attributes that define cohorts include age, gender, exposure district, water supply, consumption of home-grown foods, and consumption of locally-produced foods. Table 6-1 summarizes the initial set of cohort attributes used in TRIM.Expo for ingestion exposures. These attributes were selected based on information available in key references such as EPA’s Exposure Factors Handbook. There are fifteen primary attributes listed in this table that can be used to construct cohorts for ingestion exposure assessments, thus potentially leading to a large number of cohorts. However, many of the primary attributes can be combined (*e.g.*, home-grown foods can be aggregated into a single primary attribute instead of four separate categories as shown in Table 6-1). By combining attributes, the number of cohorts in the exposure analysis is significantly reduced.

**Table 6-1  
Primary Attributes of Exposure Cohorts**

Primary Cohort Attributes	
(1) Age	
Child	
Adult	
(2) Gender	
Male	
Female	
Exposure district	
(3) Residential	
(4) Work-school	

<b>Primary Cohort Attributes</b>
(5) Water supply
Surface water
Ground water (public well)
Ground water (private well)
Home-grown food
(6) Fruits, vegetables, grains
(7) Dairy products
(8) Eggs
(9) Meat
Locally-produced food supplies
(10) Fruits, vegetables, grains
(11) Dairy products
(12) Eggs
(13) Meat
(14) Local fishing
(15) Local hunting

### 6.1.2 TIME RESOLUTION OF EXPOSURE EVENTS

The TRIM.Expo module is designed to allow the user to specify time steps ranging from hours to years. However, because of limited data on food consumption and biotransfer factors, the time resolution of ingestion exposure events can be set to either daily or monthly time steps. The time step can be increased or decreased, depending on the pollutants being studied and the time-scale of the health effects.

### 6.1.3 EXPOSURE MEDIA CONSIDERED

The ingestion exposure media that are included in the current conceptual design of TRIM.Expo are

- Surface water;
- Ground water;
- Soil and house dust;
- Home-grown fruits, vegetables, and grains;

- Home-produced eggs, dairy products, meat and fish; and
- Locally-produced fruits, vegetables, grains, dairy products, meat, and fish.

Surface water and ground water are both considered to be sources of drinking water, but direct ingestion of surface water and ground water can also occur during swimming and other recreational activities. Ingestion of soil is modeled to occur outdoors in a residential environment, whereas ingestion of dust is assumed to occur indoors at a residence or in a work environment.

Food supplies are categorized to be home-grown, locally-grown, or some combination of the two categories. TRIM.Expo defines *home-grown* foods as those foods produced on the land associated with a household and, for the most part, consumed within that household; whereas *locally-produced* foods are those that are produced in home gardens and commercial farms in contact with air, soil, and/or water that are in the study area. For the purposes of TRIM.Expo, it is assumed that the attributes associated with the consumption of locally-grown foods is the same for all districts within a study area (*e.g.*, urban air shed) and that the quantity of food that is designated as home-grown is applied separately based on whether the exposure district is urban, suburban, or rural.

For lipophilic pollutants (*e.g.*, dioxins, furans, polychlorinated biphenyls, pesticides) and for metals (*e.g.*, lead, mercury), exposures through food have been demonstrated to be the dominant contributors to total dose for non-occupationally exposed populations (Travis and Hester 1991). However, overall uncertainties in estimating potential doses through food chains are much larger than uncertainties associated with other exposure pathways (Jones et al. 1991, McKone and Daniels 1991, McKone and Ryan 1989).

### 6.1.3.1 Ingested Water

Ingested water is defined as water that is (1) consumed directly from the tap; (2) consumed in food and beverages; and/or (3) ingested during water recreation. The primary source of ingested water is tap water that is drawn from ground water, surface water, or some combination of the two sources. Water ingested during recreation could be either surface water or ground water.

Surface water includes water obtained from estuaries, lakes, rivers, and wetlands. Therefore, exposure to surface water can occur from the use of tap water and from recreational activities, such as swimming and other water sports. Ground water is found in the saturated zone of the subsurface environment. Human exposure to ground water can occur once it is withdrawn for tap/drinking water; used in cooking and processing foods; used for irrigation; used as water supply in recreational activities (*e.g.*, to fill a swimming pool); and/or supplied to animals reared/bred for human consumption.

### 6.1.3.2 Food

Currently TRIM.Expo includes several food exposure media, such as fruits, vegetables, grains, milk, dairy products, eggs, meat, and fish. TRIM.Expo differentiates between home-grown foods and locally-produced foods, and then focuses on which of these raw foods are produced and consumed within the set of exposure districts being considered in the risk and exposure analysis.

Fruits and vegetables are further divided into categories of unprotected and protected produce. Protected produce crops have skins or shells that are not usually consumed (*e.g.*, citrus fruits, peanuts, beans). Unprotected produce typically have no outer covering or have skins or shells that are commonly consumed (*e.g.*, leafy vegetables, grapes, most grains). In addition, vegetables are distinguished between those that have edible parts that grow above the ground (*i.e.*, above-ground crops) versus those that are root crops (*i.e.*, below-ground crops). In the case of root (below-ground) crops, EPA's Exposures Factors Handbook (U.S. EPA 1997b) does not differentiate between protected or unprotected produce. Table 6-2 provides examples of fruits, vegetables, and grains defined by the above categories.

**Table 6-2**  
**Taxonomy of Food Types Categorized as Fruits, Vegetables, and Grains**

Type of Crop	Protected/ Unprotected	Fruits	Vegetables	Grains
Above-ground crops	unprotected	grapes, berries, apples	lettuce, broccoli	wheat, barely oats
	protected	citrus	beans, peas	none considered
Below-ground crops (root crops)		none considered	carrots, radishes, peanuts, potatoes	none considered

#### ***Cooked and Processed Food***

Exposures to pollutants in cooked and processed foods depend on the preparation techniques used to combine and convert raw foods into edible, consumption food products. Meats, eggs, dairy products, and grains are almost always processed and cooked prior to human consumption. Since cooking and food processing can result in the transformation of many pollutants, intermedia transfer factors are needed to characterize how preparation and cooking alter raw food products. However, for the most part, such factors are unavailable. EPA's Exposure Factors Handbook (U.S. EPA 1997b) contains some of this information.

#### ***Uncooked Food***

Most fruits and some vegetables are served uncooked, reducing the need for intermedia transfer factors to distinguish differences between ambient pollutant concentrations in the vegetation and the pollutant concentration at the time of consumption. Even though fruits and vegetables can be washed before they are eaten, current research suggests that for fine particles and pollutants dissolved in the lipid phase of the vegetation, washing does little to reduce

pollutant concentration (Jones et al. 1991) and thus, it may not be necessary to incorporate a factor that accounts for how washing alters pollutant concentrations.

### **6.1.3.3 Soil and Dust**

Three soil categories, classified by the depth of soil—surface soil, root zone soil, and vadose zone soil—are used to assess soil contamination in the outdoor environment (see the TRIM.FaTE TSD, Volumes I and II for more information; U.S. EPA 1999a, b). Both surface soil and root zone soil are considered to be sources of pollutant transfers from soil to vegetation. Surface soil is also assumed to be the primary source for direct ingestion of soil outdoors.

In the indoor environment, the hand-to-mouth activities of children and adults are assumed to give rise to contact with house dust as opposed to actual soil ingestion. House dust suspended in the indoor air environment originates from three sources: (1) airborne particles that penetrate from outdoor air to indoor air; (2) surface soil and dust tracked into buildings on shoes or clothes, by pets, or other vectors; and (3) a variety of sources related to occupant activities, material degradation, and household products. In the current version of TRIM.Expo, the pollutant concentration in house dust is assumed to be equal to that in surface soil.

## **6.1.4 EXPOSURE LOCATIONS**

The pollutant concentrations in the exposure media of drinking water, locally-grown foods, and recreational food products are likely to be either highly dependent on the original location of the media or aggregated among several exposure districts. The magnitude of exposure to an individual or cohort is not strongly dependent on the exposure district in which the receptor resides; instead, the magnitude of exposure will depend on the fraction of food and water supply that comes from local sources and on their proximity to sources of pollution. The pollutant concentrations in these exposure media are considered to be weakly dependent on the resident location of the receptor since the driving factor for exposure is the pollutant concentrations found in the locations from where water and food are obtained, rather than the pollutant concentrations found in the area where the receptor resides. In cases where food and water distribution systems are not well characterized, pollutant concentrations in all exposure media are aggregated among several exposure districts (*i.e.*, those that supply drinking water and/or food) and then delivered to the various population cohorts.

In contrast to exposure media that are weakly dependent on the receptor location, exposure media such as home-grown foods, soil, and house dust have pollutant concentration levels that depend almost completely on pollutant levels in the air and soil of the exposure district in which the exposed receptor resides.

### **6.1.4.1 Residential Exposure Locations**

For the modeling purposes of TRIM.Expo, it is assumed that ingestion exposure events occur mostly in the residential microenvironment located in the residential exposure district of the exposed receptor(s). Ingestion of home-grown foods, soil, and/or dust are assumed to occur exclusively at the primary residential location of the exposed individual or cohort. Ingestion of

water and locally-grown foods are assumed to take place primarily in the residential exposure districts. However, ingestion of the above products can also take place at work and/or at restaurants that are not necessarily in the residential exposure district of the individual or cohort. However, since these latter pollutant concentrations are aggregated among several exposure districts, the exact location where water or locally-grown foods are consumed is not important. In such cases, the information that is needed is (1) the quantity of locally-grown foods and locally-supplied water consumed by an individual or cohort and (2) the exposure districts from which the food and water are obtained.

#### **6.1.4.2 Other Exposure Locations**

As noted above, the exposure location for pollutants found in water and locally-grown foods is primarily residential, but the estimation of the pollutant levels in food and water are based on a combination of several exposure districts in which these pollutants are found. A similar approach is used for exposure to pollutants found in meat and fish derived from local hunting and fishing. The exposure location is assumed to be the residence of the cohort, but the pollutant concentrations in the watershed or habitat in which hunting and fishing take place.

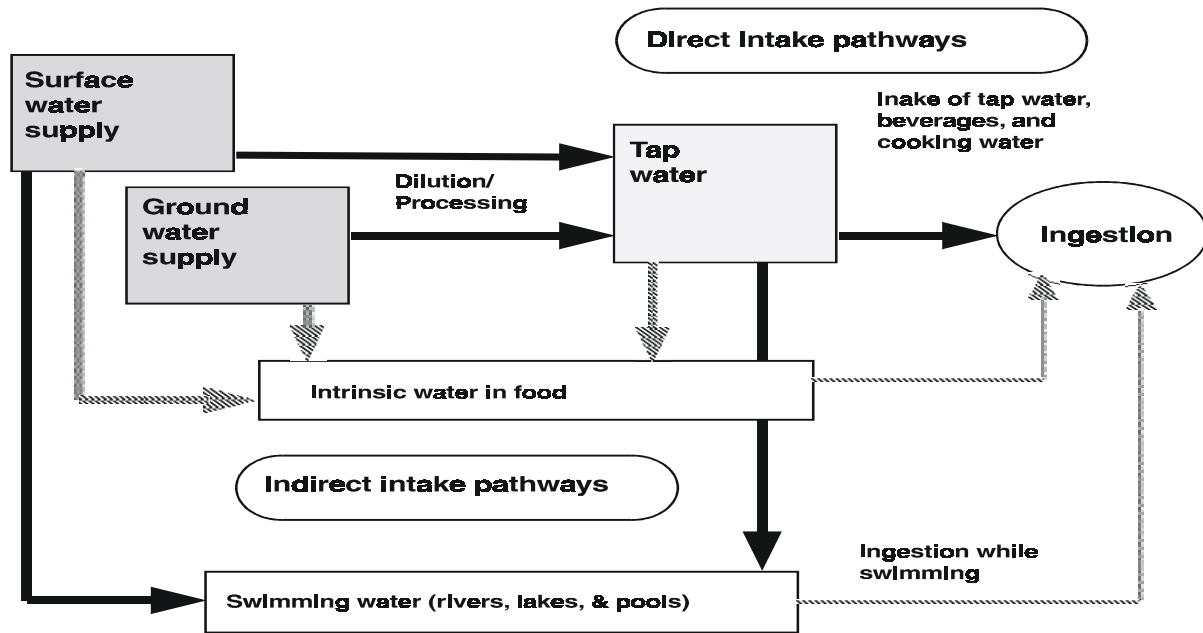
## **6.2 PRESENTATION OF THE MODEL ALGORITHMS BY EXPOSURE MEDIA**

This section presents the ingestion exposure algorithms, organized by exposure media (*i.e.*, water, soil, food) that are currently used in TRIM.Expo to express the intake of pollutant concentrations found in the environmental media.

### **6.2.1 INGESTED WATER**

Figure 6-2 illustrates the ingestion pathways of surface water and ground water for humans. TRIM.Expo currently incorporates only the direct ingestion of tap water that is derived from surface water or ground water.

Figure 6-2  
Exposure Pathways Considered for Surface and Ground Water



Tap water intake includes household drinking water that is consumed directly or consumed indirectly in a beverage (e.g., orange juice, soft drinks, coffee, tea) or in adding intrinsic water to food. For the direct ingestion of tap water, the applicable exposure algorithm is:

$$ADD_{z, tw, i}(T) = \frac{\sum_t \left( \frac{I_{z, tw}(k, l)}{BW_z} \right) C_{tw}(i, k, l, t) EF_{z, tw}(i, t) ET(t)}{T} \quad (6-2)$$

where:

$C_{tw}(i, k, l, t)$  = pollutant concentration in tap water, mg/L.

$[I_{z, tw}(k, l) BW_z]$  = the rate of intake of tap water ( $tw$ ), L/kg/d, by individual or cohort  $z$  divided by that individual's body weight ( $BW$ ). The microenvironment and activity codes  $k$  and  $l$  are not used in this calculation.

$EF_{z, tw}(i, t)$  = the exposure frequency, number of days per month equivalent, that individual or cohort  $z$  obtains tap water from exposure district  $i$  (this is likely to be location independent).



Pollutant concentration in tap water may not be directly measurable or derivable from the output of models, such as TRIM.FaTE. In such cases, intermedia transfer factors can be used to calculate the pollutant concentrations in tap water based on pollutant concentrations found in surface water and ground water:

$$C_{tw}(i,k,l,t) = PF(w) C_{sw}(i,k,l,t) \quad (6-3)$$

$$= PF(w) C_{gw}(i,k,l,t) \quad (6-4)$$

$PF(w)$  = the intermedia transfer that expresses the concentration in tap water relative to ground or surface water used in exposure district  $i$ .  $PF(w)$  is the processing dilution factor that accounts for the removal of pollutants by processing. In the current version of TRIM.Expo,  $PF(w)$  is set to 1 but can be set to a value specific to each exposure district.

The Environmental Fate and Effects Division of EPA's Office of Pesticide Programs (OPP) is in the process of producing a document that discusses the concept of the intermedia transfer ( $PF(w)$ ) that relates the pollutant concentration in tap water to that found in ground water or surface water.

## 6.2.2 INGESTION OF SOIL AND HOUSE DUST

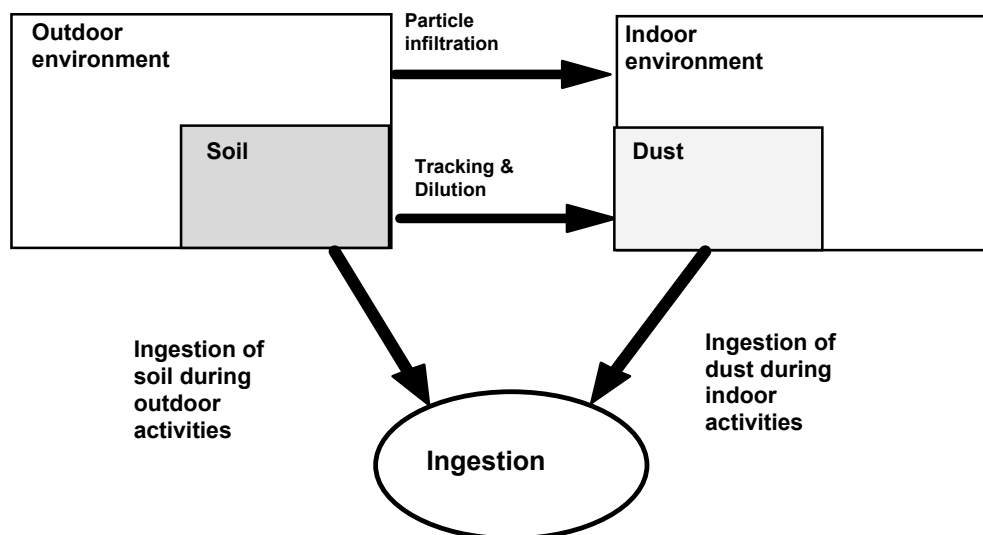
Both adults and children inadvertently ingest small amounts of soil through hand-to-mouth activities. Children who spend a great deal of time outdoors contact and ingest soil, and adults ingest soil through activities such as gardening, outdoor labor, and cleaning. In some cases, individuals suffer from a condition called *pica behavior*, and are known to intentionally consume large quantities of soil.

Several studies have been conducted to characterize soil ingestion by children (*e.g.*, see U.S. EPA 1997b, Stanek et al. 1998, Calabrese and Stanek 1995, Sedman and Mahmood 1994, Thompson and Burmaster 1991, Davis et al. 1990). Some of these studies make use of soil loading on children's hands in combination with observations of hand-to-mouth activity to estimate soil uptake. Another approach to estimating soil ingestion uses tracer elements in feces. The process involves analyzing both the feces of children and the soil in their playgrounds for elements that are thought to be poorly absorbed in the gut, such as aluminum, silicon, and titanium. Then, assuming that there are no non-soil sources of these elements and using a fecal excretion rate, the soil ingestion for each child is estimated based on the mass of each tracer element detected in the feces relative to that found in soil. In such studies, hospitalized children who have little contact with soil are often used as control groups.

Hand-to-mouth activities lead to the ingestion of pollutants in soil (outdoors) and in house dust (indoors). Pollutants in house dust are attributable in part to pollutants found in the surface soil surrounding the residence because of the resuspension of outdoor surface soil, and its infiltration through windows and openings, and its subsequent deposition onto indoor surfaces. The pollutants can also be brought indoors from the outdoor soil by soil tracking (*i.e.*, soil carried

into the house by shoes, clothing, and pets). Figure 6-3 illustrates soil ingestion pathways that are considered in TRIM.Expo.

**Figure 6-3**  
**Exposure Pathways Considered for Contact with Soil and House Dust**



### 6.2.2.1 Soil Ingestion (Outdoors)

For direct ingestion of surface soil in the residential outdoor environment, the applicable exposure algorithm is:

$$ADD_{z,ss,i}(T) = \frac{\sum_t \left( \frac{I_{z,ss}(k,l)}{BW_z} \right) C_{ss}(i,k,l,t) EF_{z,ss}(i,t) ET(t)}{T} \quad (6-5)$$

where:

$[I_{z,ss}(k,l)/BW]$  = the annually averaged daily rate of intake of surface soil (*ss*), kg/kg/d, by individual or cohort *z* divided by a representative individual's body weight (*BW*). The microenvironment and activity codes *k* and *l* are not used in this calculation.

$EF_{z,ss}(i,t)$  = the exposure frequency, which is the fraction of days in a month that individual or cohort *z* has contact with outdoor soil in exposure district *i*. This factor is used to make adjustments for time within or outside of the exposure district - the number of days

per month outside with soil contact is already accounted for in the parameter above.

$C_{ss}(i,k,l,t)$  = the pollutant concentration, mg/kg, in the surface soil or outside surface dust (of urban areas) for exposure district  $i$  during the time step  $t$ .

### 6.2.2.2 Dust Ingestion (Indoors)

For the direct ingestion of pollutants from house dust in the indoor environment, it is assumed that residential surface soil is the source of the dust pollutants. The applicable exposure algorithm is:

$$ADD_{z,hd,i}(T) = \frac{\sum_t \left( \frac{I_{z,hd}(k,l)}{BW_z} \right) C_{hd}(i,t) EF_{z,hd}(i,t) ET(t)}{T} \quad (6-6)$$

where:

$C_{hd}(i,t)$  = the pollutant concentration, mg/kg, in the house dust ( $hd$ ) of exposure district  $i$  during the time-step  $t$ .

$[I_{z,hd}(k,l)/BW]$  = the annually averaged daily rate of intake of soil, kg/kg/d, by individual or cohort  $z$  divided by a representative individual's body weight ( $BW$ ). The microenvironment and activity codes  $k$  and  $l$  are not used in this calculation,

$EF_{z,hd}(i,t)$  = the exposure frequency, fraction of days per month equivalent, that individual or cohort  $z$  has contact with house dust in exposure district  $i$ .

The concentration of a pollutant in house dust is calculated from two intermedia transfer factors:

$$C_{hd}(i,k,l,t) = f_{hds} IN_{ss}(i,t) C_{ss}(i,t) + (1 - f_{hds}) \left( \frac{IN_{ap}(i,t)}{\rho_{ap}} \right) C_{ap}(i,t) \quad (6-7)$$

$C_{ss}(i,t)$  = the pollutant concentration in soil of exposure district  $i$  during time step  $t$ , mg/kg.

$C_{ap}(i,t)$  = the pollutant concentration in the particulate phase of exposure district  $i$  during time step  $t$ , mg-m<sup>3</sup>.

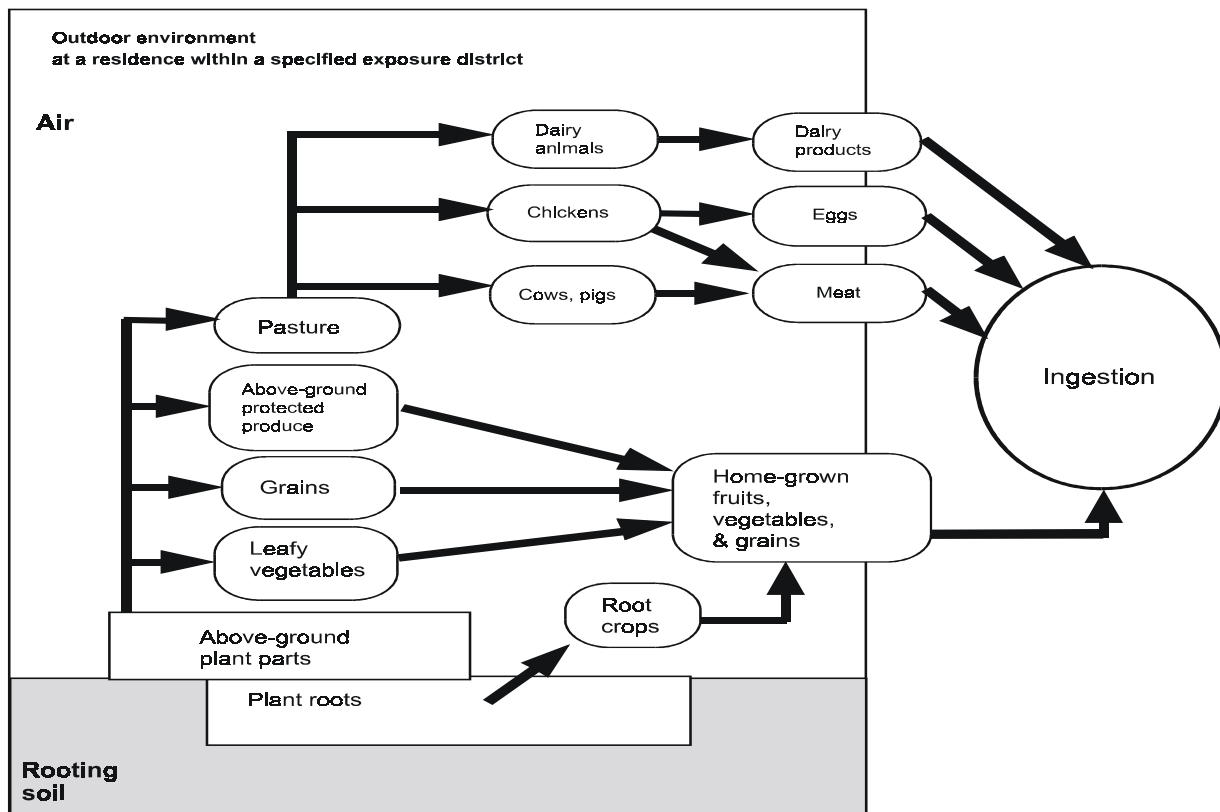
- $f_{\text{hds}}$  = the fraction of indoor dust that originates from outdoor soil. The remaining fraction is assumed to originate from particulate matter in air. Currently, this fraction is set to 0.5.
- $IN_{ss}(i,t)$  = the combined soil infiltration and soil tracking factor that expresses the likely increase or decrease of pollutant concentration in indoor soil relative to outdoor surface soil in exposure district  $i$ . TRIM.Expo currently sets  $IN_{ss}(i,t)$  to 1 but it can be set to a value specific to each exposure district and each time step.
- $[IN_{ap}(i,t)/\rho_{ap}]$  = the particle infiltration factor that expresses the likely increase or decrease of pollutant concentration in indoor dust relative to pollutant concentration in outdoor particulate matter in exposure district  $i$ .  $\rho_{ap}$  is the density of airborne particles of  $\sim 2,400 \text{ kg-m}^3$ . In the current version of TRIM.Expo,  $IN_{ap}(i,t)$  is set to 1 but can be set to a value specific to each exposure district and each time step.

### 6.2.3 INGESTION OF POLLUTANTS IN HOME-GROWN PRODUCE OR HOME-BRED ANIMALS

Soil pollutants can be transferred to the edible parts of vegetation from surface soil by resuspension and deposition, rain splash, volatilization followed by partitioning, and by root uptake for below-ground vegetation (Jones et al. 1991). The level of exposure to the soil pollutants found in vegetation food products often depends on translocation (*i.e.*, the process by which a pollutant is transferred from one part of a plant to another). Translocation can cause significant differences in pollutant concentrations in the total plant and the edible portion of the plant (*i.e.*, fruit, seeds). In addition, ingestion of contaminated soil or grains by animals reared/bred for human consumption can lead to contaminated, animal-based food products, such as meat, milk, dairy products, and eggs.

For the purposes of TRIM.Expo, home-grown foods are defined as foods grown on the land associated with a household and, for the most part, consumed within that household. Figure 6-4 illustrates the exposure pathways considered in constructing food-based exposures from home-grown foods and the algorithms used for modeling pollutant exposures from home-grown food products are discussed in the sections below. In the TRIM.Expo framework, home-grown foods are studied in a single exposure district. To calculate individual or cohort consumption of home-grown food products, the annual average consumption of the food product for individual or cohort  $z$  is derived from the national food consumption survey data (CSFII 1996) and then used to calculate the fraction that can be allocated to home-grown foods.

**Figure 6-4**  
**Exposure Pathways Considered for Contact with Food Products**



### 6.2.3.1 Vegetables, Fruits, and Grains

Vegetables, fruits, and grains include leafy vegetables (*e.g.*, cabbage, cauliflower, broccoli, celery, lettuce, spinach), exposed produce (*e.g.*, apples, pears, berries, cucumber, squash, grapes, peaches, tomatoes, string beans), protected produce or root crops (*e.g.*, carrots, beets, turnips, potatoes, legumes, melons, citrus fruits) and grains (*e.g.*, wheat, corn, rice, barley, millet).

Pollutants in the root zone soil gas and liquid can be taken up by plant roots and potentially transferred to above-ground plant parts in the transpiration stream. The ease with which non-ionized pollutants are taken up from the soil into root material is influenced by the pollutant's octanol/water partition coefficient,  $K_{ow}$ , which is commonly used as a measure of lipophilicity and water solubility. Pollutants with high  $K_{ow}$  values tend to either be strongly sorbed onto organic material in the root, making them less available for movement in the transpiration stream, or sorbed onto organic material in the soil, reducing their availability to root uptake. Increases in the water solubility of a pollutant tend to increase the amount of pollutant available for uptake from the soil water and increase the likelihood of movement with the transpiration stream; however, the root membrane of most plants restricts uptake of highly soluble or ionized species.

The algorithm for ingestion of pollutants in above-ground fruits, vegetables, and grains has the general form:

$$\begin{aligned}
 ADD_{z, fvg, i}(T) &= \frac{\sum_t \left( \frac{I_{z, g}(k, l)}{BW_z} \right) C_g(i, t) EF_{z, g}(i, t) ET(t)}{T} \\
 &+ \frac{\sum_t \left( \frac{I_{z, efv}(k, l)}{BW_z} \right) C_{efv}(i, t) EF_{z, efv}(i, t) ET(t)}{T} \\
 &+ \frac{\sum_t \left( \frac{I_{z, pfv}(k, l)}{BW_z} \right) C_{pfv}(i, t) EF_{z, pfv}(i, t) ET(t)}{T}
 \end{aligned} \tag{6-8}$$

where:

- $C_g(i, t)$  = the pollutant concentration, mg/kg, in the grains (g) of exposure district  $i$  during the time step  $t$ .
- $C_{efv}(i, t)$  = the pollutant concentration, mg/kg in the exposed fruits and vegetables (efv) of exposure district  $i$  during the time step  $t$ .
- $C_{pfv}(i, t)$  = the pollutant concentration, mg/kg in the protected fruits and vegetables (pfv) of exposure district  $i$  during the time step  $t$ .

[Note that these three concentrations must be obtained from measurements or from a model such as TRIM.FaTE].

- $[I_{z, g}(k, l)/BW_z]$  = the monthly or seasonally averaged daily rate of intake of grains, kg/kg/d, by individual or cohort  $z$  divided by a representative individual's body weight ( $BW$ ). The microenvironment and activity codes  $k$  and  $l$  are not used in this calculation.
- $[I_{z, efv}(k, l)/BW_z]$  = the monthly or seasonally averaged daily rate of intake of exposed fruits and vegetables, kg/kg/d, by individual or cohort  $z$  divided by a representative individual's body weight ( $BW$ ). The microenvironment and activity codes  $k$  and  $l$  are not used in this calculation,
- $[I_{z, pfv}(k, l)/BW_z]$  = the monthly or seasonally averaged daily rate of intake of protected fruits and vegetables, kg/kg/d, by individual or cohort  $z$  divided by a representative individual's body weight ( $BW$ ). The microenvironment and activity codes  $k$  and  $l$  are not used in this calculation,

$EF_{z,g}(i,t)$  = the exposure frequency, fraction of days per month equivalent, that individual or cohort  $z$  consumes home-grown grains in exposure district  $i$ . If the daily intake rate implicitly includes the exposure frequency, then this term is set equal to 1.

$EF_{z,efv}(i,t)$  = the exposure frequency, fraction of days per month equivalent, that individual or cohort  $z$  consumes home-grown exposed fruits and vegetables in exposure district  $i$ . If the daily intake rate implicitly includes the exposure frequency, then this term is set equal to 1.

$EF_{z,pfv}(i,t)$  = the exposure frequency, fraction of days per month equivalent, that individual or cohort  $z$  consumes home-grown protected fruits and vegetables in exposure district  $i$ . If the daily intake rate implicitly includes the exposure frequency, then this term is set equal to 1.

According to Yang and Nelson (1986), about half of all produce (*i.e.*, fruits, vegetables) consumed by humans consists of leafy vegetables and exposed produce that intercept pollutants from the atmosphere. The remaining half consists of protected produce or root crops, where pollutant transfer to the edible portion is primarily by root uptake. All grain crops are assumed to be exposed primarily to air pollutants.

### 6.2.3.2 Dairy Products

To calculate human exposures to pollutants found in dairy products, the biotransfer factors for milk versus the pollutant intake by dairy cattle must be determined, along with the parameters that describe the pasture, water, and soil intake rates of dairy cattle. For the purposes of TRIM.Expo, pasture is defined to be all foodstuffs that are grown on the farm to feed the animals (*e.g.*, open pasture grass, grains, corn).

The algorithm for ingestion of pollutants in dairy products has the form:

$$ADD_{z,dp,i}(T) = \frac{\sum_t \left( \frac{I_{z,dp}(k,l)}{BW_z} \right) C_{dp}(i,t) EF_{z,dp}(i,t) ET(t)}{T} \quad (6-9)$$

where:

$C_{dp}(i,t)$  = the pollutant concentration, mg/kg, in the dairy products ( $dp$ ) of exposure district  $i$  during the time step  $t$  obtained from measurements or from a model such as TRIM.FaTE.

$[I_{z,dp}(k,l)/BW_z]$  = the monthly or seasonally averaged daily rate of intake of dairy products, kg/kg/d, by individual or cohort  $z$  divided by a representative individual's body weight ( $BW$ ). The microenvironment and activity codes  $k$  and  $l$  are not used in this calculation.

$EF_{z,dp}(i,t)$  = the exposure frequency, expressed as the fraction of days per month equivalent, that individual or cohort  $z$  consumes home-grown dairy products in exposure district  $i$ . If the daily intake rate implicitly includes the exposure frequency, then this term is set equal to 1.

### 6.2.3.3 Eggs

To calculate human exposures to pollutants found in eggs laid by home-grown hens, the biotransfer factors for eggs versus the pollutant intake by chickens, and the parameters that describe the feed, water, and soil intake rates of chickens must be characterized.

The algorithm for ingestion of pollutants in eggs has the form:

$$ADD_{z,egg,i}(T) = \frac{\sum_t \left( \frac{I_{z,egg}(k,l)}{BW_z} \right) C_{egg}(i,t) EF_{z,egg}(i,t) ET(t)}{T} \quad (6-10)$$

where:

$C_{egg}(i,t)$  = the pollutant concentration, mg/kg, in eggs in the exposure district  $i$  during the time step  $t$  obtained from measurements or from a model such as TRIM.FaTE.

$[I_{z,egg}(k,l)/BW_z]$  = the monthly or seasonally averaged daily rate of intake of eggs, kg/kg/d, by individual or cohort  $z$  divided by a representative individual's body weight ( $BW$ ). The microenvironment and activity codes  $k$  and  $l$  are not used in this calculation,

$EF_{z,egg}(i,t)$  = the exposure frequency, expressed as the fraction of days per month equivalent, that individual or cohort  $z$  consumes home-grown eggs in exposure district  $i$ . If the daily intake rate implicitly includes the exposure frequency, then this term is set equal to 1.



### 6.2.3.4 Meat and Poultry

To calculate human exposures to pollutants found in meat, the biotransfer factors for meat versus pollutant intake by animals reared/bred for human consumption and the parameters that describe the pasture, water, and soil intake rates of these animals must be quantified. For the purposes of TRIM.Expo, cattle is used to represent **all** animals that are reared/bred for human consumption.

The algorithm for ingestion of pollutants found in meat has the form:

$$ADD_{z, mp, i}(T) = \frac{\sum_t \left( \frac{I_{z, mp}(k, l)}{BW_z} \right) C_{mp}(i, t) EF_{z, mp}(i, t) ET(t)}{T} \quad (6-11)$$

where:

$C_{mp}(i, t)$  = the pollutant concentration, mg/kg in the home-grown meat and poultry (*mp*) of exposure district *i* during the time step *t* obtained from measurements or from a model such as TRIM.FaTE.

$[I_{z, mp}(k, l)/BW_z]$  = the average daily rate of intake of meat and poultry, kg/kg/d, by individual or cohort *z* divided by a representative individual's body weight (*BW*). The microenvironment and activity codes *k* and *l* are not used in this calculation.

$EF_{z, mp}(i, t)$  = the exposure frequency of meat and poultry consumption of individual or cohort *z* in exposure district *i* (expressed as the fraction of days per month equivalent). If the daily intake rate implicitly includes the exposure frequency, then this term is set equal to 1.

## 6.2.4 LOCALLY-GROWN COMMERCIAL FOODS

The following subsections describe algorithms for estimating intake of pollutants found in locally-grown foods. These types of algorithms have been previously developed by McKone and Ryan (1989), McKone and Daniels (1991), Travis and Blaylock (1992), and McKone (1993a, b, c). The form and ranges of values used in these models have been validated for a limited number of compounds by Bennett (1981, 1982) and by Travis and Blaylock (1992).

Locally-grown foods (*i.e.*, grown in home gardens and commercial, local farms) are defined as foods that are not only produced, but also consumed within the same urban air shed being modeled by TRIM.Expo. The pollutant concentrations in air, soil, and/or water that are used to assess concentrations in locally-grown foods make use of the average pollutant concentration in the locations of farms producing such foods. For modeling purposes, it is ideal

if distributions for describing the local concentrations of pollutants in produce, grain, milk and dairy products, meat, eggs, and fish are available; but if these values are not available, they must be developed.

#### 6.2.4.1 Vegetables, Fruits, and Grains

The algorithms used to calculate intake of pollutants in locally-grown vegetables, fruits, and grains are the same as those provided in Section 6.2.3.1 with the following replacements:

$EF_{z,g}(i,t)$  = the exposure frequency, fraction of days per month equivalent, that individual or cohort  $z$  consumes locally-produced grains in exposure district  $i$ . As with home-grown produce and home-bred animals, if the daily intake rate of locally-grown produce implicitly includes the locally-grown produce exposure frequency, then this term is set equal to 1.

$EF_{z,efv}(i,t)$  = the exposure frequency, fraction of days per month equivalent, that individual or cohort  $z$  consumes locally-produced exposed fruits and vegetables in exposure district  $i$ . As with home-grown produce and home-bred animals, if the daily intake rate of locally-grown produce implicitly includes the locally-grown produce exposure frequency, then this term is set equal to 1.

$EF_{z,pfv}(i,t)$  = the exposure frequency, fraction of days per month equivalent, that individual or cohort  $z$  consumes locally-produced protected fruits and vegetables in exposure district  $i$ . As with home-grown produce and home-bred animals, if the daily intake rate of locally-grown produce implicitly includes the locally-grown produce exposure frequency, then this term is set equal to 1.

$C_g(avg,t)$  replaces  $C_g(i,t)$ , where  $C_g(avg,t)$  is the averaged pollutant concentration, mg/kg, in grains based on the average concentration in the locations where local foods are produced during the time step  $t$ .

$C_{efv}(avg,t)$  replaces  $C_{efv}(i,t)$ , where  $C_{efv}(avg,t)$  is the averaged pollutant concentration, mg/kg, in exposed fruits and vegetables based on the average concentration in the locations where local foods are produced during the time step  $t$ .

$C_{pfv}(avg,t)$  replaces  $C_{pfv}(i,t)$ , where  $C_{pfv}(avg,t)$  is the averaged pollutant concentration, mg/kg, in protected fruits and vegetables based on the average concentration in the locations where local foods are produced during the time step  $t$ .

### 6.2.4.2 Dairy Products

The algorithms used to calculate intake of pollutants from locally-produced dairy products are the same as those provided in Section 6.2.3.2 with the following replacements:

$EF_{z,dp}(i,t)$  = the exposure frequency, expressed as the fraction of days per month equivalent, that individual or cohort  $z$  consumes locally-produced dairy products in exposure district  $i$ . As with home-grown produce and home-bred animals, if the daily intake rate of locally-produced dairy products implicitly includes the locally-produced dairy products exposure frequency, then this term is set equal to 1.

$C_{dp}(avg,t)$  replaces  $C_{dp}(i,t)$ , where  $C_{dp}(avg,t)$  is the spatially averaged pollutant concentration, mg/kg, in the milk derived from all suburban and rural exposure districts where local dairy products are produced during the time step  $t$ .

### 6.2.4.3 Eggs

The algorithms used to calculate intake of pollutants found in locally-produced eggs are the same as those provided in Section 6.2.3.3 with the following replacements:

$EF_{z,egg}(i,t)$  = the exposure frequency, fraction of days per month equivalent, that individual or cohort  $z$  consumes locally-produced eggs in exposure district  $i$ . As with home-grown produce and home-bred animals, if the daily intake rate of locally-produced eggs implicitly includes the locally-produced eggs exposure frequency, then this term is set equal to 1.

$C_e(avg,t)$  replaces  $C_{egg}(i,t)$ , where  $C_{egg}(avg,t)$  is the averaged pollutant concentration, mg/kg, in eggs based on the average concentration in the locations where eggs are produced locally during the time step  $t$ .

### 6.2.4.4 Meat and Poultry

The algorithms used to calculate intake of pollutants found in locally-produced meat and poultry are the same as those provided in Section 6.2.3.4 with the following replacements:

$EF_{z,mp}(i,t)$  = the exposure frequency, number of days per month equivalent, that individual or cohort  $z$  consumes locally-produced meat products in exposure district  $i$ . As with home-grown produce and home-bred animals, if the daily intake rate of locally-produced meat products implicitly includes the locally-produced meat products exposure frequency, then this term is set equal to 1.

$C_{mp}(avg,t)$  replaces  $C_{mp}(i,t)$ , where  $C_{mp}(avg,t)$  is the averaged pollutant concentration, mg/kg, in meat based on the average concentration in the locations where local meat products are produced during the time step  $t$ .

#### 6.2.4.5 Fish (Commercial, Subsistence, and Recreational)

Exposures to pollutants that are found in fish are assumed to occur only on a local scale, with no residential (home) scale exposures. The algorithm for ingestion of pollutants found in fish has the form:

$$ADD_{z,f,i}(T) = \frac{\sum_i \left( \frac{I_{z,f}(k,l)}{BW_z} \right) C_f(avg,t) EF_{z,f}(i,t) ET(t)}{T} \quad (6-12)$$

where:

- $[I_{z,f}(k,l)/BW_z]$  = the average daily rate of intake of fish ( $f$ ), kg/kg/d, by individual or cohort  $z$  divided by a representative individual's body weight ( $BW$ ). The microenvironment and activity codes  $k$  and  $l$  are not used in this calculation.
- $C_f(avg,t)$  = the spatially or market averaged pollutant concentration, mg/kg, in the fish of all exposure districts in the air shed being considered during the time step  $t$ .
- $EF_{z,f}(i,t)$  = the exposure frequency, expressed as the fraction of days per month or its equivalent), that individual or cohort  $z$  in exposure district  $i$  consumes locally-caught fish. When the daily intake rate implicitly includes exposure frequency this term can be set equal to 1.

The TRIM.Expo module utilizes three types of cohorts to reflect differences in the exposure frequency to fish – those who buy and consume locally-raised fish, but do not catch their own fish; those who consume locally-raised fish that they also catch on their own (*e.g.*, recreational fishermen); and those who are subsistence fishermen who catch fish for a living and also eat the fish that they catch.

#### 6.2.5 RECREATIONAL SPORT MEAT (HUNTING)

Exposures to pollutants found in game animals (*e.g.*, deer, water fowl) are assumed to occur only on a local scale, with no residential (home) scale exposures. The algorithm for ingestion of pollutants in meat from game animals is as follows:

$$ADD_{z, sm, i}(T) = \frac{\sum_t \left( \frac{I_{z, sm}(k, l)}{BW_z} \right) C_{sm}(avg, t) ET(t)}{T} \quad (6-13)$$

where

$[I_{z, sm}(k, l)/BW_z]$  = the time-step averaged daily rate of intake of sport meat (*sm*), kg/kg/d, by individual or cohort *z* divided by a representative individual's body weight (*BW*). The microenvironment and activity codes *k* and *l* are not used in this calculation.

$C_{sm}(avg, t)$  = the averaged pollutant concentration, mg/kg, in the meat of game animals residing in the air shed being considered during the time step *t*.

There is currently no separate algorithm available in TRIM.Expo to determine concentrations in game animal tissues. This information must be obtained from available data or can be obtained from the output of TRIM.FaTE.

### 6.3 INTEGRATION OF EXPOSURES ACROSS MULTIPLE INGESTION MEDIA

The integration of ingestion exposures across multiple media for an individual or cohort is based on matching time scales. All ingestion intakes within a given time step are summed, and currently, relatively large time steps (monthly) are used in TRIM.Expo, such that the time aggregation of ingestion exposures is straight forward and does not introduce a significant source of uncertainty or confusion. Even daily aggregation of ingestion exposures should not be difficult since TRIM.Expo is capable of working in hourly time steps. However, more importantly, if TRIM.Expo is used to integrate ingestion exposures in hourly time steps, then a comprehensive inventory of micro-activity data on the daily water and food intake and hand-to-mouth activities of cohorts and individuals are needed. Such data are not yet available.

With regard to ingestion, some products are bolous exposures which are discrete while others are aggregated (*e.g.*, a beef meal would be associated with a specific farm and have a spatially dependent concentration, while milk would likely be a diluted exposure composed of a mixture of milk from all neighboring dairy farms). Therefore, where appropriate these exposures should be modeled on a meal-by-meal basis (*i.e.*, for each meal, the source of the food item is randomly selected based on the proportion of its contribution to the total commodity load and, thus, the pollutant concentration in the food item would be specific to that farm). Probabilistic approaches would be repeated for each meal to get a more representative estimate of dietary exposure. This process is described in more detail in EPA's guidance on health risks associated with multiple exposure pathways to combustor emissions (U.S. EPA 1997d).

The population risk (*i.e.*, incidence of effects) from pollutants that are believed to exhibit non-threshold mechanisms (*i.e.*, linear carcinogens) can be estimated based on the amount of pollutants entering the food supply each year (U.S. EPA 1997d). This method, as specified in EPA guidance (U.S. EPA 1997d), uses the annual amount of food produced in various food-producing regions of the study area as the metric of concern and then estimates the subsequent exposures to pollutants in the food.

## 6.4 DISCUSSION OF ALGORITHM INPUTS AND VALUES

An important attribute of exposure models is the ability to account for factors that control variation in human contact (*i.e.*, age, gender, location, activity patterns). Exposure assessments for ingestion pathways use of a number of factors that are both variable and uncertain. For each relevant population cohort, a number of exposure factors described in the previous sections can be used to characterize contact and intake. These factors are used to describe specific ingestion behaviors (*e.g.*, rates of ingestion for specific media such as fish and water for specific cohorts) or to describe the characteristics of the populations themselves (*e.g.*, body weight). For each of these parameters, it is necessary to develop a range of values that represent the population cohorts. Currently, OAQPS is compiling and evaluating data for each parameter for TRIM.Expo. The EPA's Exposure Factors Handbook (U.S. EPA 1997b) is one source being used extensively to derive such factors. EPA's National Center for Environmental Assessment (NCEA) is currently conducting research on how to derive distributions for many of the ingestion exposure factors identified in this chapter. When these distributions become available, they will be adopted as appropriate for use in TRIM.Expo. In the meantime, efforts are underway by OAQPS and other EPA program offices to develop exposure factors and associated distributions for specific parameters for use in risk assessments. When these are available, they will be published and be the subject of subsequent reviews.

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## APPENDIX A

### Glossary

- Absorbed dose** The amount of pollutant that crosses a specific absorption barrier (*e.g.*, the exchange boundaries of skin, lung, or digestive tract) through uptake processes. Absorbed dose is calculated from the intake and absorption efficiency and is usually expressed as the mass of pollutant absorbed into the body per unit time (mg/kg/d). For inhalation exposure, absorbed dose is the amount of material that passes from the lung volume into the blood. For ingestion exposure, absorbed dose is the quantity of pollutant that passes from the volume of the gastrointestinal tract across the gut wall and into the blood stream. For dermal exposure, absorbed dose is the quantity of material that passes through the stratum corneum into the living cells of the epidermis and dermis and then into the blood stream. Sometimes referred to as internal dose.
- Absorption barrier** Any of the exchange boundaries of the body (*e.g.*, the skin, lung tissue, digestive tract, gastrointestinal tract wall) that allow differential diffusion of various pollutants across the boundary.
- Activity pattern** A series of discrete events of varying time intervals describing information about an individual's lifestyle and routine. The information contained in an activity pattern typically includes the locations that the individual visited (usually described in terms of microenvironments), the amount of time spent in those locations, and a description of what the individual was doing in each location (*e.g.*, sleeping, eating, exercising). All of the information for an activity pattern is gathered during an "activity pattern survey," usually through the use of questionnaires or diaries. Each activity pattern survey is designed to collect information on activities needed for a particular study or purpose. Activity patterns are also referred to as "time/activity patterns."
- Applied dose** The amount of a pollutant given in mg/kg/d that comes in contact with the living tissue of an organism by entering into the lungs, by entering the gastrointestinal tract, and/or by crossing the stratum corneum into the living cells of the epidermis. In some experimental designs, the applied dose is referred to as the administered dose.
- Average daily dose (ADD)** Dose rate within a population averaged over body weight and an averaging time and typically expressed in terms of mg/kg/d.

- Biologically effective dose** The amount of a deposited or absorbed pollutant that reaches the cells or target site where an adverse effect occurs or where that pollutant interacts with a membrane surface.
- Breathing zone** A zone of air in the vicinity of an organism from which respired air is drawn. Personal monitors are often used to measure pollutants in the vicinity of the breathing zone.
- Cohort** A group of people within a population who are assumed to have similar exposures are taken from the same probability distribution during a specified exposure period.
- The use of cohorts is useful when modeling the exposures of a large population. Since adequate data on the exposures of each individual in a population does not exist, information about people who are expected to have similar exposures are aggregated together in order to make better use of the limited data that is available.
- Cohorts can be defined for each application or situation. In the latest pNEM/CO model, for example, cohort exposure was taken to be a function of demographic group, location of residence, location of work place, and type of cooking fuel (natural gas or other). Specifying the home and work district of each cohort provided a means of linking cohort exposure to ambient CO concentrations. Specifying the demographic group provided a means of linking cohort exposure to activity patterns which vary with age, work status, and other demographic variables. Specifying the type of cooking fuel provided a means of linking cohort exposure to proximity to a particular emission source. In some analyses, cohorts are further distinguished according to factors relating to time spent in particular microenvironments. In the pNEM analyses, the population-of-interest is divided into a set of cohorts such that each person is assigned to one and only one cohort.
- Demographic group** A group of people within a population sharing common demographic characteristics such as gender, race, household income, working status, or incidence of a particular disease or ailment. These groups can be defined differently depending on the study or application and much of this information can be gathered from the census.
- Dermal** The external skin surface of an organism.

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<b>Dermal exposure</b>	The contact between a pollutant and the external skin surface of a biological organism.
<b>Dose</b>	The quantity of energy or pollutant available for interaction with metabolic processes or biological receptors after crossing the outer boundary of an organism. See related terms: absorbed dose, applied dose, biologically effective dose, delivered dose, internal dose, and potential dose.
<b>Dose rate</b>	Dose per unit time (mg/d). Dose rate is often expressed on a per-unit-bodyweight-basis ( <i>e.g.</i> , mg/kg/d) and may be expressed as an average over a long time period ( <i>e.g.</i> , a lifetime). Also referred to as dosage.
<b>Environmental media</b>	The components of the physical environment that carry a pollutant, and through which pollutants can move and reach the organisms. The environmental media in TRIM.Expo include ambient air, ground water, surface water, surface soil, root zone soil, vadose zone soil, and several classes of vegetation.
<b>Exposure</b>	The contact between a target organism and a pollutant at the outer boundary of the organism. Exposure may be quantified as the amount of pollutant available at the boundary of the receptor organism per specified time period. As an example, inhalation exposure over a period of time may be represented by a time-dependent profile of the exposure concentrations.
<b>Exposure assessment</b>	Measurement or estimation of the magnitude, frequency, duration, and route of exposure of biological organisms to pollutants in the environment for a specified time period. An exposure assessment also describes the nature of exposure and the size and nature of the exposed populations.
<b>Exposure district</b>	A geographic location within a defined physical or political region where there is potential contact between an organism and a pollutant, and for which environmental media concentrations have been estimated either through modeling or measurement.
<b>Exposure event</b>	A human activity that results in contact with a contaminated medium within a specified microenvironment at a given geographic location.
<b>Exposure factor</b>	A normalizing or standardizing factor used in an exposure assessment as a surrogate for specific information that is not available for a particular subject, cohort, or demographic group. These factors are often drawn from a distribution or a range of data

[see for example, EPA's *Exposure Factors Handbook* (U.S. EPA 1997b)].

<b>Exposure media</b>	The part of the physical environment that surrounds or contacts organisms at the time of an exposure. The exposure media in TRIM.Expo include outdoor air, indoor air (multiple microenvironments), tap water, home-grown food, locally-produced food, prepared food, breast milk, house dust, soil, swimming pools, and other recreational surface water.
<b>Exposure pathway</b>	The physical course of a pollutant from the source to the exposed organism. An exposure pathway describes a unique mechanism by which an individual or population is exposed to pollutants or physical agents at, or originating from, a site. Each exposure pathway includes a source, or release from a source, an exposure point, and an exposure route. If the exposure point differs from the source, a transport/exposure medium (such as air) or media (in cases of intermedia transport, such as water to air) is also included.
<b>Exposure route</b>	The way a pollutant enters an organism after contact, including inhalation, ingestion, or dermal absorption.
<b>Fixed-site monitoring</b>	Sampling of an environmental or ambient medium for a pollutant's concentration at the same location continuously or repeatedly over some length of time.
<b>Ingestion</b>	An exposure route whereby pollutants enter the body by the mouth for digestion or absorption.
<b>Ingestion exposure</b>	The contact between a pollutant and the boundary in the area surrounding the mouth at the time of ingestion. The contact boundary is often defined for each particular situation or study.
<b>Inhalation</b>	An exposure route whereby air and pollutants are drawn into the lungs via the nasal or oral respiratory passages.
<b>Inhalation exposure</b>	The contact between an airborne pollutant and a human, or other animal, at the time of inhalation.
<b>Intake</b>	The process by which a pollutant crosses the outer boundary of an organism prior to passing an absorption barrier ( <i>e.g.</i> , through ingestion or inhalation).
<b>Intermedia transfer</b>	An algorithm for "linking" the environmental media with the microenvironmental media that exposed individuals occupy ( <i>e.g.</i> , air compartments) or the exposure media with which they come in



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	contact ( <i>e.g.</i> , air, water, food, soil). An intermedia transfer algorithm relates the pollutant concentration in a microenvironmental medium to the concentration in an ambient environmental medium that provides an input to that microenvironment.
<b>Internal dose</b>	See absorbed dose.
<b>Lifetime average daily dose</b>	LADD is the average daily dose within a population when the averaging time is the expected individual lifetime and is usually expressed in terms of mg/kg/d for compounds with carcinogenic or chronic effects.
<b>Microenvironment</b>	A defined space in which human contact with an environmental pollutant takes place and which can be treated as a well-characterized, relatively homogeneous location with respect to pollutant concentrations for a specified time period.
<b>Monte Carlo technique</b>	A statistical method that uses repeated random sampling from the distribution of values for each of the parameters in a generic (exposure or dose) equation to derive an estimate of the distribution of (exposures or doses in) the population.
<b>Multipathway exposure</b>	Exposure in which the pollutant travels via more than one environmental medium from its source to the point of contact with the exposed organism. For example, a pollutant which is released into the air, but is then deposited into a water body before coming in contact with a person.
<b>Potential dose</b>	An approximation to the applied dose that is simply the amount of a pollutant in the material ingested, air inhaled, or material applied to the skin. The potential dose for inhalation and ingestion is analogous to the administered dose in a dose-response experiment. For the dermal route, the potential dose is the amount of pollutant applied or the amount of pollutant in the exposure medium applied to the skin.
<b>Risk</b>	The probability of deleterious effects that may result from an action or inaction.
<b>Risk assessment</b>	The process of evaluating the toxic properties of a pollutant and the conditions of human exposure to the pollutant in order to ascertain the likelihood that exposed humans will be adversely affected and to characterize the nature of the effects they may experience. Risk assessments historically have included the following four steps: (1) hazard identification (determination of whether or not a particular

pollutant is causally linked to a particular adverse health effect); (2) exposure assessment (determination of the amount of the pollutant that humans are exposed to and the conditions of that exposure); (3) dose-response assessment (quantification of how adverse effects change with dose); and (4) risk characterization (the final analysis that integrates the scientific findings of the previous three components to assess the overall conclusions about potential human risk including a description of the expected nature and severity of harm associated with the risk).

**Uptake**

The process in which a pollutant crosses an absorption barrier and is absorbed into the body.

## APPENDIX B

### Comparison/Critique of Exposure Models

This appendix provides a review of several existing and emerging concentration and human exposure assessment models. The review in this chapter is organized according to the general characteristics of the concentration and human exposure models. To begin the review, models were generally classified according to whether they were (1) concentration models or (2) exposure models. Models were then further characterized into more specific categories. For example, the concentration models were further subdivided into outdoor air (Section B.1) and indoor air (Section B.2) concentration models. The exposure models were subdivided according to the exposure media represented: air (Section B.3), consumer products (Section B.4), dietary (Section B.5), and multimedia (Section B.6). Exposure simulation modeling systems were also reviewed (Section B.7). These are not individual models *per se*, rather they are a compilation of various components that are integrated through a common computer system. The parts of this system can include such varied components as air quality models (*e.g.*, atmospheric dispersion models or other types of fate/transport models), Geographic Information System (GIS) capabilities, environmental and various other databases, as well as exposure models and physiologically-based pharmacokinetic (PBPK) models.

This appendix is organized by model categories – air concentration models (*i.e.*, indoor and outdoor air quality models) and human exposure models, therefore facilitating comparison of models with similar characteristics. For the air concentration models (Section B.1 & B.2), “Summary Features” are provided that display the key attributes of each model.

#### B.1 OUTDOOR AIR CONCENTRATION MODELS

Three models were identified that primarily assess outdoor air concentrations: TOXLT, TOXST, and ASPEN. Both TOXLT and TOXST can be accessed via the EPA’s Exposure Models Library (EML) (U.S. EPA 1996c).

##### B.1.1 TOXLT (Toxic Modeling System Long-Term)

The Toxic Modeling System Long-Term (TOXLT) is a PC-based model that was developed in conjunction with the release of the EPA’s Industrial Source Complex (ISC2) Dispersion Models (U.S. EPA 1992b). Both the TOXLT and ISC2 models coincided with the promulgation of the EPA’s guidance entitled, “A Tiered Modeling Approach for Assessing the Risks due to Sources of Hazardous Air Pollutants” (U.S. EPA 1992c). The TOXLT computer system was established by OAQPS to examine both the lifetime cancer risks and the chronic noncancer hazard indexes associated with toxic pollutants. The purpose of TOXLT is to assist in the evaluation of the lifetime cancer risks and chronic noncancer hazards that may result from long-term exposure to toxic air pollutants. The ISCLT2 model is used to simulate annual average pollutant concentrations which are then used to estimate cancer risk levels or hazard index values at each user-specified receptor. These outputs presume (1) a hypothetical individual exists at each receptor; (2) no contribution from “background” sources (*i.e.*, sources not specifically included in the simulation); and (3) pollutant contributions in a mixture are additive

(i.e., there are no synergistic or antagonistic interactions between pollutants).

Summary Features – TOXLT

Environmental media:	Ambient air
Pollutants:	Multiple gas- and particle-phase agents
Time scale:	Long-term (annual average)
Stochastic:	No
Variability:	No
Uncertainty:	No

**B.1.2 TOXST (Toxic Modeling System Short-Term)**

The former Integrated Toxic Expected Exceedance Model (INTOXX), which was based on the superseded version of the Industrial Source Complex Short-Term (ISCST) Model, was revised to become the Toxic Modeling System Short-Term (U.S. EPA 1994b). TOXST addresses the problem of estimating expected exceedances of specified short-term health effects thresholds in the vicinity of continuous and intermittent toxic pollutant releases. Certain industrial facilities emit airborne toxic chemicals known to be harmful when their concentrations exceed a specified health effect threshold value for a specified length of time. However, releases of such chemicals often occur intermittently. This random emission pattern makes it difficult to predict the frequency with which ambient concentrations will exceed the health effect threshold. TOXST attempts to avoid the problems of underestimation and overestimation of exceedance rates resulting from random emission patterns by using the Monte Carlo simulation of source emissions of user-specified durations and rates at randomly selected points in time over a simulated long period of time. In addition, TOXST maintains the capability of simulating continuous emission sources along with intermittent emission, thereby providing a more realistic simulation of actual industrial operations.

Summary Features – TOXST

Environmental media:	Ambient air
Pollutants:	Multiple gas- and particle-phase agents
Time scale:	Short term to long-term (~ 1 hour to continuous)
Stochastic:	Yes
Variability:	Yes
Uncertainty:	No

**B.1.3 ASPEN (Assessment System for Population Exposure Nationwide)**

The Assessment System for Population Exposure Nationwide (ASPEN) was originally developed with support from EPA's Office of Policy (OP) [formally the Office of Policy, Planning, and Evaluation (OPPE)]. The model is being applied by OAQPS as part of their National Air Toxics Assessment (NATA) activities. ASPEN, which is used for hazardous air pollutants, consists of three separate modules (SAI 1999):

1. A dispersion module estimates ambient concentration increments at a set of fixed receptor locations in the vicinity of an emission source;

2. A mapping module interpolates ambient concentration increment estimates from the grid receptors to census tract centroids and sums contributions from all modeled sources; and
3. An exposure module, currently under development, will estimate the average concentration increment to which the population of a census tract is exposed, accounting for time spent in both indoor and outdoor microenvironments and time spent in other census tracts.

The ASPEN dispersion module, like its predecessors HEM and SCREAM2, uses a Gaussian model formulation and climatological data to estimate long-term average concentrations. For each source, the model calculates ground-level concentrations as a function of radial distance and direction from the source for a set of receptors laid out in a radial grid pattern. The concentrations represent the steady-state concentrations that would occur with constant emissions and meteorological parameters. For each grid receptor, concentrations are calculated for each combination of stability class, wind speed, and wind direction. These concentrations are then averaged together. The resulting output of ASPEN's dispersion module is a grid of annual average outdoor concentration estimates for each source/pollutant combination. Improvements to HEM and SCREAM2 that have been incorporated into ASPEN include:

- Expansion of reactive decay options;
- Inclusion of simple treatment of secondary formation;
- Improvement of the deposition algorithm;
- Improved treatment of locations near major point sources; and
- Improved treatment of area and mobile source emissions.

The annual average concentration estimates from ASPEN's dispersion module are then interpolated from the grid receptors to census tract centroids with ASPEN's mapping module. The contributions from all modeled sources are summed to give estimates of cumulative ambient concentration increments in each census tract. The concentration estimates are designed to represent population-weighted concentration averages for each census tract.

The number of emission sources, receptors, and pollutants for an ASPEN application are virtually unlimited. It has been applied to more than 200,000 point, area, and mobile emission sources of 148 hazardous air pollutants to estimate outdoor concentrations in the more than 60,000 census tracts in the contiguous U.S. Work is underway to link an appropriate exposure module to ASPEN.

*Summary Features – ASPEN*

Environmental media:	Ambient air
Pollutants:	Multiple gas- and particle-phase agents
Time scale:	Long-term (annual average)
Stochastic:	No
Variability:	No
Uncertainty:	No

## B.2 INDOOR AIR CONCENTRATION MODELS

Several approaches have been used to estimate expected indoor air pollutant concentrations (for a review, see Wadden and Scheff 1983). These approaches include deterministic models based on a pollutant mass balance around a particular indoor air volume; a variety of empirical approaches based on statistical evaluation of test data and (usually) a least-squares regression analysis; or a combination of both approaches – empirically fitting the parameters of a mass balance model with values statistically derived from experimental measurements. All three approaches have advantages and disadvantages. The mass balance models provide more generality in their application, but often the information on various input parameters is unavailable to carry out a mass balance approach. The empirical models, when applied within the range of measured conditions for which they were fitted, provide more accurate information. Mass balance models include single and multiple compartment models. Often the component of the indoor air mass balance models that is most difficult to represent is the role of indoor surfaces as sources or sinks for pollutants.

### B.2.1 INDOOR, EXPOSURE, and RISK (EPA ORD Indoor Air Quality Models)

INDOOR, EXPOSURE, and RISK are a series of three indoor air quality models developed by the Indoor Air/Radon Mitigation Branches of EPA's National Risk Management Research Laboratory within the Office of Research and Development (ORD). The first model, INDOOR, was designed to calculate the indoor pollutant concentrations from indoor sources. The second model, EXPOSURE, extended INDOOR to allow calculation of individual exposure. The RISK model extends EXPOSURE to allow analysis of individual risk to indoor pollutant sources. Risk estimates generated by models such as RISK are useful mainly for the purpose of comparing scenarios, rather than for estimating risks to individuals or populations.

The RISK model uses data on source emissions, room-to-room air flows, air exchange with the outdoors, and indoor sinks to predict concentration-time profiles for all the rooms. The concentration-time profiles are then combined with individual activity patterns to estimate exposure. Risk is calculated using a risk calculation framework. The model allows analysis of the effects of air cleaners located in the central air circulating system and/or individual rooms on IAQ and exposure. The model allows simulation of a wide range of sources including long-term steady state sources, intermittent sources, and decaying sources. Several sources can be modeled in each room. The model allows the analysis of the effects of sinks and sink re-emissions on IAQ. The results of test house experiments were compared with model predictions. The agreement between predicted concentration-time profiles and the test house data was good. The model is designed to run in the Windows operating environment.

#### *Summary Features – INDOOR, EXPOSURE, RISK*

Environmental media:	User-specified indoor sources
Pollutants:	Multiple chemicals and radon
Time scale:	Annual average
Stochastic:	No
Variability:	Yes
Uncertainty:	No

### B.2.2 MAVRIQ (Model for Analysis of Volatiles and Residential Indoor Air Quality)

The Model for Analysis of Volatiles and Residential Indoor Air Quality (MAVRIQ) (Wilkes et al. 1992) was developed jointly at Carnegie Mellon University and the University of Pittsburgh. It is a compartmental mass balance model that was developed to address human exposure to volatile organic compounds released from showers and other household water uses. In MAVRIQ, the indoor environment is divided into multiple compartments with constant or varying air flows. Based on water supply concentrations as an input, MAVRIQ accounts for pollutant generation, chemistry, and transport kinetics and characteristics of the exposed individual (*i.e.*, water use activity, location, breathing rates).

#### Summary Features – MAVRIQ

Environmental media:	Ground or surface water
Pollutants:	Volatile organic compounds
Time scale:	Short-term to long-term (~ 1 hour to continuous)
Stochastic:	Yes (but, only for parts of the model)
Variability:	Yes (must be entered repetitively)
Uncertainty:	No

### B.2.3 CONTAM (various versions)

The National Institute of Standards and Technology (NIST) has over the past several years developed a series of public domain computer programs for calculating air flow and pollutant dispersal in multi-zone buildings, including CONTAM86, CONTAM87, and CONTAM94. These programs take a multi-zone network approach to airflow analysis. Airflow paths include doorways, small cracks in the building envelope, and a simple model of the air handling system. CONTAM94, the most recent version of CONTAM, works on an Intel®-based PC in the DOS environment. A graphical interface is used to create and edit building descriptions. Future versions of this program are expected to include the capability for carrying out exposure assessments.

#### Summary Features – CONTAM

Environmental media:	User-specified indoor sources
Pollutants:	Generic
Time scale:	Short term to long-term (~ 1 hour to continuous)
Stochastic:	No
Variability:	No
Uncertainty:	No

### B.2.4 AMEM (ADL Migration Exposure Model)

The ADL Migration Exposure Model was developed by EPA's Office of Pollution Prevention and Toxics (OPPT) to estimate the migration of chemicals from polymeric materials such as television cabinets, water pipes, curtain backings, plastic toys, or other products containing polymers in home environments where these chemicals could become sources of indoor air pollution or contaminate potable water. Once the fraction of chemical that can migrate

from a product is estimated, external models can be used to estimate the exposures and risk to people from contaminated indoor air or water. The AMEM provides estimates for screening-level assessments when data are not available. The goal of the model is to identify concentrations that result in possible health concerns to justify further emission testing of the product for polymeric materials.

*Summary Features – AMEM*

Environmental media:	Indoor environment
Pollutants:	Chemicals emitted by polymeric materials
Time scale:	Short term
Stochastic:	No
Variability:	No
Uncertainty:	No



### B.3 HUMAN INHALATION EXPOSURE MODELS

Most human exposure models have the capability to track humans, either as individuals or in groups (*i.e.*, cohorts<sup>1</sup>) through their daily routines. The tracking process includes knowing where the person is, what they are doing (*i.e.*, their activities, including knowledge of the physical demand that the person is exerting during an activity), and the concentration of the pollutants that they come into contact with as they move about.

With the knowledge that outdoor air pollutants are able to penetrate into the interior of buildings and that many air pollutants are emitted by both outdoor and indoor sources, a great deal of work has focused on combining the features of both indoor and outdoor exposure models. These models differ in their approach, but all of them estimate exposures to outdoor pollutants that penetrate into buildings. The building type of greatest concern for estimating indoor exposures is probably residential buildings. A national study on human activities found that on average, U.S. citizens spend 69 percent of their time indoors at home (U.S. EPA 1996a). This percentage can be higher for some subsets of the population; for example, the very young or the elderly. Therefore, it is important to be able to model the pollutants of concern to human health that can penetrate a building's structure. The models in this section have, through various techniques, attempted to develop an integrated assessment of the exposure mechanisms associated with airborne pollutants from both indoor and outdoor sources. Descriptions of the models are provided below.

#### B.3.1 NEM and pNEM [The (probabilistic) National Ambient Air Quality Standards Exposure Models]

The EPA has used the NEM modeling methodology since the late 1970s when three pollutant-specific versions of the NAAQS Exposure Model (NEM) were developed for ozone (O<sub>3</sub>), carbon monoxide (CO), and particulate matter. The early versions of the NEM were referred to as "deterministic" as they did not attempt to model the random processes of people's activities as part of the exposure simulation. The models simulate the movements of specific subgroups or cohorts within a population through zones of varying air quality. Each zone is typically defined by a geographic location and a microenvironment. The movements of each cohort are determined by the use of activity diary data specific to the demographic characteristics of the cohort. The activity data are also specific to day of the week, season, and temperature. Depending on the application, cohort movements may account for trips to work places or to schools.

From its inception, NEM was designed to treat human exposure to airborne pollutants as a time series of a joint set of human activities occurring in a particular microenvironment and air quality (as measured by the concentration of a pollutant) in that same microenvironment. Maintaining the time series allows estimates for alternative exposure and dose metrics to be developed, a capability that has proven invaluable (McCurdy 1997).

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<sup>1</sup> A cohort is comprised of persons with similar demographic characteristics. A cohort is defined by a specific combination of home district (where they reside), work district (their place of employment), and demographic variables (*e.g.*, gender, age).

In 1988, the Monte Carlo technique for randomly selecting important variables was incorporated into the model simulations. These models were referred to as “probabilistic” and hence are known as probabilistic NEM, or pNEM. The models are pollutant specific. To identify one version of the model from another, the chemical symbol is appended to the pNEM-acronym; hence, the model for ozone is pNEM/O<sub>3</sub> and for carbon monoxide is pNEM/CO. These two models are the most commonly used pNEM models today. Developing the probabilistic versions of the model was an important step because it meant that the entire distribution of available data for each variable in a model could now be used. This makes it easier to address variability and uncertainty regarding the variables that were in the model (McCurdy 1997).

The first pNEM developed was that for ozone, or pNEM/O<sub>3</sub>. The early pNEM/O<sub>3</sub> used a regression-based relationship to estimate indoor concentrations of ozone using concentrations measured outdoors. Then, in 1991, a new version of pNEM applicable to carbon monoxide (pNEM/CO) was developed (Johnson et al. 1992b). This model was the first to use a mass balance model to estimate indoor pollutant concentrations. The mass balance model is based on the generalized mass balance model presented by Nagda et al. (1987). In general terms, the mass balance model can be described as:

$$\begin{aligned} \text{The change in indoor pollution concentration} = & \\ & \text{the pollutant entering from outside} \\ & + \text{the indoor generation of pollutant} \\ & \quad - \text{pollutant leaving the indoor microenvironment} \\ & \quad \quad - \text{removal of the pollutant by an air cleaning device} \\ & \quad \quad \quad - \text{decay of the pollutant indoors.} \end{aligned}$$

Another version of the pNEM/O<sub>3</sub> soon followed which also used a mass balance model to estimate indoor ozone concentrations. Several other refinements were included in this new version of the pNEM/O<sub>3</sub>. Some of these include the use of more recent census data for determining demographic information, a new commuting algorithm, and an increase in the number of fixed-site monitors able to represent each urban area.

Early in 1994, a special version of pNEM/O<sub>3</sub> applicable to outdoor workers was developed and used to estimate ozone exposures for outdoor workers in several cities in the U.S. (Johnson et al. 1996c). In a follow-up effort, another version of pNEM/O<sub>3</sub> specific to children who were active in outdoor activities was developed (Johnson et al. 1996c).

More recently, enhancements have been completed on the pNEM/CO. The latest version of the model is pNEM/CO (Version 2.0). Improvements to this model include the use of an expanded human activity database. This database is called the Comprehensive Human Activity Database (CHAD) (McCurdy 1999). The CHAD is comprised of over 17,000 person-days of activity pattern data. The data have been collected and organized from eight human activity pattern surveys. The CHAD contains the sequential patterns of activities for each individual, which is particularly important to estimating the dose profile for CO by the model. Another enhancement to pNEM/CO (Version 2.0) is the inclusion of a special commuting database developed by the Bureau the model for creating an “origin-destination” table to indicate the

patterns of commuting trips made by working cohorts among the defined exposure districts (Johnson et al. 1999).

Improvements have been made to both the algorithms and inputs to the mass balance model in pNEM/CO (ver. 2.0). The pNEM/CO methodology includes a mass balance model, which is used to estimate CO concentrations when a cohort is assigned to an indoor or motor vehicle microenvironment. The mass balance model is based on the generalized mass balance model presented by Nagda et al. (1987). As originally proposed, this model assumed that pollutant concentration decays indoors at a constant rate. For use in pNEM/CO, the Nagda model was revised to incorporate an alternative assumption that the indoor decay rate is proportional to the indoor concentration (Johnson et al. 1999). This alternative assumption is believed to more closely model the actual decay rate that takes place indoors. In addition, new databases and improved algorithms have been included for determining air exchange rates, the probability of gas stove use, gas stove-burner emission rates, pilot light emission rates, and residential volumes used in the mass balance model (Johnson et al. 1999).

The pNEM/O<sub>3</sub> and pNEM/CO are part of a small group of exposure models in which attempts have been made to evaluate their results using personal exposure monitoring data. Johnson et al. (1996c) describes initial efforts to evaluate the pNEM/O<sub>3</sub>. In this effort, pNEM/O<sub>3</sub> exposure estimates for Houston, Texas were compared with personal exposure monitoring data collected in 1981 during the Houston Asthmatic Study (HAS) (Stock et al. 1985). A special version of the pNEM/O<sub>3</sub> was created, which corresponded to the data collection criteria for the HAS. Results were compared for distributions of both one-hour ozone exposure estimates and one-hour daily maximum ozone exposure estimates. In general, the results suggested that the model overpredicted the HAS exposures in the range below 70 ppb and underpredicted exposures above 70 ppb. Developers of the pNEM/O<sub>3</sub> believed that the exposure estimates of the model were particularly sensitive to the distribution of ozone decay rates used in the model's mass balance algorithm (Johnson et al. 1996c).

During early model development, the execution of the pNEM series of models was conducted only on an EPA mainframe computer because of the large input and output data files required to run the model. However, in the summer of 1999, pNEM/CO (Version 2.0) was migrated (that is transferred) to run on a PC. OAQPS and ORD's NERL are continuing to support efforts to improve the efficiency of pNEM on a PC and to provide documentation and user's guides for the PC version. The documentation and code for the PC version of pNEM/CO should be available for public release in 2000.

The pNEM/CO (Version 1) was evaluated using CO exposure data collected during the Denver Personal Exposure Monitoring Study conducted during the winter of 1982/83 (Akland et al. 1985). Researchers analyzed the Denver data to determine the one-hour daily maximum and the 8-hour daily maximum CO exposures associated with each person-day of data. Then, the pNEM/CO was run to simulate the conditions of the Denver Personal Exposure Monitoring Study. The exposure estimates from this application were tabulated according to the classification of each cohort with respect to the type of cooking fuel used (*i.e.*, natural gas or other). The researchers found relatively good agreement between the observed and estimated distributions for the one-hour daily maximum analyses, except for the values above the 99<sup>th</sup>

percentile. They did not find as good agreement between the observed and estimated distributions for the eight-hour daily maximum exposures. The researchers reported that in each case, the distribution obtained from pNEM/CO overestimated the exposure values at low exposures and underestimated the exposure values at high exposures. The researchers point out that the estimated and observed distributions for the eight-hour daily maximum exposures agreed most closely in the range of CO concentrations between 5 and 12 ppm (Johnson et al. 1992b).

The pNEM/CO (Version 1) was evaluated similarly to the Johnson et al. (1992b) evaluation effort but with the additional use of the Kolmogorov-Smirnov test statistic to compare the observed and simulated cumulative frequency distributions for the one-hour daily maximum exposure (1DME) and the eight-hour daily maximum moving average exposure (8DME) (Law et al. 1997). A similar effect to that seen in the evaluation of the pNEM/O<sub>3</sub> occurred for pNEM/CO. For 1DME, the pNEM/CO exposure estimates agreed most closely with observed exposures within the middle of the distribution; that is, in the range of approximately 6 to 13 ppm. However, the model overestimated values at low exposures (*i.e.*, less than 6 ppm) and underestimated values at high exposures (*i.e.*, greater than 13 ppm). For 8DME, the estimated exposures agreed well with observed exposures in the range of CO concentrations between about 5.5 and 7 ppm. However, the model overestimated values below 5.5 ppm and underestimated values above 7 ppm (Law et al. 1997).

### **B.3.2 HAPEM (The Hazardous Air Pollutant Exposure Model)**

In 1985, the EPA's Office of Mobile Sources (OMS) developed a model for estimating human exposure to nonreactive pollutants emitted by mobile sources. This model is similar to the pNEM in that it simulated the movements of population groups between home and work locations and through various microenvironments. However, they differed in the temporal resolution used for expressing the exposure estimates. The pNEM provided hourly exposure estimates which could be averaged over longer time periods, whereas the HAPEM provided annual average exposure estimates. The HAPEM included a facility for estimating cancer incidence through the use of risk factors developed by the EPA, but the pNEM does not include this capability.

Then, in 1991, OMS extended this modeling methodology to estimate annual average carbon monoxide (CO) exposures in urban and rural areas under specified control scenarios. The model was now called the Hazardous Air Pollutant Exposure Model for Mobile Sources (HAPEM-MS). The annual average CO exposures could be used to estimate annual average exposures to various hazardous air pollutants associated with mobile sources. In each case, it was necessary to assume that the annual average exposure to a particular hazardous air pollutant was linearly proportional to the annual average CO exposure. The model was executed for specified urban areas that had ambient fixed- te CO monitors.

Shortly after, under the direction of EPA's Office of Research and Development (ORD), an enhanced version of the HAPEM-MS was developed. This model was labeled the HAPEM-MS2. It sub-divided the annual exposures by calendar quarter (*i.e.*, 3-month periods) to better estimate exposures to mobile sources as a consequence of outdoor air temperature. The HAPEM-MS2 also increased the number of microenvironments to 37, increased the number of

demographic groups<sup>2</sup> to 23, and increased the size of the activity pattern database (Johnson et al. 1993a).

In 1996, the EPA's ORD further enhanced the HAPEM by creating another generation of the model called the HAPEM-MS3. The enhancements included adding the ability to customize the demographic groups, updating the census data by using the 1990 census, and developing an algorithm for estimating ambient impacts in residences with attached garages (Palma et al. 1996).

Until the spring of 1998, execution of the HAPEM-MS3 operated only on an EPA mainframe computer. During early model development, this limitation was necessary as the model requires large data files for storage and large internal arrays for calculation. Then, by 1998, with advances in computing technology, it became possible to have the HAPEM-MS3 executed on a "workstation." To this end, in the spring of 1998, the HAPEM-MS3 was migrated (that is transferred) to the UNIX operating system on a workstation. During the migration, further enhancements to the model were made, including a new time-activity database derived from the CHAD, a new air quality program that automatically selects sites, and a more efficient implementation of the commuting algorithm.

Immediately after the release of the UNIX-version of the HAPEM-MS3, the ORD again made substantial improvements to the model. The newest model had two distinct improvements over the 1998 UNIX-version. First, the areal extent of the model was expanded to include the entire contiguous United States at the census tract-level. In order to make this possible, the second innovation to the model was the facility to use modeled air quality data as well as AIRS data. With this improvement, the model for the first time was able to *directly* estimate exposures to hazardous air pollutants; hence, the model was renamed again by dropping the mobile source (-MS) acronym. This latest version of the model, called the HAPEM4, has other enhancements as well. These include broader flexibility in defining the study area (this can range from a census tract up to the entire contiguous U.S.), an updated database of temperatures, an updated commuting algorithm, population data for all census tracts in the country, and the ability to change internal modeling parameters such as the number of microenvironments and the demographic group designations.

### **B.3.3 HAPEM-PS (The Hazardous Air Pollutant Exposure Model for Point Sources)**

The Hazardous Air Pollutant Exposure Model for Point Sources (HAPEM-PS) was initially developed for OAQPS. In its original form, HAPEM-PS was intended to be applied to factories, refineries, and other stationary point emission sources. The HAPEM-PS requires an air quality indicator (*e.g.*, annual mean concentration) for each point in a receptor grid surrounding the point source under evaluation. Receptor air quality values are typically determined through the use of emissions data and a dispersion model. The HAPEM-PS has not had the same extensive enhancements that the HAPEM-MS has had since the early 1990s.

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<sup>2</sup> A demographic group is defined by specific demographic characteristics taken from the census. For example, in HAPEM demographic groups are typically defined by gender, age, race, and working status (*i.e.*, either working or non-working).

Like the HAPEM-MS, HAPEM-PS defines exposures for sets of cohorts. However, the population of concern in HAPEM-PS is usually defined as all persons residing within a specified distance from a particular emission source. The pollutant concentrations at the receptors are typically estimated by the ISCLT dispersion model. Input data for the ISCLT model include local meteorological data and an estimate of the pollutant emissions from the source. In a typical HAPEM-PS application, the ISCLT model is used to estimate the annual average pollutant concentrations at the centroid of each of the census units used to define the home and work districts and at regularly-spaced receptors along the emission source property line. The HAPEM-PS output provides a histogram of the total number of people exposed at pollutant concentration level intervals. The HAPEM-PS output also provides the annual cancer incidence by home district, the home district population, and the cancer incidence per million individuals for each home district. Finally, the output includes the value and cohort of the maximum exposure and the values and home districts of the maximum lifetime cancer incidence and incidence rate (Johnson et al. 1993b).

### **B.3.4 AirPEX (Air Pollution Exposure Model)**

The AirPEX was developed at the National Institute of Public Health and the Environment in the Netherlands as a tool for analyzing the inhalation exposures of the Dutch population to air pollutants. The model was designed to assess and evaluate the time- and space-dependency of inhalation exposures of humans. It can be used to evaluate individuals, as well as populations and subpopulations.

The AirPEX estimates personal exposure for one-hour time intervals. The exposure parameters calculated include (1) the potential exposure concentrations (the air concentration as a function of time and space (*i.e.*, microenvironments)), (2) the actual exposure concentration (the concentration that a person moving through the microenvironment experiences as a function of time), (3) the intake rate (the rate at which a pollutant enters the respiratory tract per unit time), (4) the standardized intake rate (the intake rate standardized to the target organ (*e.g.*, lung, body mass)), (5) the frequency and time fraction that a person is in contact with concentrations above a certain threshold value, (6) the critical intake (the excess intake at exposure concentrations above critical concentrations) (Freijer et al. 1997). Averages for each of these variables can be obtained for an exposure period by integrating them over the whole period and dividing by the time span of the period.

Population exposures are approximated by repeating individual calculations for a large sample of individuals taken randomly from the whole population. The distribution of the calculated individual average exposures are approximated for the whole population by the probability density function. Analysis of the distribution in terms of percentiles yields information on the median, and extremes in the exposure levels are quantified by the 10<sup>th</sup> and 90<sup>th</sup> percentiles (Freijer et al. 1997).

The model itself consists of three modules assembled in the Windows<sup>®</sup> environment. The program retrieves data from two databases and uses numerous compound specific parameters. Default values for benzene, B(a)P, ozone, and PM are included in the program. Users can

override the default values and supply their own values for these four compounds, as well as for other compounds. The main module calculates individual exposure measures from time-series of air quality data and human activity patterns. Exposures are estimated in 15-minute discrete time-steps for various microenvironments. The AirPEX currently uses a database containing 4,985 daily activity patterns with 15-minute time resolution for the population in the Netherlands. Time series of air quality are supplied with one-hr resolution. A second module selects records from the activity pattern database. It estimates population exposures by repeating individual exposure calculations for all selected activity patterns and then combining this information to construct normalized frequency distributions. A third module displays the results of the exposure calculations and analyzes the distributions by percentiles. An important feature is the ability to analyze the socioeconomic characteristics of the individuals having the highest exposures to enable identification of high risk groups.

### **B.3.5 HEM (Human Exposure Model)**

In 1980, the EPA's OAQPS developed the Human Exposure Model (HEM). The model was designed to screen point sources of air pollutant emissions efficiently, ranking the sources according to their potential cancer risks. Then, in 1990, an updated version (HEM-II) that had additional modeling capabilities needed to address issues related to the analysis of toxic air pollutants was released. The HEM-II was intended for use in evaluating potential human exposure and risks from sources of toxic air pollutants (U.S. EPA 1991). HEM-II retained the capability of screening point sources for a single pollutant in order to rank sources according to cancer risks. The HEM-II also allows more refined analyses of individual point sources and study of entire urban areas that include multiple point sources, multiple pollutants, area sources, and dense population distributions.

The HEM-II uses the Industrial Source Complex Long-Term (ISCLT) Model for estimating dispersion. The HEM-II also provides the ability of moving the exposed population into up to ten microenvironments. These may include indoors at home, indoors at work, in transit, and movement out of the study area. For each application, parameters can be defined for indoor-outdoor concentration ratios for each microenvironment, the percentage of the exposed population to be assigned to the microenvironment, and the amount of time, on an annual basis, estimated to be spent in each microenvironment. New to this revised version of the model is the quantification of several key uncertainties. Using the Monte Carlo technique, six input variables can be described by distributions. They are the unit risk factor, the emission rate, microenvironmental concentrations, the time spent in a microenvironment, years spent in current residence, and the variability in concentrations predicted at the receptors. A choice of several statistical distributions can be selected for each input variable.

The HEM-II contains a limited STability ARray (STAR) database within the model. Complex emissions inventories can also be modeled. This includes modeling area sources (*e.g.*, mobile sources, residential heating) simultaneously with point sources. A choice of grid systems, including a Cartesian grid that will accommodate areas with high population density and numerous air pollution sources, is offered for calculating exposures. Population growth can be simulated, either from the base year of the population database to the current year or to a future

year. The model allows the user to account for differences between microenvironments (*i.e.*, indoor and outdoor concentrations). Census coverages are for the entire U.S. at the block group level. The results of the model's output can be shown graphically.

### **B.3.6 SHAPE (Simulation of Human Activities and Pollutant Exposure)**

EPA's ORD developed the Simulation of Human Activities and Pollutant Exposure (SHAPE) (Ott et al. 1988). SHAPE generates carbon monoxide inhalation exposure profiles for different human subgroups. It considers exposure to carbon monoxide in air through the inhalation pathway only. The model has two major input components: (1) human location patterns, and (2) microenvironmental carbon monoxide concentrations. It matches available location/activity data with environmental concentration data to obtain exposure profiles for 24-hour periods. Exposure concentrations are obtained by applying a superposition principle to contributions from the ambient and different microenvironments. In addition to the limited evaluations conducted on pNEM, SHAPE is one of the only other exposure models where attempts were made to evaluate the model's estimates using personal exposure data. The EPA's Denver/Washington, D.C. personal exposure database was used to test the model's predictions against 24-hour exposure profiles for more than 1,200 persons (Ott et al. 1988).

### **B.3.7 BEAM (Benzene Exposure Assessment Model)**

The Benzene Exposure Assessment Model's (BEAM) initial development by EPA's ORD in the late 1980s was spurred, at least in part, as a result of benzene being listed as a hazardous air pollutant by the Clean Air Act and because benzene is regarded as a human carcinogen (U.S. EPA 1990a). The model utilizes microenvironmental benzene concentration data coupled with human activity pattern data to estimate exposure to benzene. The BEAM estimates benzene inhalation exposure profiles for different human subgroups. It considers exposure to benzene in air through the inhalation pathway only. The model has three major input components: 1) human location patterns, 2) ambient (background) benzene concentrations, and 3) microenvironmental benzene concentrations. It matches available location/activity data with environmental concentration data to obtain exposure profiles for 24-hour periods. Exposure concentrations are obtained by applying a superposition principle to contributions from the ambient and different microenvironments. Inhalation dose is then obtained by applying inhalation rate to exposure concentrations. The BEAM was patterned after the Simulation of Human Air Pollution Exposure (SHAPE) model.

The Total Exposure Assessment Methodology (TEAM) studies conducted between 1979 and 1988 by the U.S. EPA have been cited as providing the impetus for developing a human exposure assessment model for benzene. The TEAM studies strongly indicated that human exposure to certain classes of volatile organic compounds (VOC), including benzene, occurs primarily within the confines of very restrictive microenvironments, primarily indoors, but outdoors as well. The TEAM studies also suggested that the traditional method of estimating exposures to benzene (as well as most VOCs) did not adequately account for the contribution of benzene from small, nearby sources. Therefore, the developers of the BEAM endeavored to



develop an exposure simulation model for benzene that utilized microenvironmental benzene concentrations data coupled with human activity pattern data to estimate human exposure to benzene (U.S. EPA 1990a, U.S. EPA 1993a). The BEAM is one of the models included in EPA's THERdbASE (see Section B.7.2).

### **B.3.8 pHAP (probabilistic Hazardous Air Pollutant exposure model)**

The probabilistic Hazardous Air Pollutant (pHAP) exposure model was developed by the EPA to estimate exposures to HAPs for the population residing in a specified study area. The model uses census data, ambient air quality data, meteorological data, and human activity pattern data to simulate exposures to the population from several different HAPs. The original version of the pHAP model was developed for a mainframe computing system. The mainframe version was developed and used to estimate benzene exposures to residents of a study area in Phoenix, Arizona for the year 1990. Subsequent to that development, a PC-version of the model was developed and tested using the same study area. The PC-version of the model is called, pHAP-PC. The pHAP-PC model utilizes a Graphical User Interface (GUI) to provide a Windows®-like environment (Panguluri et al. 1998).

### **B.3.9 CPIEM (California Population Indoor Exposure Model)**

The California Population Indoor Exposure Model was developed for the California Air Resources Board's (ARB) Indoor Program to evaluate indoor exposures for the general California population as well as certain subgroups such as individuals who may be highly sensitive to indoor air pollutants. The ARB required a model which could estimate the average and peak indoor exposures for the population and sensitive subgroups. The CPIEM combines indoor air concentration distributions with Californians' location and activity information to produce exposure and dose distributions for different types of indoor environments. This task is achieved through a Monte Carlo simulation whereby a number of location/activity profiles that were collected in ARB studies are combined with airborne pollutant concentrations for specific types of microenvironments (*e.g.*, residences, office buildings).

Concentration distributions for many pollutants and microenvironments are included in the CPIEM database. However, for pollutants and microenvironments not included in the database, the CPIEM presents two alternatives. The first is to estimate indoor air concentration distributions based on distributional information for mass balance parameters described below. The second is for the user to directly specify concentration distributions. The concentration values for a particular environment are then sampled from the distributions.

The simulation of indoor concentrations accounts for various types of indoor sources as well as outdoor concentrations, air exchange rates, and losses to indoor sinks. The concentration component (called a module) of the model uses a mass balance equation, based on the principle of conservation of mass, to estimate concentration distributions for specific types of indoor environments such as residences, offices, and schools. This module samples values from user-specified distributions for parameters such as emission rates for indoor sources, building

volumes, outdoor air concentrations, and indoor-outdoor air exchange rates, which are used as inputs to the mass balance equation.

Multiplication of the concentration values by breathing rates determined from the location/activity profiles and pulmonary ventilation data yields an estimate of the potential inhaled dose distribution for each modeled environment. The model then aggregates the environment-specific exposure and dose estimates to develop distributions of “total indoor air” exposures and doses. That is, the portion of the total (24 hour) exposure/dose associated with time spent indoors. Because outdoors are included as one of the environments in the model, it is also possible to simulate the total (both indoor and outdoor) exposure and dose distributions (CARB 1998).

## **B.4 CONSUMER PRODUCT EXPOSURE MODELS**

A few exposure models have been developed to assess potential exposures associated with the use of household consumer products. This type of exposure model is not as numerous as those found in the previous three sections because these models deal solely with pollutants emitted by the consumer products. The emissions from these products occurs primarily indoors where relatively few regulations exist for controlling toxic emissions. However, unlike the exposure models in the previous section that estimated exposures exclusively by the inhalation route, two of the models in this section can also estimate exposures by ingestion and/or dermal contact.

### **B.4.1 CONSEXPO (CONSUMER EXPOSURE MODEL)**

The CONSUMER product EXPOSURE model (CONSEXPO) (Van Veen 1995) developed by the National Institute of Public Health and the Environment (RIVM) [Netherlands] uses simple exposure and uptake models to assess the potential health impacts of consumer products. In order to cope with the diversity in consumer products, it is based on a general model framework that provides a general setting for widely differing exposure situations, and, secondly, it offers a number of predefined exposure/uptake models, which the user can link to build a complete exposure/uptake model. The starting points are the inhalation, dermal, and ingestion exposure pathways. For each of these pathways, a limited number of models is available to model exposure/uptake. The program reports several important exposure variables, namely, the per event concentration, the yearly averaged concentration, the fraction taken up, the amount taken up during a year (per year and summed), and the uptake per kilogram body weight per day. The program also allows for stochastic parameters, in order to propagate the effects of variable and/or uncertain parameters to the final exposure/uptake estimates. If one uses the stochastic parameters, the resultant distributions can be displayed and studied.

### **B.4.2 SCIES (SCREENING CONSUMER INHALATION EXPOSURE SOFTWARE)**

The Screening Consumer Inhalation Exposure Software (SCIES) was developed to assist the Economics, Exposure, and Technology Division of U.S. EPA's Office of Pollution Prevention and Toxics in performing screening-level assessments of the potential dose rates resulting from inhalation of new and existing chemicals in consumer products. The model calculates screening-level estimates of average individual inhalation potential dose rates to components of consumer products that can be classified into 11 different product categories. The model estimates potential dose rates for both actively-exposed users of the product and passively-exposed non-users. Default values are suggested for each parameter required to run the model for each product category. These values are based on exposure scenarios, volatility classifications, and residence occupancy patterns. The model combines results of an effort to measure ventilation flows within residences with a 2-zone mass balance model to allow estimation of potential dose rates to both consumer product users and non-users.

### **B.4.3 DERMAL**

DERMAL was developed to assist the Economics, Exposure, and Technology Division of U.S. EPA's Office of Pollution Prevention and Toxics in performing screening-level assessments of the potential dose rates resulting from dermal contact with consumer products containing new and existing chemicals in consumer products. The model calculates screening-level estimates of annual individual dermal potential dose rates to components of 16 consumer product categories. Exposures are calculated based on the weight fraction of the chemical of interest in the consumer product and assuming deposition of a film of liquid on to the dermal surface from contact with the product. Conservative default values are provided for most of the input parameters required to run the model for each of the 16 consumer product categories.

### **B.4.4 MCCEM (Multi-Chamber Concentration and Exposure Model)**

The MCCEM is an interactive model developed for the EPA's OPPT and updated for the EPA's ORD. It allows users to model indoor air contamination for use in assessing potential inhalation exposures caused by consumer products. The objective of MCCEM is to allow users to be able to assess the risk from exposure to pollutants emitted by consumer products. The model uses a spreadsheet format to estimate indoor concentrations for, and individual exposures to, chemicals released from products in residences. Concentrations can be modeled in as many as four zones within a house. The model can supply air exchange rates and interzonal airflows for different types of residences. Time-varying emission rates can be input for a pollutant in each zone of the residence, for outdoor concentrations, and for the zone where an individual is located. In this way, the model develops a time-series exposure profile for the individual.

The MCCEM allows the user to explore the sensitivity of the model results to changes in one or more of the input parameters. The parameters that can be modified in the sensitivity analysis include the infiltration rate, the source rate, the decay rate, and the outdoor concentration.

## **B.5 DIETARY EXPOSURE MODELS**

### **B.5.1 DEPM (Dietary Exposure Potential Model)**

The Dietary Exposure Model (DEPM) is a model and database system developed by U.S. EPA's ORD to correlate food information in a format for dietary exposure modeling. Currently, the database system includes information from several national, government-sponsored surveys and monitoring programs. In the model, food consumption is based on 11 food groups, containing approximately 800 core food types, established from over 6500 common food items. A unique feature of the DEPM is the use of recipes, developed for exposure analysis, that link consumption survey data to the pollutant residue information. The summary databases are aggregated in a fashion to allow the analyst selection of demographic factors, such as age/sex groups, geographical regions, ethnic groups and economic status. The model was developed for personal computers with the data files designed in dBASE IV with FoxPro for Windows applications programs for queries and reporting.

## **B.6 MULTIMEDIA EXPOSURE MODELS**

This section presents a review of a number of multimedia models that address exposure links among multiple ambient environmental media and multiple exposure media.

### **B.6.1 The Exposure Commitment Method**

One of the earliest approaches for systematically assessing multipathway exposures to environmental pollutants is termed the Exposure Commitment Method, developed by Bennett (1981). The basic objective of this approach is to calculate exposure commitments (*i.e.*, pollutant concentration in human tissue), which are calculated from transfer factors that are estimated as the ratios of the steady-state concentrations of a pollutant in adjoining compartments of an exposure pathway. An exposure commitment is determined by multiplying the transfer factors associated with the adjoining compartments of a given pathway of exposure, for example; air to plants to livestock to diet. This method has been applied to organic chemicals and metals. The published applications of the exposure commitment methodology depend on measured concentrations of the substances in different compartments to estimate transfer factors. The retrospective nature of this approach limits its usefulness for predicting exposures to chemicals for which there is little or no monitoring data available.

### **B.6.2 Layton et al. (1992) Indoor/Outdoor Air/Soil Transport Model**

In recent years various researchers have begun to model algorithms that address the movement of fine and coarse particles in the indoor environment by processes such as resuspension, deposition, and soil tracking (see Raunemaa et al. 1989; Nazaroff and Cass 1989; Allott et al. 1992). Nevertheless, none of these algorithms provide an integrated simulation of major transport processes and indoor/outdoor relationships for toxic substances in air, water and soil. In order to estimate concentrations of pollutants in the media identified here, one needs an indoor transport model that simulates (1) the movement of pollutants from the outdoor environment (air and soils) to the indoor environment and (2) the resulting concentrations in indoor media (air and floor dusts) resulting from both outdoor and indoor sources of the target pollutants.

Layton et al. (1992) have developed for particle bound radio nuclides a pollutant transport model that accounts for (1) the movement of pollutants from the outdoor environment (air and soils) to the indoor environment and (2) the resulting levels in human contact media ( $\mu\text{g}/\text{m}^2$  of floor dust and  $\mu\text{g}/\text{m}^3$  in air) derived from both outdoor and indoor sources. This model can be linked directly to the multimedia model to evaluate indoor/outdoor relationships. This model was used to evaluate the relative importance of various kinds of human factors in mediating human contacts with substances in air and dust. The loading of soil/dust on floor surfaces and the resuspension of particles from floors, for example, should increase as the number of household occupants increases. Increased loading of soil/dust on floors should in turn lead to more cleaning/vacuuming that redistributes pollutants onto contact surfaces throughout a house. For example, the tracking-in process, vacuuming, and particle penetration of a building shell tend to produce smaller sized particles in the indoor environment, making them more bioavailable.

### **B.6.3 CalTOX (California Total Exposure Model for Hazardous Waste Sites)**

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. 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 waste sites (McKone 1993a, b, c). 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 be used to 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 models encompass twenty-three exposure pathways. The exposure assessment process consists of relating pollutant concentrations in the multimedia model compartments to pollutant concentrations in the media with which a human population has contact (personal air, tap water, foods, household dusts soils).

### **B.6.4 MMSOILS: Multimedia Contaminant Fate, Transport, and Exposure Model**

MMSOILS was developed by EPA's ORD to estimate the human exposure and health risk associated with releases of contamination from hazardous waste sites (U.S. EPA 1992d). It is a multimedia model addressing the transport of a chemical in ground water, surface water, soil erosion, the atmosphere, and accumulation in food. The human exposure pathways considered in the methodology include: soil ingestion, air inhalation of volatiles and particulates, dermal contact, ingestion of drinking water, consumption of fish, consumption of plants grown on contaminated soil, and consumption of animals grazing on contaminated pasture. For multimedia exposures, the methodology provides estimates of human exposure through individual pathways and combined exposure through all pathways considered. The risk associated with the total exposure dose is calculated based on chemical-specific toxicity data. The intended use of MMSOILS is for screening and relative comparison of different waste sites, remediation activities, and hazard evaluation. The methodology can be used to provide an estimate of health risks for a specific site, but the uncertainty of the estimated risk may be quite large (depending on the site characteristics and available data) and this uncertainty must be considered in any decision-making process.

### **B.6.5 RESRAD (RESidual RADiation)**

The Residential Radiation (RESRAD) model was developed by Argonne National

Laboratory to evaluate residual concentrations of radio nuclides in soil, concentrations of airborne radon decay products, external gamma radiation levels, surface contamination levels, and radio nuclide concentrations in air and water and to determine radiation dose and excess lifetime cancer risks to an on-site resident (a maximally exposed individual or a member of a critical population group).

RESRAD was developed for the U.S. DOE and is accepted for use in remedial action activities. RESRAD determines site-specific residual radioactive material cleanup guidelines based on calculations of the radiation dose to hypothetical residents or workers on the site. The nine environmental pathways considered in RESRAD are direct exposure, dust inhalation, radon, and ingestion of plant foods, meat, milk, aquatic foods, water, and soil.

RESRAD code has been adapted to include both chemical and radiological health risks. Other recent RESRAD developments include the incorporation of uncertainty analysis and decontamination and decommissioning analysis capabilities. The development of the code is funded by the DOE.

#### **B.6.6 USES (Unified System for the Evaluation of Substances)**

The Uniform System for the Evaluation of Substances (USES) (RIVM 1994), was developed in the Netherlands by the National Institute of Public Health and the Environment (RIVM); Ministry of Housing, Spatial Planning and Environment (VROM); and the Ministry of Welfare, Health, and Cultural Affairs (WVC). USES provides a single framework for comparing the potential risks of difference chemical substances released to multiple media of the environment. It is an integrated modeling system that includes multiple environmental media and multiple human exposure pathways. The exposure assessment in USES starts with an estimate of substance emissions to water, soil, and air during the various life-cycle stages of a substance and follows its subsequent distribution in the total environment. The result of this type of multi-media assessment are the Predicted Environmental Concentrations (PECs) and an estimate of the daily intake by human receptors. In general, PECs are compared to "no-effects" levels for organisms in the environment, which are derived by extrapolating single-species toxicity tests to field situations. The estimated daily intake by humans is compared to the "no-observed-adverse-effect" level for mammals or to the "no-effect" level for humans.

#### **B.6.7 BEADS (The Benzene Exposure and Absorbed Dose Simulation)**

BEADS (MacIntosh et al. 1995) was developed at the Harvard School of Public Health through support from EPA's ORD. It is a population-based, multiple exposure pathway microenvironmental model of 24-hour average inhalation exposures and total absorbed doses of benzene. The model was developed: (1) to provide a tool for estimating the distribution of benzene personal air concentrations and total absorbed doses for a large population, (2) to examine the determinants of inter-individual variability of exposures and absorbed doses of benzene, and (3) to explore the accuracy and precision of predictions of population exposures and absorbed doses of benzene made with monitoring results from past field studies. A



two-dimensional Monte Carlo simulation approach is used in the model to estimate the uncertainty about the predicted population exposure and absorbed dose distributions. A principal advantage of this approach to uncertainty analysis is that the relative contribution of the input variables to prediction uncertainty can be easily identified. Decisions can then be made regarding the appropriate measures to be taken to reduce the parameter uncertainty, where the overall goal is to minimize prediction uncertainty.

The BEADS model includes a probabilistic non-sequential (non-temporal) simulation of time activity patterns (TAP) and an anthropometric module used to correlate exposure factors in order to estimate absorbed dose (from inhalation, ingestion, and dermal absorption). Short term, high concentration exposures are not accounted for. The multimedia exposure and absorbed dose model underwent preliminary evaluation to estimate the benzene distribution of personal air concentration that would be expected for a large population depending on a microenvironment and exposure scenario in air (all via inhalation) or water (via ingestion, dermal uptake, or inhalation). Estimated distributions of personal and microenvironmental benzene exposures compared well with previous monitoring results (TEAM–Total Exposure Assessment Methodology) except at the upper ends.

### **B.6.8 DERM (Dermal Exposure Reduction Model)**

The physical-stochastic model DERM, was developed by Stanford's Environmental Engineering and Science Group to estimate personal dermal exposure incurred via multiple contact mechanisms as a function of time (Zartarian 1996). This is the first exposure model to calculate dermal exposure as a function of actual human activity data. An important output of DERM is the dermal exposure profile, which plots mass of pollutant loading on the skin as a function of time. Such profiles are the basis of understanding the pathways by which dermal and non-dietary ingestion exposure are incurred (*e.g.*, liquid immersion, surface contact with liquids, soil, or dust, aerosol deposition, hand-to-mouth contact). DERM is a personal, physical-stochastic model designed to evaluate the sources of uncertainty in the calculations, to understand the important dermal exposure contact pathways, and to help determine the best ways to control those factors that contribute most significantly to exposure. DERM has also been designed to assess ingestion exposures for hand-to-mouth activities.

### **B.6.9 SCREAM2 (South Coast Risk and Exposure Assessment Model, ver. 2)**

The SCREAM2 (Rosenbaum et al. 1994) was developed with support from California's South Coast Air Quality Management District and provides the ability to model both inhalation and multipathway non-inhalation exposures. A submodel, called MULTPATH, calculates population exposures to air toxics through non-inhalation pathways. The MULTPATH submodel includes the following pathways: soil ingestion, soil dermal contact, home-grown produce ingestion, commercial (locally-grown) produce ingestion, commercial (locally-raised) animal product ingestion, surface drinking water (local source) ingestion, fish (local source) ingestion, and breast milk ingestion. Average daily doses of a pollutant to the population are estimated from concentrations in each medium on the basis of age-specific ingestion rates and

body weights and local population age profiles. Exposure estimates are made with respect to contamination of commercial foodstuffs (produce and animal products) and surface water used for drinking and/or fishing by assuming that they are consumed entirely and uniformly by the population of the modeled area in proportion to the average ingestion rates for each age group. The individual carcinogenic health risk associated with ingestion exposure over a 70-year lifetime is estimated as the product of the dose and a cancer potency slope. MULTPATH requires site-specific information on the locations and yields of all commercial produce and commercial animal-raising operations. In addition, the locations and information on certain physical parameters of all water bodies used as sources of drinking water or fishing are required.

For inhalation exposures, the 24-hourly concentrations for each census block group are estimated using a Gaussian air dispersion- and mapping modules. For each source, the model calculates ground-level concentrations as a function of radial distance and direction from the source for a set of receptors laid out in a radial grid pattern. The concentrations represent the steady-state concentrations that would occur with constant emissions and meteorological parameters.

The inhalation exposure module accounts for mobility patterns of the population, indoor-outdoor exposure concentration differences, and physical exercise levels. The module estimates exposures for each individual census block group, aggregating exposure throughout the modeled area for a number of subregions, called exposure districts. Exposure is estimated for 12 basic population age/occupation groups which are further subdivided into 56 subgroups, distinguished by their hourly activity patterns. For each hour, a subgroup is assigned to a geographic location (*i.e.*, either a home or work district), one of several different indoor or outdoor microenvironments, and one of three physical exercise levels (low, moderate, or heavy). There are population activity patterns defined for weekdays, Saturdays, and Sundays.

In order to track the geographic locations of the population from hour to hour, the inhalation exposure/risk module again divides the 56 subgroups into cohorts, defined on the basis of common age-occupation groupings, and again by home and work exposure districts. The population composition and mobility data are compiled at the exposure-district level, while concentrations are for the smaller census block-group level.

SCREAM2 can use the Indoor Air Quality Model (IAQM) submodel to calculate indoor pollutant concentrations. IAQM simulates indoor air quality by means of a dynamic mass balance equation, with a building being represented by a single compartment. Outdoor air is permitted to leak into and out of the building, and indoor recirculation and makeup air can be supplied as appropriate through simulation of a heating, ventilation, and air conditioning (HVAC) system. In addition, indoor sources, which are specified in terms of source strength and time profile, can be modeled with the IAQM. Pollutant losses indoors are simulated in terms of adsorption onto surfaces or deposition due to settling, with surface reactivity or deposition rates dependent on the pollutant.

### **B.6.10 Integrated Spatial Multimedia Compartmental Model (ISMCM)**

The Integrated Spatial Multimedia Compartmental Model has been under development with the School of Engineering and Applied Science at the University of California Los Angeles for approximately the last 15 years. A newer version of the ISMCM, called MEND-TOX, is currently undergoing evaluation at the EPA ORD's National Exposure Research Laboratory (NERL).

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

The ISMCM is not structured to incorporate uncertainty/variability analyses directly into the model operation. Furthermore, the links and compartments (spatial configuration) of the ISMCM are predetermined, thereby making it less useful in a system that is to be fully integrated.

### **B.6.11 Indirect Exposure Methodology (IEM) Model**

The U.S. EPA began developing the Indirect Exposure Methodology (IEM) in the 1980s. The IEM consists of fate and transport algorithms that estimate the media concentrations resulting from the multipathway transfer of air pollutants to soil, vegetation, and water bodies. The algorithms in IEM are designed to predict exposures for pollutants for which indirect 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 summarizing the IEM methodology was published in 1990 (U.S. EPA 1990b), and a major addendum was issued in 1993 (U.S. EPA 1993b). 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 1998e). The algorithms in IEM are under continuous refinement, and revised documentation addressing SAB and public comments on the 1993 Addendum is pending (U.S. EPA 1999h). This revised document no longer uses the IEM terminology; instead, the document refers to MPE (multiple pathways of exposure) assessment.

The IEM estimates human exposure to pollutants via several routes, including inhalation, dermal contact, and food, water, and soil ingestion. Exposures are estimated using environmental media concentrations, transfer factors (*e.g.*, bioaccumulation factors) where appropriate, and measures of human activity and exposure characteristics (*e.g.*, consumption rates for food types) such as those available in EPA's *Exposure Factors Handbook* (U.S. EPA 1997b). The IEM is designed to estimate intakes for specific, predetermined receptor scenarios (*e.g.*, subsistence gardener, recreational fisher, average urban resident) that may be indicative of high-end or average exposures to a pollutant.

Because it is designed to estimate exposure for individuals classified into specific scenarios, IEM does not readily allow for the modeling of a distribution of exposures within a population. It is not designed to provide estimates of population exposures. In addition, IEM is set up to model a long-term emission source, and the fate and transport component of IEM consists of a set of linked, one-way algorithms that do not allow for tracking transformations between different chemical species or feedback between different media. Pollutants are input to the model as annual average air concentrations and wet and dry deposition rates for a specific location or as areal averages for a given space (*e.g.*, a watershed). Thus, the model cannot provide a detailed time series estimation of media concentrations and the resulting human exposures, and spatial variations in exposure can be approximated only through substantial site-specific model adjustment and repeated model runs. In addition, IEM is a deterministic model and is not designed to estimate the uncertainty or variability associated with exposure estimates. These characteristics make IEM suitable for scenario-specific, screening-level exposure assessments and the determination of exposure routes of potential concern for a long-term emission source but less appropriate for estimating distributions of population exposures over time and space and across various pathways.

## **B.7 EXPOSURE SIMULATION MODEL SYSTEMS**

In addition to exposure models, there are a number of exposure modeling systems. These are systems or libraries that can contain transport models, exposure models, data files, and the associated software for linking these models with the various input and output files.

### **B.7.1 GEMS (Graphical Exposure Modeling System)**

The EPA's OPPT developed the Graphical Exposure Modeling System (GEMS) to support exposure and risk assessments by providing access to single medium and multimedia fate and exposure models, physical and chemical properties estimation techniques, statistical analysis, and graphics and mapping programs with related data on environments, sources, receptors, and populations. Under development since 1981, GEMS provides analysts with an interactive, easily learned interface to various models, programs, and data needed for exposure and risk assessments. PC-GEMS (GSC 1988) is a stand-alone version of GEMS that can be run on a personal computer.

The environmental models in GEMS are atmospheric, surface water, land unsaturated (soil) and saturated (ground water) zones, and multimedia in nature. Methods for estimating octanol-water partition and adsorption coefficients, bioconcentration factor, water solubility, melting and boiling point, vapor pressure, Henry's constant, acid dissociation constant, lake/stream volatilization rate, and atmospheric half-life are available. Data sets are related to environmental characteristics (climate, soil, rivers, ground water, vegetation), source releases (POTWs and industrial water discharges, Census business patterns, RCRA permit sites), and receptors (population and household estimates for 1970, '80, '90, and '95 by small area census district; and drinking water facility information).

### **B.7.2 THERdbASE (Total Human Exposure Risk database and Advanced Simulation Environment)**

THERdbASE has been developed by EPA's ORD as a PC-based computer modeling and database system that contains exposure and risk related information. The system provides a framework for the construction of a suite of exposure and risk related models within the Modeling Engine by using information available in data files within the Database Engine. Data can be viewed as a table, coded fields can be viewed as decoded fields, fields can be set to "show" or "hide" mode, and multiple data files can be viewed at the same time. In the "advanced" mode, user files can be edited. Data records can be queried and simple statistics (summary statistics — mean; standard deviation; minimum and maximum; percentile values at desired intervals; and linear regression on two numerical data fields) can be performed. Data can be printed, saved, or exported. New user files can be created and data can be imported. Input to models is achieved through a standardized procedure. Inputs can be provided as single values, custom distributions (normal, lognormal), distributions based on data files present in THERdbASE, or as specific percentile values. Efficient algorithms are provided to optimally access input data, to perform the numerical simulations, and to generate appropriate output data. Multiple model runs can be done through a batch process. Results can be output as either THERdbASE data files or as pre-set graphs (U.S. EPA 1998g).

Information about THERdbASE is available on the EPA's Internet website (<http://www.epa.gov/nerlpage/head/therdbase.htm>). The Internet version of THERdbASE includes the following models:

- Location Patterns
- Chemical Source Release - Instantaneous Emission
- Chemical Source Release - Timed Application
- Indoor Air (2-Zone)
- Indoor Air (N-Zone)
- Exposure Patterns For Chemical Agents
- Benzene Exposure Assessment Model (Beam)
- Source Based Exposure Scenario (Inhalation + Dermal)
- Film Thickness Based Dermal Dose
- PBPK Based Dermal Dose

The Internet version of THERdbASE also includes the following databases:

- 1990 Bureau of Census Population Information
- California Adult Activity Pattern Study (1987 - 88)
- AT&T-sponsored National Activity Pattern Study (1985)
- 1992-94 National Human Activity Patterns Study (NHAPS)
- Chemical Agents from Sources
- Chemical Agent Properties
- Air Exchange Rates
- Information from EPA's TEAM (Total Exposure Assessment Methodology) Studies
- Information from EPA's NOPES (Non-Occupational Pesticides Exposure Study) Studies

- Human Physiological Parameters

### **B.7.3 MEPAS (Multimedia Environmental Pollutant Assessment System)**

The Multimedia Environmental Pollutant Assessment System (MEPAS) (Streng and Chamberlain 1995, Droppo et al. 1992) was developed by Battelle Pacific Northwest Laboratory (PNL) for the U.S. Department of Energy. The system was developed to rank DOE sites having potential hazardous chemical and radioactive releases. The key objective of MEPAS is to rank sites by calculating human health risk to the population surrounding the site. MEPAS calculates “hazard potential index” (HPI) values for a site by summing up risk factors associated with various exposure scenarios. This system has wide applicability to a range of environmental problems using air, ground water, surface water, overland, and exposure models. MEPAS integrates source, transport, and exposure models into a single system. The algorithms in MEPAS accommodate the following ten components: 1) source terrain, 2) overland pathway, 3) ground water (vadose and saturated zones) pathway, 4) surface water pathway, 5) atmospheric pathway, 6) exposure routes, 7) hazard assessment (chemical carcinogens / non-carcinogens; radio nuclides), 8) pollutant/transport and exposure scenarios, 9) a user-friendly PC shell, and 10) a chemical database.

Pollutant transport media are ground water, overland flow, surface water, and atmosphere. Human uptake occurs through ingestion (of contaminated water, soil, crops, animal products, and aquatic foods), inhalation (of airborne pollutants), and dermal contact (with chemicals and radio nuclides). The hydrologic media consists of the hydrologic source term, unsaturated and saturated ground water zones, and surface water/runoff. The source term can be computed internally or specified at receptor locations or by specified flow. The source term geometries include point, line, and area sources. Limitations of the hydrologic pathway include negligible leaching of the source by ground water, and flow in the virtual direction only.

The atmospheric pathway consists of the atmospheric source term and atmospheric transport processor. Source terms consist of point sources and area sources. Atmospheric transport of pollutants utilizes an enhanced Gaussian plume model, and computes long term exposure for a sixteen sector grid using average stack parameters. Enhancements to the plume model include deflection of wind speed to account for variability in local surface roughness, and can consider radioactive decay depletion and first order chemical reactions. Only simple sources can be modeled, and particulate pollutants originate from area sources only.

MEPAS calculates an average dose over 70 years time increments for a number of user specified receptor locations. Dose is calculated for each transported pollutant. For radioactive pollutants the dose is expressed as the effective dose equivalent from each pollutant. MEPAS uses the ICRP dose conversion factors to convert the rate of exposure to dose.

### **B.7.4 EML/IMES (Exposure Models Library / Integrated Model Evaluation System)**

The Exposure Models Library (EML) was developed by the U.S. EPA’s ORD and is a collection of exposure models distributed in a CD-ROM (U.S. EPA 1996c). The purpose of this disk is to provide a compact and efficient means to distribute exposure models, documentation,

and the Integrated Model Evaluation System (IMES). The EML disk contains over 120 models which may be used for exposure assessments and transport modeling. The model files may contain source and/or executable code, sample input files, and other data files, sample output files, and in many cases, model documentation in WordPerfect<sup>®</sup>, ASCII text, or other similar formats. IMES assists in selecting appropriate models, provides literature citations on model validations, and demonstrates model uncertainty protocols. The IMES software is an MS-DOS application, can be used on an Intel-based PC, and is capable of running on a network. Model codes and documentation can be downloaded from the CD-ROM to a hard drive. The most recent version, which is the third edition, has an HTML interface to view model directories and Internet source for some models.

### **B.7.5 MENTOR (Modeling ENvironment for TTotal Risk)**

The Modeling ENvironment for TTotal Risk (MENTOR) project, is being developed through funding from EPA's National Exposure Research Laboratory (NERL). The objective of the on-going MENTOR project is to develop, apply through case studies, and evaluate state-of-the-art computational tools, that will support multipathway, multiscale source-to-dose studies and exposure assessments for a wide range of environmental pollutants. Particular emphasis in MENTOR is placed on integrating methods for prognostic and diagnostic exposure/dose analyses, by utilizing, in combination, environmental, microenvironmental, and biomonitoring information to evaluate assumptions regarding routes and pathways of exposure.

MENTOR merges the methods and tools of the comprehensive Exposure and Dose Modeling and Analysis System (EDMAS) with those currently available in pNEM, and extends them for application to situations that are relevant to multimedia and multipathway exposures. EDMAS is an expandable library of interlinked computation modules (Georgopoulos et al. 1997). MENTOR incorporates models, databases, and analytic tools which can probabilistically estimate exposures (and doses) to individuals, populations, and susceptible subpopulations as well as predict and diagnose the complex relationships between source and dose. MENTOR is designed as a multiscale modeling system, that allows following in a mechanistically consistent manner the evolution of physicochemical phenomena over spatial scales ranging from geographic regions to personal and residential microenvironments. It provides a consistent link with biological uptake and disposition models. MENTOR is also multiscale in time, designed to support modeling of processes in ranges from minutes to decades.

MENTOR has a modular structure with an interface that offers linkage to both a Geographic Information System (ArcView and ArcInfo) and a relational database management system (Oracle) for "defining" an application or case study. MENTOR incorporates libraries of environmental and biological process models, including macroenvironmental, ecological/food-web, local multimedia, microenvironmental, activity pattern/exposure event, biological fate and transport, and dose response modules. MENTOR will eventually provide an extensible set of ready-to-use methodological tools, as well as linkages to relevant databases, for performing assessments of exposure/dose for populations or specific individuals, and for a variety of user-defined scenarios.

The MENTOR development and application effort is being pursued at the Computational Chemodynamics Laboratory (CCL) of the Environmental and Occupational Health Sciences Institute (EOHSI), which is a joint project of the University of Medicine and Dentistry of New Jersey (UMDNJ) and Rutgers University.

### **B.7.6 MODELS-3/Multimedia Integrated Modeling System (MIMS)**

The U.S. EPA ORD's NERL is developing Models-3 Community Multi-scale Air Quality (CMAQ) modeling system. It is a flexible software system designed to simplify the development and use of environmental assessment and decision support tools for a wide range of applications from regulatory and policy analysis to understanding the interactions of atmospheric chemistry and physics. This newest generation of environmental modeling software has been under development for the past seven years.

Models-3, in combination with CMAQ, form a third generation air quality modeling and assessment system. First generation air quality models dealt with tropospheric air quality with simple chemistry at local scales using Gaussian plume formulation as the basis for prediction. Second generation models covered a broader range of scales (*i.e.*, local, urban, and regional) and pollutants, addressing each scale with a separate model and often focusing on a single pollutant. Third generation models treat multiple pollutants simultaneously up to continental scales and incorporate feedback between chemical and meteorological components. Future development is planned for a fourth generation system which would extend linkages and process feedback to include air, water, land, and biota to provide a more holistic approach to simulation of transport and fate of chemical and nutrients throughout an ecosystem (U.S. EPA 1998f). This system, called the Multimedia Integrated Modeling System (MIMS), is described below.

Models-3 has a unique framework and science design that enables scientists and regulators to build their own modeling systems to suit their needs. The CMAQ system has capabilities for urban to regional-scale air quality simulation of tropospheric ozone, acid deposition, visibility, and fine particles. The Models-3 framework contains components that assist the model developer with creating, testing, and performing comparative analysis of new versions of air quality models and enables the user to execute air quality simulation models and visualize the results. The overall goal of Models-3 is to simplify and integrate the development and use of complex environmental models, beginning with air quality and deposition models (U.S. EPA 1998f).

MIMS will have capabilities to represent the transport and fate of nutrients and chemical stressors over multiple scales. It will be designed to improve the environmental management community's ability to evaluate the impact of air and water quality and watershed management practices on stream and estuarine conditions. The system will provide a computer-based problem solving environment for testing understanding of multimedia (atmosphere, land, water) environmental problems, such as the movement of chemicals through the hydrologic cycle, or the response of aquatic ecological systems to land-use change, with initial emphasis on the fish health endpoint. The design will attempt to combine the state-of-the-art in computer science, system design, and numerical analysis (*i.e.* object oriented analysis and design, parallel processing, advanced numerical libraries including analytic elements) with the latest



advancements in process level science (process chemistry, hydrology, atmospheric and ecological science). The problem solving environment will embrace the watershed/airshed approach to environmental management, and build upon the latest technologies for environmental monitoring and geographic representation.

### **B.7.7 SHEDS (Stochastic Human Exposure and Dose Simulation) Model**

The Stochastic Human Exposure and Dose Simulation (SHEDS) Model is a probabilistic, physically-based model that simulates aggregate exposure and dose for population cohorts and multimedia pollutants of interest. It is being developed by the U.S. EPA ORD's NERL. At present the model is applied to assess children's exposures to pesticides (SHEDS-Pesticides) and population exposures to PM (SHEDS-PM). The key objectives of SHEDS are: (1) to improve the risk assessment process by predicting both inter-individual variability and uncertainties associated with the upper percentiles (*e.g.*, >90<sup>th</sup> percentile) of population exposure and dose distributions; (2) to improve the risk management process by identifying critical exposure routes and pathways; and (3) to provide a framework for identifying and prioritizing measurement needs and to formulate the most appropriate hypotheses and designs for exposure studies.

SHEDS-PM estimates the population distribution of PM exposure by sampling from distributions of ambient PM concentrations and from distributions of emission strengths for indoor sources of PM, such as cigarette smoking and cooking. A steady-state mass balance equation is used to calculate PM concentrations for the home microenvironment. The physical factors data used in the equation (*e.g.*, air exchange rate, penetration rate, deposition rate) are also sampled from distributions. Non-residential microenvironmental concentrations are calculated based on penetration of outdoor PM and indoor sources. Additional model inputs include demographic data for the population being modeled and human activity pattern data from the National Human Activity Pattern Survey (NHAPS). Output from the SHEDS-PM model includes distributions of PM exposures in various microenvironments (*e.g.*, indoors at home, in vehicles, outdoors) and the relative contributions of these various microenvironments to the total exposure.

The first generation of SHEDS-PM has been applied to the population of Vancouver, Canada using spatially interpolated ambient PM<sub>10</sub> measurements (Özkaynak et al. 1999a, b). Subsequent generations will focus on modeling both PM<sub>10</sub> and PM<sub>2.5</sub> exposure and dose in a selected U.S. city.

SHEDS-Pesticides predicts children's aggregate population exposure and dose to pesticides. It simulates individuals from the user-specified population cohort by selecting daily sequential time/location/activity diaries from surveys contained in EPA's CHAD (*e.g.*, the National Human Activity Pattern Survey). For each individual, SHEDS-Pesticides constructs daily exposure and dose time profiles for the inhalation, dietary and non-dietary ingestion, and dermal contact exposure routes, then aggregates the dose profiles across routes. A single-compartment pharmacokinetic component has been incorporated into the first generation SHEDS-Pesticides model to predict real-time pollutant or metabolite concentrations in the blood compartment or eliminated urine. Exposure and dose metrics of interest (*e.g.*, peak, time-averaged, time-integrated) are extracted from the individual's profiles, and the process is

repeated thousands of times to obtain population distributions. This approach allows identification of the relative importance of routes, pathways, and model inputs. Two-stage Monte-Carlo sampling is applied to predict the range and distribution of aggregate doses within the specified population and the uncertainties associated with percentiles of interest.

SHEDS-Pesticides samples, for each individual, location-specific air, dust, soil, and surface residue levels; meal-specific food and beverage residues; exposure factors (*e.g.*, residue-to-skin transfer efficiency, saliva and washing removal efficiency, soil adherence, surface area contacted); uptake factors (*e.g.*, inhalation and dietary absorption fractions); and pharmacokinetic rate constants (*e.g.*, dermal absorption, gastrointestinal absorption, elimination) from user-specified probability distributions. For each location/activity combination in the individual's diary, SHEDS-Pesticides combines the air concentration, activity-specific inhalation rate (derived from distributions of MET energy expenditures), and inhalation absorption fraction to estimate real-time inhalation absorbed dose. For each eating or drinking event, SHEDS-Pesticides combines the mass residue ingested by the ingestion absorption fraction to obtain mass in the gastrointestinal tract, then applies a gastrointestinal absorption rate constant to estimate real-time mass in the blood compartment. If the eating event is non-dietary, the mass of residue ingested is that on the object mouthed or the skin at that instant in time. The dermal loading over time is obtained by simulating exposures from discrete dermal contact events (*i.e.*, contacts between the skin surface and different objects such as smooth surfaces, textured surfaces, mouth, turf) within each macro-activity. Probabilities of skin contacts with different surfaces for a given contact event are obtained from the contact frequency and duration information collected via videography studies. For each dermal contact event, the model combines available mass on the skin by a dermal absorption rate constant to estimate real-time dermal absorbed dose.

To help meet the requirements of the Food quality Protection Act of 1996 (FQPA), the initial focus of the SHEDS-Pesticides model has been residential exposures of children to pesticides. Model estimates for chlorpyrifos have been obtained for several application methods (*i.e.*, broadcast, crack, and crevice) and age groups (0-4 years, 5-9 years) for acute, short-term, and chronic post-application time periods, and then weighted with available pesticide use and frequency information to develop aggregate population estimates. A paper describing the initial SHEDS-Pesticides modeling framework, presenting the chlorpyrifos case study, and demonstrating that the modeled estimates compare well against available published measurement data has been submitted for publication (Zartarian et al. 1999).

While the first generation SHEDS-Pesticides model was developed with a special emphasis on characterizing critical exposure pathways and factors for residential exposures of children to pesticides, the next generation will characterize both aggregate and cumulative dose associated with human exposure (*i.e.*, for both adults and children) to a variety of environmental pollutants in addition to pesticides, including other persistent organic pollutants, metals, and air toxics. SHEDS-Pesticides will eventually be expanded to include source-to-concentration (*i.e.*, fate and transport models) and more complete exposure-to-dose models (pharmacokinetic or dosimetric models).

Each iteration of SHEDS will use the best available data to identify critical pathways of human exposure and dose and the major uncertainties in those pathways. Model inputs and

assumptions will continue to be reined as new measurement data become available (e.g., pesticide usage survey data, residue and concentration distributions in space and time, residue-to-skin transfer efficiencies, uptake data, microlevel activity data, emission source strengths, air exchange rates, penetration rates). The model will be tested against field measurement programs for refinement and subsequent evaluation.

**Table B-1  
Model Features and the Exposure Models Associated with Each Feature**

Feature	Model	Remarks
Short-term (≤ 1 h) exposure events	CPIEM	Other built-in time scales include: 24 hours, 12 hours (daytime), 12 hours (nighttime), and 8 hours.
	pNEM	Inhalation exposures can be calculated for i minute to 24 hours depending on the pollutant. Exposures are generally for 1-hour (5-minute duration for SO <sub>2</sub> ). However, activities can be as short as 1-minute in duration.
	HAPEM-PS	Annually averaged 1-hour increments.
	HAPEM	Seasonally (3-month) averaged 1-hour increments.
	AirPEX	15-minutes
	SHAPE	Exposures are generally for 1-hour. However, activities can be as short as 1-minute in duration.
	DERM	Dermal exposures are estimated over the day based on dermal contact events ranging from seconds to minutes.
	SHEDS (under development)	Inhalation exposures can be calculated for 1 minute to 12 hours, depending on the pollutant and diary selected. Dermal and non-dietary ingestion exposures can be as short as a 5-second duration. Diaries are used to determine ingestion events. Modeled dietary ingestion exposures for each eating and drinking event are assumed instantaneous, but absorption is calculated on a 30-minute time scale.
	BEAM	1 hour.
pHAP	1 hour.	
Long-term exposure events	CalTOX	Annual.
	SHEDS (under development)	Daily exposure and dose profiles could be repeated over longer durations based on multi-day activity and contact frequency information.
	HEM	Annual.
	SCREAM2	Annual.
Exposure media	CPIEM	Indoor air (multiple microenvironments).
	pNEM	Indoor air and outdoor air.
	HAPEM	Indoor air and outdoor air.
	AirPEX	Indoor air and outdoor air.

APPENDIX B  
COMPARISON/CRITIQUE OF EXPOSURE MODELS

Feature	Model	Remarks
	HEM	Indoor air and outdoor air.
	SHAPE	Indoor air and outdoor air.
	BEAM	Indoor air and outdoor air.
	pHAP	Indoor air and outdoor air.
	CONSEXPO	Indoor air, personal air, and contact with surfaces (both oral and dermal).
	CalTOX	Indoor air; outdoor air; soil; house dust; tap water; food from home gardens and locally-produced fruits, vegetables, grains, fish, meat, milk, eggs; and dairy products.
	SHEDS (under development)	Indoor air; outdoor air; soil; house dust; surface residues (indoor and lawn); hand and object residues; tap water; food and beverage residues
	MMSOILS	Indoor air; outdoor air; soil; house dust; tap water; food from home gardens and locally-produced fruits, vegetables, grains, fish, meat, milk, eggs; and dairy products.
	USES	Indoor air; outdoor air; soil; house dust; tap water; food from home gardens and locally-produced fruits, vegetables, grains, fish, meat, milk, eggs; and dairy products.
	BEADS	Indoor air, outdoor air, and tap water.
	SCREAM2	Indoor air; outdoor air; soil; tap water; food from home gardens; locally-grown produce; locally-raised animal products, including fish; and breast milk.
	DERM	Liquid, air, soil on surfaces, dust on surfaces, residues on surfaces.
	DERMAL	Contact with surfaces (dermal).
Models inhalation only	CPIEM	Designed for indoor exposures to numerous pollutants.
	pNEM	Models are pollutant-specific (e.g., ozone, carbon monoxide, sulfur dioxide). Current development is on CO-version.
	HAPEM	For criteria and modeled air toxic pollutants.
	AirPEX	Default values available for benzene, B(a)P, ozone, and PM.
	HEM	Multiple gas- and particle-phase agents from outdoor sources.
	SHAPE	Model designed for inhalation exposures to CO.
	BEAM	Model for benzene only.
	pHAP	Multiple gas- and particle-phase agents from outdoor sources. Has been tested using benzene.
Models non- inhalation routes of exposure	CONSEXPO	Inhalation, ingestion, and dermal contact of chemicals from consumer products. Indoor sources only.
	CalTOX	Inhalation, ingestion, and dermal contact of organic chemicals and some metals.

Feature	Model	Remarks
	MMSOILS	Inhalation, ingestion, and dermal contact of organic chemicals and metal species from hazardous waste sites.
	USES	Inhalation, ingestion, and dermal contact of organic chemicals and some metal species.
	BEADS	Inhalation, ingestion, and dermal contact to benzene only.
	SHEDS (under development)	Inhalation, dietary and non-dietary ingestion, dermal contact for multimedia pollutants.
	SCREAM2	Inhalation, ingestion, and dermal contact to numerous modeled air toxics.
	DERM	Dermal exposure to pesticides.
	DERMAL	Calculates screening-level estimates of annual individual dermal potential dose rates to components of 16 consumer product categories.
Explicit treatment of variability	CPIEM	Several parameters are sampled from distributions, including the concentration data. A variety of formats for describing the concentration distribution is allowed by the model, including provision of a data file containing the concentration values. A random number seed can be selected by the user or the model can use the system's clock to determine the seed.
	CalTOX	Variability in exposure factors and in landscape factors are explicitly represented by probability distributions.
	pNEM	Environmental, demographic (e.g., activity pattern and ventilation data), and mass balance inputs are characterized by distributions.
	HAPEM	Most input parameters are characterized by distributions.
	AirPEX	Exposure distributions for the population are characterized by the normalized cumulative frequency distribution.
	SHEDS (under development)	Model samples from user-specified input probability distributions for residues and exposure factors. Monte Carlo sampling allows analyses of input and output variability.
	HEM	
	SHAPE	Model generates a hypothetical population, sampling each descriptive parameter of an individual (e.g., age, gender, body mass) from a user-specified distribution function.
	DERM	Variability quantified by applying bootstrap method to dermal exposure estimates for individuals
	BEAM	
pHAP		
Explicit treatment of uncertainty	CPIEM	User specifies all inputs. Then, the model is run several times with all inputs kept constant except the random number seed. Variability for each output parameter across repeated model runs is characterized through a measure such as the coefficient of variation.
	SHEDS (under development)	Two-stage Monte Carlo sampling allows for explicit characterization of both uncertainty and variability. Model samples from user-specified input probability distributions and their associated uncertainty distributions.

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Feature	Model	Remarks
	CalTOX	All chemical-specific property data are represented by probability distributions.
	HEM	
	pNEM	The model is generally run 10 times using a Monte Carlo simulation approach for each regulatory scenario analyzed.
Mass balance approach for indoor concentrations	pNEM	Mass balance model accounts for outdoor concentration, air exchange rate, building volume, building penetration rate, deposition rate, and indoor emission rates and usage patterns for some indoor sources.
	SHEDS (under development)	Mass balance model accounts for outdoor concentration, air exchange rate, building volume, and indoor emission rates, and usage patterns
	CPIEM	Uses a mass balance equation, based on the principle of conservation of mass, to estimate concentration distributions for specific types of indoor environments such as residences, offices, and schools.
	SCREAM2	Optional use of mass balance model that accounts for outdoor concentration, air exchange rate, and indoor emission rate.
Regression or I/O ratios for indoor concentrations	HAPEM	Uses microenvironmental factors.
	AirPEX	Parameters relating concentration measured at monitoring site to four macroenvironments (rural, urban, city, and transit) which are in turn related to three indoor microenvironments (home, vehicle, elsewhere) by I/O ratios. Also, three additive terms account for indoor sources in the same three microenvironments.
	SHEDS (under development)	For certain microenvironments, empirical mass balance models in the form of regressions are used.
	HEM	Uses I/O ratios for microenvironments.
	SHAPE	Exposure concentrations are obtained by applying a superposition principle to contributions from the ambient and different microenvironments.
	BEAM	Same as SHAPE.
	SCREAM2	Optional use of I/O ratios for microenvironments.
Includes ventilation rate	pNEM	Ventilation rate ( $V_E$ ) value estimated based on estimated body mass, gender, and other information from energy expenditure literature for each exposure event.
	SHEDS (under development)	Ventilation rate ( $V_E$ ) value estimated based on estimated body mass, gender, and other information from energy expenditure literature for each exposure-event.
	CPIEM	Breathing rates supplied by the model are specific to three age/gender groups (adult males, adult females, and children under age 12) and four activity levels (resting, light, moderate, and heavy).
	SCREAM2	For each hour, the activity pattern of each subgroup is assigned to one of three activity levels (low, moderate, or heavy). The user may designate enhancement of inhaled dosage of the pollutant for the various activity levels with scaling factors.

Feature	Model	Remarks
	AirPEX	Ventilation rate is a function of a person's body mass and level of activity. Uses five levels of activity, ranging from "sleeping" to "heavy exercise."
Can estimate dose	pNEM	The CHAD database provided an activity indicator for each exposure event. Each activity type was assigned a distribution of values for the metabolic equivalent of work (MET). The MET is dimensionless, given by the ratio of the rate of energy expenditure during a particular activity (expressed in kcal/min) and a person's typical resting metabolic rate (also expressed in kcal/min).
	SHEDS (under development)	<p>Inhalation: For each modeled individual's sequential location/activity combination in daily diaries, model combines air concentration, activity-specific inhalation rate (derived via METs), and absorption fraction to estimate inhalation absorbed dose. Next generation will include more PK models to calculate dose.</p> <p>Ingestion: For each eating and drinking event, model combines mass residue ingested and absorption fraction to obtain mass in gastrointestinal (GI) tract, then applies a GI absorption rate constant to estimate mass in blood compartment.</p> <p>Dermal: For each dermal contact event, model combines available mass on skin and dermal absorption rate constant to estimate dermal absorbed dose.</p> <p>To obtain aggregate absorbed and eliminated dose, model sums time profiles across all routes.</p>
	CPIEM	Breathing rates and activity levels are used by the model to calculate the potential inhaled dose received by each individual in each microenvironment.
	SCREAM2	Average daily doses of a pollutant to the population are estimated from concentrations in each medium on the basis of age-specific ingestion rates and body weights and local population age profiles.
Includes indoor sources	CPIEM	The model samples values from user-specified distributions for emission rates for indoor sources.
	SHEDS (under development)	The model samples values from user-specified distributions for indoor source concentrations.
	pNEM	Includes CO emitted by gas stove operation and passive smoking.
	HAPEM	Includes an additive term for indoor source contributions (user specified).
	SCREAM2	Includes an additive term for indoor source contributions (user specified).
Includes smoking as a source	pNEM	Contribution from smoking is modeled.
	SHEDS (under development)	Contribution from smoking is modeled.

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Feature	Model	Remarks
Calculates exposures of commuters	pNEM	<p>The populations of the commuting cohorts (assumed to include all working cohorts) were determined by the expression:</p> $Com(d,h,f,w) = Pop(d,h,f) \times Com(h,w)/Work(h)$ <p>where <math>Com(d,h,f,w)</math> is the number of persons in the commuting cohort associated with demographic group <math>d</math>, home district <math>h</math>, cooking fuel <math>f</math>, and work district <math>w</math>; <math>Pop(d,h,f)</math> values provided an estimate of the population of each non-commuting cohort residing within home district <math>h</math>; <math>Com(h,w)</math> is the number of workers in all demographic groups that commute from home district <math>h</math> to work district <math>w</math>; and <math>Work(h)</math> is the total number of workers in home district <math>h</math>. Estimates of <math>Work(h)</math> were developed from census data specific to each district. The in-vehicle concentration is calculated using a mass balance model.</p>
	SHEDS (under development)	Exposures of commuters are modeled. A similar approach to pNEM is being considered.
	HAPEM	Commuting patterns of workers between exposure districts are modeled. The "travel time to work" data from the 1990 census are used to develop the commuting patterns. A program uses these data to build an array of probabilities of the movement of working commuters for each census tract-to-tract combination.
	SCREAM2	Commuting patterns of workers between exposure districts are modeled. The patterns were estimated from travel survey data collected by the Southern California Association of Governments in a manner similar to pNEM/CO.
Includes dispersion algorithms to calculate outdoor air concentrations	SCREAM2	Uses a Gaussian model formulation and climatological data to estimate long-term average concentrations as a function of radial distance and direction from a source for a set of receptors laid out in a radial grid pattern.
	SHEDS (under development)	Uses Bayesian spatial and temporal interpolation methods to estimate outdoor air concentrations in different census tracts.
	HEM	Uses the Industrial Source Complex Long-Term (ISCLT2) Model for estimating dispersion.



**Table B-2<sup>3</sup>**  
**Strengths and Weaknesses of Different Models and Modeling Systems**

Model	Strengths	Weaknesses
<i>pNEM/CO</i> (inhalation)	<ol style="list-style-type: none"> <li>1. Most input parameters are probabilistic.</li> <li>2. Can calculate delivered dose as a function of the pollutant concentration and ventilation rate values assigned to the event and the demographic characteristics of the cohort.</li> <li>3. Mass balance model for indoor microenvironments.</li> <li>4. Calculates the exposures to the portion of the population that commute to work.</li> <li>5. Estimates exposures to those exposed to passive smoking.</li> </ol>	<ol style="list-style-type: none"> <li>1. Single exposure route (inhalation) only.</li> <li>2. Each version of pNEM is specific to a single pollutant.</li> </ol>
<i>CalTOX</i> (multimedia)	<ol style="list-style-type: none"> <li>1. Multipathway and multimedia.</li> <li>2. All input parameter values are distributions.</li> <li>3. Explicit treatment of pollutant concentrations in various environmental media.</li> <li>4. Mass balance model.</li> </ol>	<ol style="list-style-type: none"> <li>1. Does not allow spatial tracking of a pollutant.</li> <li>2. Limited number of chemical species for which the model is applicable.</li> <li>3. Limited in the extent of the environmental settings for which it can be applied.</li> </ol>
<i>HAPEM4</i> (inhalation)	<ol style="list-style-type: none"> <li>1. Most input parameters are probabilistic.</li> <li>2. Model can use both measured air quality data and modeled data from the ASPEN model or from air dispersion models.</li> <li>3. Can model population exposures down to the census tract-level.</li> <li>4. User can easily specify different demographic groups (providing they have data for the groups).</li> <li>5. User can specify a "lag" factor for calculating indoor concentrations from pollutants penetrating from outside.</li> </ol>	<ol style="list-style-type: none"> <li>1. Single exposure route (inhalation) only.</li> <li>2. The sequence of exposure events for activities is not preserved.</li> <li>3. Does not provide any estimate of ventilation rate or delivered dose.</li> <li>4. Currently, does not account for exposures to passive smoking.</li> </ol>

<sup>3</sup> This table only includes models and modeling systems that are currently publicly available. OAQPS will continue to monitor and incorporate into TRIM.Expo, where appropriate, features, algorithms, and/or models that are under development. This includes ongoing work by the U.S. EPA on models and modeling systems, such as MENTOR and SHEDS.

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Model	Strengths	Weaknesses
<i>IEM</i> (multimedia)	<ol style="list-style-type: none"> <li>1. Establishes procedures for estimating the indirect human exposures and health risks that can result from the transfer of air pollutants to soil, vegetation, and water bodies.</li> <li>2. Addresses exposures via multiple routes (inhalation, food, water, and soil ingestion, and dermal contact).</li> <li>3. Has undergone extensive scientific review.</li> <li>4. Has been widely used in EPA screening-level risk assessments.</li> <li>5. Relatively simple spreadsheet model.</li> </ol>	<ol style="list-style-type: none"> <li>1. Based on annual average air concentrations and deposition rates.</li> <li>2. Structured as a one-way process through a series of linked models. Not a truly coupled multimedia model. Does not have the ability to model feedback loops between media or secondary emissions.</li> <li>3. Not designed to readily address spatial variability in exposures.</li> <li>4. Not designed for probabilistic variability and uncertainty analysis.</li> <li>5. Not suitable for estimating population exposures.</li> <li>6. Does not provide a detailed time series of media concentrations or the resulting exposures.</li> <li>7. Can only be applied to chemicals that are emitted into the air.</li> </ol>
<i>ISMCM</i> (multimedia)	<ol style="list-style-type: none"> <li>1. Considers all media, biological and non-biological, in one integrated system.</li> <li>2. Includes both spatial and compartmental modules to account for complex transport of pollutants through the ecosystem.</li> <li>3. Mass conserving model.</li> <li>4. Includes estimation of intermedia transfer factors.</li> </ol>	<ol style="list-style-type: none"> <li>1. Links and spatial compartments are predetermined.</li> <li>2. Not structured to incorporate uncertainty/variability directly into the model operation.</li> </ol>
<i>SCREAM2</i> (multimedia)	<ol style="list-style-type: none"> <li>1. Can calculate indoor pollutant concentrations using the Indoor Air Quality Model (IAQM) or by using indoor/outdoor ratios.</li> <li>2. Multipathway: inhalation, ingestion, and dermal.</li> <li>3. Results reported in terms of both concentrations/dosages and risks.</li> <li>4. Includes air dispersion algorithms to calculate air concentrations from emissions.</li> </ol>	<ol style="list-style-type: none"> <li>1. Deterministic.</li> <li>2. Results reported for annual average exposures only.</li> </ol>

**Table B-3  
Model Features for pNEM/CO**

Attribute	Component	Remarks
General	Model name	pNEM/CO
	Pollutants of concern	Carbon monoxide
	Reference	Johnson et al. 1999. for U.S. EPA, OAQPS. Estimation of Carbon Monoxide Exposures and Associated Carboxyhemoglobin Levels in Denver Residents Using pNEM/CO (Version 2.0).
	Model status	Operates on either mainframe or PC. Further enhancements are currently ongoing.
	Contact/Affiliation	Harvey Richmond (U.S. EPA, OAQPS) (919) 541-5271
	Stochastic?	Yes – most variables chosen stochastically.
	Variability?	Yes – year-long exposure-event sequences (EES) use data from multiple subjects to better represent the variability of exposure that is expected to occur among the persons included in the cohort.
	Uncertainty?	Yes
Modeled area, study population, and modeling period	Study areas where model has been applied	Most recently to Denver. Application to Los Angeles is planned.
	Spatial designation of study area	50 km radius surrounding the city center of Denver.
	Sub-area designations	Six exposure districts, each 10 km in radius, surrounding fixed site CO monitors.
	Exposure duration for modeling	Typically one year.
	General population of interest	Typically defined as people with specific demographic or health status characteristics (e.g., adults with ischemic heart disease).
	Special subgroups or designations	Demographic groups (DG): 1. Children 0 to 17 years; 2. Males, 18 to 44, working; 3. Males, 18 to 44, non-working; 4. Males 45 to 64, working; 5. Males 45 to 64, non-working; 6. Males 65+; 7. Females, 18 to 44, working; 8. Females, 18 to 44, non-working; 9. Females 45 to 64, working; 10. Females 45 to 64, non-working; 11. Females 65+
	Special attributes for subgroups	Each DG further subdivided into cohorts identified as a distinct combination of (1) home district, (2) demographic group, (3) work district (if applicable), (4) residential cooking fuel, and (5) replicate number.

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Attribute	Component	Remarks
	Source of demographic data for study population	1990 Bureau of the Census.
Exposure events	Environmental media	Ambient air.
	Exposure media	Indoor air, outdoor air.
	Pathways	Ambient air and indoor air to personal air.
	Routes	Inhalation.
	Time resolution of exposure events	<u>Inhalation:</u> One minute.  <u>Ingestion:</u> N/A
	Integration of exposures across multiple media	N/A.
	Method for determining pollutant contact rate	<u>Inhalation:</u> Ventilation rate ( $V_E$ ) value estimated for each exposure-event. $V_E$ expressed as liters of air respired per minute (liters $\text{min}^{-1}$ ).  <u>Ingestion:</u> N/A.
	Activity pattern methodology	In typical pNEM applications, the EESs are determined by assembling activity diary records relating to individual 24-hour periods into a year-long series of records. Each exposure event within an EES was defined by (1) district, (2) CHAD location descriptor, (3) microenvironment, (4) CHAD activity descriptor, and (5) passive smoking status.
	Source of activity pattern data	Comprehensive Human Activity Database (CHAD).
	Time resolution of activity patterns	One minute.
	Microenvironments (Inhalation)	1. Indoors – residence 2 - 6. Indoors – nonresidence A - E 7. Indoors – residential garage 8. Outdoors – near roadway 9. Outdoors – other locations 10. Vehicle – automobile 11. Vehicle – other 12. Outdoors – public parking or fueling.
	Exposure locations (Ingestion)	N/A.
Model calculates exposure of commuters	Yes – the number of commuters in each working cohort is calculated based on census data. In vehicle concentrations are estimated using a mass balance model (see Concentrations and Sources).	
Concentrations and sources	Outdoor concentration determination method	Hourly-average CO concentrations for outdoor microenvironments based on data from fixed-site monitor and statistical relationship between fixed-site data and personal monitoring for outdoor microenvironments from a previous personal exposure study in Denver. Exposure districts are defined by monitor locations.

Attribute	Component	Remarks
	Indoor concentration determination method	Mass balance model used to estimate CO concentrations when a cohort is assigned to an indoor or motor vehicle microenvironment.
	In-vehicle concentration estimation	Mass balance model which accounts for outdoor concentration, air exchange rate, and passive smoking status of occupants.
	Passive smoking	CO contribution from indoor and in-vehicle passive smoking is modeled using a mass balance model.
	Other indoor sources	Gas stoves.
Extrapolation to study population	Method of allocating estimated exposures to study population	Entire population is simulated through the use of cohorts and census data relating cohorts to study area population.

**Table B-4**  
**Model Features for CalTOX**

Attribute	Component	Remarks
General	Model name	CalTOX (California Total Exposure Model for Hazardous Waste Sites).
	Pollutants of concern	Potential toxic chemicals placed in landfills and in controlled and formerly uncontrolled hazardous waste sites. Chemicals on the Toxic Release Inventory (TRI) list emitted to air or water.
	References	McKone, T.E. 1993. CalTOX, A Multimedia Total-Exposure Model for Hazardous Wastes Sites. Lawrence Livermore National Laboratory, Livermore, CA, UCRL-CR-111456. Part I: Executive Summary; Part II: The Dynamic Multimedia Transport and Transformation Model; Part III: The Multiple-Pathway Exposure Model.
	Model status	Two versions of CalTOX are currently available from Cal-EPA: the original version developed for soil clean-up goals and a second version used for waste classification. A third version has been developed for use with the Environmental Defense Fund (EDF) Scorecard project.
	Contact/Affiliation	Tom McKone, Lawrence Berkeley National Laboratory (510-642-8771). Cal-EPA version: Ned Butler (916-323-3751).
	Stochastic?	Yes — all model inputs are represented by a mean value, coefficient of variability, and default distribution.
	Variability?	Yes — variability in exposure factors and in landscape factors are explicitly represented by probability distributions.
	Uncertainty?	Yes — all chemical-specific property data are represented by probability distributions.
Modeled area, study population, and modeling period	Study areas where model has been applied	For setting soil clean-up goals and for assessing residual risk at municipal landfills, CalTOX was used to represent the variability among all California land areas. For the EDF Scorecard project, CalTOX was used to represent the fate of air and water emissions in all 48 conterminous U.S. states.
	Spatial designation of study area	The designated study area is the environment impacted by either a waste site, air emissions, or water releases. 5,000 GIS land units were used to establish variability among California locations. For the EDF version, county-level climate and land data are used to establish state-level variability.
	Sub-area designations	The exposure location can be modeled with a residential, agricultural, commercial, or industrial scenario.
	Exposure duration for modeling	Exposure duration is variable depending on how long the exposure individual remains at the exposure location. Values as long as 70 years can be used.
	General population of interest	Populations in the landscape impacted by a waste site, air release, or water release.

Attribute	Component	Remarks
	Special subgroups or designations	Residential populations: Children (0 to 12 years) Adults (12 to 70 years). Agricultural populations. Those working or shopping at a commercial site. Those working at an industrial site.
	Special attributes for subgroups	Those with home gardens have been singled out for special attention.
	Source of demographic data for study population	EPA Exposure Factors Handbook.
Exposure events	Environmental media	Ambient air, surface soil, root zone soil, surface water and ground water.
	Exposure media	Indoor air; outdoor air; soil; house dust; tap water; food from home gardens and locally-produced fruits, vegetables, grains, fish, meat, milk, eggs; and dairy products.
	Pathways	Twenty-three pathways linking ambient media to exposure media.
	Routes	Inhalation, ingestion, dermal contact.
	Time resolution of exposure events	<u>Inhalation</u> : 1 day resolution to build the exposure scenario that is repeated over longer duration based on exposure frequency. <u>Ingestion</u> : 1 year. <u>Dermal contact</u> : 1 day resolution to build the exposure scenario that is repeated over a longer duration based on exposure frequency data.
	Integration of exposures across multiple media	Exposures are aggregated across all media and pathways to construct a total intake by route--inhalation, ingestion, and dermal contact.
	Method for determining pollutant contact rate	<u>Inhalation</u> : Activity adjusted breathing rate per unit body weight. <u>Ingestion</u> : Food consumption per unit body weight for each major food category is adjusted by fraction of food consumed within the contaminated landscape. <u>Dermal contact</u> : Activity data are used to establish long-term average rate and duration of contact with tap water and soil.
	Activity pattern methodology	For inhalation, the day is divided into the amount in each microenvironment and a breathing rate is assigned to each microenvironment. For ingestion, consumption of each major food category is divided into local and non-local sources. For dermal contact, the number and duration of water or soil contact events in a day are used.
	Source of activity pattern data	EPA Exposure Factors Handbook.

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Attribute	Component	Remarks
	Time resolution of activity patterns	1 to 24 hours for inhalation. Annual consumption patterns for ingestion. Minutes to hours for dermal contact.
	Microenvironments (Inhalation)	Outdoors at home, Outdoors away from home, Indoors at home, Indoors in the bathroom.
	Exposure locations (Ingestion)	Residential environment.
	Model calculates exposure of commuters	No
Concentrations and sources	Outdoor concentration determination method	Multimedia mass balance using a dynamic regional fugacity model. Sources to air, soil, and water are allowed.
	Indoor concentration determination method	Based on a simple penetration model for outdoor air, a dust tracking model for soil pollutants, a transfer model for soil gas drawn into home, and a transfer model from water to indoor air.
	In-vehicle concentration estimation	Not explicitly represented; assumed to be equal to outdoor concentration.
	Passive smoking	Not included.
	Other indoor sources	Stripping of chemicals. Household water uses. Tracking of soil to house. Transfer of volatile chemicals from soil gas below homes.
Extrapolation to study population	Method of allocating estimated exposures to study population	Entire population is simulated through the use of probability distributions to represent variability and uncertainty in source-to-dose relationships.



**Table B-5  
Model Features for HAPEM4**

Attribute	Component	Remarks
General	Model name	HAPEM4 (Hazardous Air Pollutant Exposure Model)
	Pollutants of concern	Criteria pollutants for which measured data, or HAPs for which modeled data can be obtained. Most recent application was for benzene.
	Reference	
	Model status	Operates on UNIX workstations.
	Contact/Affiliation	Ted Palma (U.S. EPA, OAQPS) (919) 541-5470
	Stochastic?	Yes – most variables chosen stochastically.
	Variability?	Yes – distributions available for many input variables.
	Uncertainty?	Not explicitly handled by the current model.
Modeled area, study population, and modeling period	Study areas where model has been applied	Most recently Houston and Phoenix. *Note – HAPEM4 may also be run in a <i>measured data mode</i> using data from fixed-site monitors. In this mode, the spatial designation and study areas are similar to those in pNEM.
	Spatial designation of study area	Houston and Phoenix Metropolitan Statistical Areas (MSAs). *In measured data mode: study areas are typically a circle with a predetermined radius surrounding the city center.
	Sub-area designations	Census tracts. *In measured data mode: up to 18 exposure districts surrounding fixed-site monitors can be chosen for each MSA.
	Exposure duration for modeling	Typically one year (results are currently aggregated and reported as 3 month “seasons”).
	General population of interest	Typically defined as all persons described by the demographic groups for each sub-area designation.

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Attribute	Component	Remarks
	Special subgroups or designations	Demographic groups (DG) in latest version (other groups for which census data are available may be input by the user): <ol style="list-style-type: none"> <li>1. Caucasians;</li> <li>2. African-Americans;</li> <li>3. All people not in DG 1 or 2;</li> <li>4. Children 0 to 5 years;</li> <li>5. Children 6 to 11 years;</li> <li>6. Children 12 to 17 years;</li> <li>7. Males 18 to 64;</li> <li>8. Females 18 to 64;</li> <li>9. Males 65+;</li> <li>10. Females 65+;</li> <li>11. People with gas stoves at home;</li> <li>12. People without gas stoves at home;</li> <li>13. People with attached garages at home;</li> <li>14. People without attached garages at home;</li> <li>15. People age 18 and older who work and were outdoors for at least 240 minutes (4 hrs) on the day recorded;</li> <li>16. All persons.</li> </ol>
	Special attributes for subgroups	No further sub-designations of population for this application. However, in future development, cohorts may be identified for commuting by specifying a home district and work district. Other cohort attributes may also be specified in future versions.
	Source of demographic data for study population	1990 Bureau of the Census.
Exposure events	Environmental media	Ambient air.
	Exposure media	Indoor air and outdoor air.
	Pathways	Ambient air and indoor air to personal air.
	Routes	Inhalation.
	Time resolution of exposure events	<u>Inhalation:</u> 1 to 60 minutes; obtained from CHAD.  <u>Ingestion:</u> N/A.
	Integration of exposures across multiple media	N/A.
	Method for determining pollutant contact rate	<u>Inhalation:</u> N/A.  <u>Ingestion:</u> N/A.

Attribute	Component	Remarks
	Activity pattern methodology	<p>Information on the time spent in various microenvironments (<math>\mu</math>e) for each individual are used.</p> <p>* Note, this is not an activity sequence, rather it is the total time spent in each <math>\mu</math>e during each 1-hour block of time throughout the day.</p> <p>A daily record (comprised of 24 separate hours) is chosen using the Monte Carlo technique. The record chosen is matched to the day being modeled by using the maximum outdoor temperature for each hour. The number of minutes spent in a particular <math>\mu</math>e for each individual selected and for each hour of the day are calculated. The exposures reported for each DG are the averages of all individuals sampled from each group.</p>
	Source of activity pattern data	Comprehensive Human Activity Database (CHAD).
	Time resolution of activity patterns	1 to 60 minutes.
	Microenvironments (Inhalation)	<ol style="list-style-type: none"> <li>1. In vehicle – car</li> <li>2. In vehicle – bus</li> <li>3. In vehicle – truck</li> <li>4. In vehicle – other</li> <li>5. Indoors – public garage</li> <li>6. Outdoors – parking lot/garage</li> <li>7. Outdoors – near a road</li> <li>8. Outdoors – motorcycle</li> <li>9. Indoors – service station</li> <li>10. Outdoors – service station</li> <li>11. Indoors – residential garage</li> <li>12. Indoors – other repair shop</li> <li>13. Indoors – residence, no inside sources of CO</li> <li>14. Indoors – residence, gas stove present</li> <li>15. Indoors – residence with attached garage</li> <li>16. Indoors – residence with stove and attached garage</li> <li>17. Indoors – office</li> <li>18. Indoors – store</li> <li>19. Indoors – restaurant</li> <li>20. Indoors – manufacturing facility</li> <li>21. Indoors – school</li> <li>22. Indoors – church</li> <li>23. Indoors – shopping mall</li> <li>24. Indoors – auditorium</li> <li>25. Indoors – health care facility</li> <li>26. Indoors – other public building</li> <li>27. Indoors – other location</li> <li>28. Indoors – not specified</li> <li>29. Outdoors – construction site</li> <li>30. Outdoors – residential grounds</li> <li>31. Outdoors – school grounds</li> <li>32. Outdoors – sports arena</li> <li>33. Outdoors – park/golf course</li> <li>34. Outdoors – other location</li> <li>35. Outdoors – not specified</li> <li>36. In vehicle – train/subway</li> <li>37. In vehicle – airplane.</li> </ol>
	Exposure locations (Ingestion)	N/A.

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Attribute	Component	Remarks
	Model calculates exposure of commuters	Yes – commuting patterns of workers between exposure districts are modeled. The “travel time to work” data from the 1990 census are used to develop the commuting patterns. A program uses this to build an array of probabilities of the movement of working commuters for each census tract-to-tract combination.
Concentrations and sources	Outdoor concentration determination method	<i>Modeled air quality mode:</i> The model is currently configured to read output at the census tract-level from the ASPEN (Assessment System for Population Exposure Nationwide) model. <i>Measured data mode:</i> Hourly-average CO concentrations taken from fixed-site monitors. Exposure districts defined by monitor locations.
	Indoor concentration determination method	Uses microenvironmental factors. These factors are obtained from field studies through a linear regression of microenvironmental concentrations against fixed-site monitoring concentrations.
	In-vehicle concentration estimation	Microenvironmental factor (same as indoor concentration determination method above).
	Passive smoking	N/A.
	Other indoor sources	Gas stoves and residences with attached garages through the use of additive factors (user supplied).
Extrapolation to study population	Method of allocating estimated exposures to study population	Entire population is simulated through the use of cohorts and census data relating cohorts to study area population.

**Table B-6  
Model Features for SCREAM2**

Attribute	Component	Remarks
General	Model name	SCREAM2 (South Coast Risk and Exposure Model, Version 2.0).
	Pollutants of concern	HAPs for which emissions data can be obtained.
	Reference	Rosenbaum, A.S. User's Guide for an Enhanced Version of the South Coast Air Quality Management District's Air Toxics Risk and Exposure Assessment Model (SCREAM2 – PC version).
	Model status	Operates on UNIX workstations and PCs.
	Contact/Affiliation	Unix: Henry Hogo, South Coast Air Quality Management District, (909) 396-3100. PC: Arlene Rosenbaum, ICF Consulting Group, (415) 507-7192.
	Stochastic?	No.
	Variability?	No.
	Uncertainty?	No.
Modeled area, study population, and modeling period	Study areas where model has been applied	California's South Coast Air Basin.
	Spatial designation of study area	All block groups in the South Coast Air Basin as defined by the Bureau of the Census.
	Sub-area designations	Block group centroids.
	Exposure duration for modeling	One year.
	General population of interest	Typically defined as all persons described by the demographic groups for each sub-area designation.
	Special subgroups or designations	Default demographic groups (other groups for which census data are available may be input by the user): <ol style="list-style-type: none"> <li>1. Students 18 and over;</li> <li>2. Managers and professionals;</li> <li>3. Sales workers;</li> <li>4. Clerical and kindred workers;</li> <li>5. Craftsmen and kindred workers;</li> <li>6. Farmers;</li> <li>7. Operatives and laborers;</li> <li>8. Service, military, and private household workers;</li> <li>9. Housepersons;</li> <li>10. Unemployed and retired persons;</li> <li>11. Children under 5;</li> <li>12. Children 5 to 17.</li> </ol>
	Special attributes for subgroups	Each demographic group is further sub-divided into cohorts identified as a distinct combination of (1) home district, (2) demographic group, and (3) work district (if applicable).

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COMPARISON/CRITIQUE OF EXPOSURE MODELS

Attribute	Component	Remarks
	Source of demographic data for study population	1990 Bureau of the Census and Southern California Association of Governments (commuting).
Exposure events	Environmental media	Ambient air, soil, surface water, food crops.
	Exposure media	Indoor air, outdoor air, soil ingested or contacted, drinking water, food ingested, and breast milk.
	Pathways	Ambient air; indoor air to personal air; soil to ingested soil, contacted soil; soil to root crops and leafy crops to ingested food; soil and surface water to animal food sources to ingested food; ambient air and soil to surface water to drinking water; ingested food and drinking water to ingested breast milk.
	Routes	Inhalation, ingestion, dermal contact.
	Time resolution of exposure events	<u>Inhalation</u> : 1 hour. <u>Ingestion</u> : daily.
	Integration of exposures across multiple media	Yes.
	Method for determining pollutant contact rate	<u>Inhalation</u> : N/A. <u>Ingestion</u> : N/A.
	Activity pattern methodology	Information on the fraction of time spent in various microenvironments by each demographic group for each of 24 hours is used.
	Source of activity pattern data	Roddin, Ellis, and Siddiqee (1979) "Background Data for Human Activity Patterns, Vols. I and II." SRI International.
	Time resolution of activity patterns	1 hour.
	Microenvironments (Inhalation)	1. Indoors – residence 2a. Indoors – office 2b. Indoors – school 3. In vehicle 4. Outdoors – near a road 5. Outdoors – other location.
	Exposure locations (Ingestion)	Home
	Model calculates exposure of commuters	Yes – commuting patterns of workers between exposure districts are modeled. Commuting data provided by the Southern California Association of Governments.
Concentrations and sources	Outdoor concentration determination method	Estimated from data on emission sources with the air dispersion module.
	Indoor concentration determination method	Alternative 1: the Indoor Air Quality Model (IAQM), a mass balance model using outdoor concentration, air exchange rates, filtration rates, and mixing ratios. Alternative 2: indoor/outdoor concentration ratios obtained from field studies.
	In-vehicle concentration estimation	Same as for indoor concentration determination method.
	Passive smoking	N/A.
	Other indoor sources	Additive factors (user supplied).

Attribute	Component	Remarks
Extrapolation to study population	Method of allocating estimated exposures to study population	Entire population is simulated through the use of cohorts and census data relating cohorts to study area population.

**Table B-7**  
**Model Features for CPIEM**

Attribute	Component	Remarks
General	Model name	CPIEM (California Population Indoor Exposure Model)
	Pollutants of concern	Benzene, benzo[a]pyrene, CO, chloroform, formaldehyde, NO <sub>2</sub> , PM <sub>10</sub> , perchloroethylene, trichloroethylene, and PAHs. User has the ability to input data for other chemicals.
	Reference	California Air Resources Board. 1998. Development of a model for assessing indoor exposure to air pollutants. Sacramento, CA. Report No. A933-157. January 1998.
	Model status	Operates on PCs.
	Contact/Affiliation	Susan Lum (California Air Resources Board) (916) 323-5043
	Stochastic?	Yes.
	Variability?	Yes.
	Uncertainty?	The model needs to be run several times with all inputs the same except the random number seed. Variance in each output parameter across the repeated model runs is then used to characterize the uncertainty through a measure such as the coefficient of variation.
Modeled area, study population, and modeling period	Study areas where model has been applied	Most recently applied to the South Coast region (encompasses Los Angeles and surrounding areas).
	Spatial designation of study area	South Coast region, San Francisco Bay area, or the remainder of the State of California.
	Sub-area designations	County.
	Exposure duration for modeling	Varies (user-defined).
	General population of interest	California population.
	Special subgroups or designations	Certain identified subgroups of the population such as individuals who may be sensitive to indoor pollutants.
	Special attributes for subgroups	For purposes of calculating potential dose, the population was further segregated into the following groups: adult males, adult females, and children (age 12 and younger).
	Source of demographic data for study population	
Exposure events	Environmental media	Indoor air and outdoor air.
	Exposure media	Indoor air and outdoor air.
	Pathways	Ambient air and indoor air to personal air.
	Routes	Inhalation



Attribute	Component	Remarks
	Time resolution of exposure events	<p><u>Inhalation</u>: 1-hour periods; but these may be aggregated into an 8-hour exposure event. Also, a 12- or 24-hour exposure event may be specified (the basis for these are a single activity per individual).</p> <p><u>Ingestion</u>: N/A.</p>
	Integration of exposures across multiple media	N/A.
	Method for determining pollutant contact rate	<p><u>Inhalation</u>: Breathing rates are supplied by the model for three age/sex groups (adult males, adult females, and children under age 12) and four activity levels (resting, light, moderate, heavy). Using information sampled on the quantity of time spent in an environment and the concentration in each environment, combined with the breathing rates, the model calculates the potential inhaled dose received by each individual in each environment.</p> <p><u>Ingestion</u>: N/A.</p>
	Activity pattern methodology	<p>Location codes were grouped into nine types of environments. Then, the time spent was summed across locations within each environment type. This was done separately for each individual for a 24-hour period, 12-hour daytime and nighttime periods, 24 sequential 1-hour periods, and 24 running 8-hour periods. Within each of the nine environment types, each individual's time was further disaggregated according to four activity levels (resting, light, moderate, heavy). In addition, demographic information (e.g., age, gender, location of residence, month and day of week when the activity was recorded, work status, income) on each person was matched to their location/activity information. An index number was assigned sequentially to each record of each file in order to enable linking the information.</p>
	Source of activity pattern data	<p>Two ARB-sponsored studies: The first for a target population of adults (18 years and older) and adolescents (12 to 17 years), provided 1,762 profiles; the second, for a target population of children (aged 11 years and younger), provided 1,200 profiles.</p>
	Time resolution of activity patterns	One minute.
	Microenvironments (Inhalation)	<p>Environment types: residences (numerous microenvironments); offices (office, bank, or post office); industrial plants; school; travel in enclosed vehicles (several microenvironments); stores and other public buildings (several microenvironments); restaurants and lounges; other indoor locations (several microenvironments); outdoors (several microenvironments).</p>
	Exposure locations (Ingestion)	N/A.
	Model calculates exposure of commuters	Distributional data on concentrations for travel in enclosed vehicles were taken from studies identified in the literature.

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COMPARISON/CRITIQUE OF EXPOSURE MODELS

Attribute	Component	Remarks
Concentrations and sources	Outdoor concentration determination method	Two options are provided for inputting outdoor concentrations: daily-average values and hourly-average values. Sources of data identified for input (for formaldehyde, several VOCs, B(a)P, PM <sub>10</sub> , NO <sub>2</sub> , and CO) include state/local ambient air monitoring networks and some indoor air monitoring studies where outdoor concentrations were measured in conjunction with indoor measurements.
	Indoor concentration determination method	Mass balance model. Each source is associated with both a pollutant (a source may be associated with more than one pollutant) and a source category ( long-term, episodic, or frequent). For each source category, different input parameters are required by the model which are sampled from distributions. The model calculates the initial indoor concentration and the hourly emission rates. These contributions are then used by the mass balance routine to calculate the indoor concentrations.
	In-vehicle concentration estimation	Distributional data on concentrations for travel in enclosed vehicles were taken from studies identified in the literature.
	Passive smoking	
	Other indoor sources	Examples of the indoor sources considered for pollutants provided with the model are tobacco smoking, unburned natural gas (leaks), various consumer products, wood burning, range cooking, range pilot light, chlorinated water supply, pressed wood products, vacuuming/sweeping, and dry-cleaned clothes. <i>*Note– Data are not available for each pollutant being emitted from each of these identified sources.</i>
Extrapolation to study population	Method of allocating estimated exposures to study population	

**Table B-8**  
**Model Features for SHEDS**

Attribute	Component	Remarks
General	Model name	SHEDS (Stochastic Human Exposure and Dose Simulation) Model
	Pollutants of concern	pesticides, particulate matter, and other POPs, metals, and air toxics
	References	Zartarian V.G., Özkaynak H., Burke J.M., Zufall M.J., Rigas M.L., and Furtaw Jr. E.J. A Modeling Framework For Estimating Children's Residential Exposure and Dose to Chlorpyrifos Via Dermal Residue Contact and Non-Dietary Ingestion. Submitted to Environmental Health Perspectives. September 1999.  Özkaynak H., Zufall, M., Burke, J., Xue, J., Zidek, J. 1999a. Predicting population exposures to PM10 and PM2.5. Presented at PM Colloquium, Durham, NC. June, 1999.  Özkaynak H., Zufall, M., Burke, J., Xue, J., Zidek, J. 1999b. A Probabilistic Population Exposure Model for PM10 and PM2.5. Presented at 9 <sup>th</sup> Conference of the International Society of Exposure Analysis, Athens, Greece. September 5-8, 1999.
	Model status	Prototype first-generation SHEDS-Pesticides model has been developed. A case study for children and chlorpyrifos has been conducted using 1-stage Monte Carlo sampling. Currently case study is being completed for 2-stage Monte Carlo sampling to conduct variability and uncertainty analyses. Next generation will focus on pesticides and other multimedia, multipathway pollutant for different population cohorts, and will assess both cumulative and aggregate dose.  Prototype first-generation SHEDS-PM model has been developed. A PM10 case study for Vancouver, Canada has been conducted using 1-stage Monte Carlo sampling. Subsequent generations will focus on modeling both PM10 and PM2.5 exposure and dose in a selected U.S. city, using 2-stage Monte Carlo sampling.
	Contact/Affiliation	Halûk Özkaynak, U.S. EPA National Exposure Research Laboratory (919-541-5172) Valerie Zartarian (SHEDS-Pesticides), U.S. EPA National Exposure Research Laboratory (703-648-5538) Janet Burke (SHEDS-PM), U.S. EPA National Exposure Research Laboratory (919-541-0820) Maria Zufall (SHEDS-PM), U.S. EPA National Exposure Research Laboratory (919-541-5461)
	Stochastic?	Yes - all model inputs are represented by a probability distribution

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Attribute	Component	Remarks
	Variability?	Yes - variability of inputs is explicitly represented by user-specified probability distributions and Monte Carlo sampling is applied to quantify variability in model outputs.
	Uncertainty?	Yes - for each input parameter probability distribution, associated uncertainty distributions can also be specified. 2-stage Monte Carlo sampling is applied to analyze uncertainty in model outputs.
Modeled area, study population, and modeling period	Study areas where model has been applied	<p>First-generation SHEDS-Pesticides model has been applied to estimate children's indoor and outdoor (home lawn) exposures and doses to chlorpyrifos. Children were sampled from the National Human Activity Pattern Survey, which includes all 48 conterminous U.S. states.</p> <p>First-generation SHEDS-PM model has been applied to estimate PM10 exposures to individuals in Vancouver, Canada.</p>
	Spatial designation of study area	The designated study area is the geographic location associated with the user-specified cohort from national time/location/activity surveys in EPA's Consolidated Human Activity Database (CHAD).
	Sub-area designations	Sub-area designations are the set of locations (microenvironments) occupied by individuals sampled from the time/location/activity pattern surveys in EPA's Consolidated Human Activity Database (CHAD).
	Exposure duration for modeling	Daily exposure and dose profiles are modeled for each individual. The time scales used to generate these profiles differ by route. For inhalation, the time scale ranges from 1 minute to 12 hours, depending on the pollutant and diary selected. For dermal contact and non-dietary ingestion, the time scale is 5 seconds. For dietary ingestion, the time scale for ingestion is instantaneous for each eating/drinking event, but absorption is calculated on a 30-minute time scale after each ingestion event. The daily profiles correspond to time periods associated with the user-specified environmental concentrations (e.g., <1 day, 1-7 days, 8-30 days, 30-365 days post-pesticide application).
	General population of interest	The U.S. population as represented by individuals in time/location/activity surveys contained in EPA's Consolidated Human Activity Database (CHAD).
	Special subgroups or designations	<p>The first generation of SHEDS-Pesticides focuses on residential exposures to children (0-4 years and 5-9 years). The next generation will be able to address residential, non-residential, and occupational exposures for other cohorts of interest.</p> <p>The first generation of SHEDS-PM estimates exposures by gender and age category.</p>
		Special attributes for subgroups
Source of demographic data for study population		Time/location/activity surveys in EPA's CHAD.

Attribute	Component	Remarks
Exposure events	Environmental media	SHEDS is a concentration-to-dose model in which the user enters distributions for residues or concentrations in exposure media rather than environmental media (except for ambient air and surface soil).
	Exposure media	indoor air; outdoor air; commuting/in-vehicle air; soil; house dust; surface residues (indoor and lawn); hand and object residues; tap water; food and beverages
	Pathways	Ingestion of residues in food and beverages by eating/drinking event; Dermal contact with soil, dust, or residues on surfaces; Non-dietary ingestion of residues on skin and objects mouthed; Inhalation of pollutants in indoor, outdoor, and commuting/in-vehicle locations
	Routes	Inhalation, Dietary Ingestion (food, drinking water, other beverages), Non-Dietary Ingestion (hand-to-mouth and object-to-mouth), Dermal Contact
	Time resolution of exposure events	<u>Inhalation</u> : Daily profiles with down to 1 minute resolution. <u>Dermal and Non-Dietary Ingestion</u> : Daily profiles with 5-second resolution. <u>Dietary Ingestion</u> : Daily profiles with 30-minute resolution for absorption; residues ingested by eating events assumed to be instantaneous.
	Integration of exposures across multiple media	Exposures are estimated for each route and pathway via sequential exposure profiles. Corresponding dose profiles for each route and pathway are calculated then summed across routes.
		Method for determining pollutant contact rate
	Dietary Ingestion: For sampled individual's daily sequential time/location/activity diary events, combine total residue mass ingested during each eating/drinking event (sampled from measured or modeled distributions) with dietary absorption fraction.	
	Dermal Contact: For sampled individual's daily sequential time/location/activity diary events, simulate sequences of microlevel object contact events using probabilities developed from videography study data. For each discrete microlevel contact event, combine surface residue, transfer or removal efficiency, and dermal or GI absorption rate constant.	

Attribute	Component	Remarks
	Activity pattern methodology	Daily time/location/activity profiles are obtained from surveys contained in EPA's CHAD (e.g., NHAPS, CARB, U. Michigan). For inhalation, the day is divided into 1-minute to 12 hour sequential activities (depending on the pollutant and diary selected). For ingestion, the day is divided into 30-minute sequential macro-activities and eating/drinking events. For dermal and non-dietary ingestion, the day is divided first into 30-minute sequential macro-activities, then each macro-activity is divided into 5-second contact events. Daily activity pattern time profiles for each route are combined with concentrations, exposure factors, and dose factors to yield daily exposure and dose profiles.
	Source of activity pattern data	For macrolevel activity patterns, time/location/activity surveys contained in EPA's CHAD (e.g., NHAPS, CARB, U. Michigan) are used. For microlevel activity patterns, data on contact frequency and duration for different body parts and surfaces are obtained from available videography studies.
	Time resolution of activity patterns	Inhalation: 1 minute to 12 hours, depending on the pollutant and diary selected.. Dietary ingestion: Daily consumption patterns, with instantaneous ingestion assumed for each eating/drinking event, and 30-minute time steps for GI absorption. Dermal and non-dietary ingestion: 5-second time steps for contact events occurring within each macro-activity.
	Microenvironments (Inhalation)	In the first-generation of SHEDS: indoors at home and outdoors at home, non-residential locations (SHEDS-PM), and in vehicles (SHEDS-PM)
	Exposure locations (Ingestion)	Microenvironments in time/location/activity surveys in which sampled individuals ingest food or beverages.
	Model calculates exposure of commuters	First generation of SHEDS calculates in-vehicle exposures, but does not explicitly incorporate pollution gradients during commuting. Next generation will include air concentrations in specified cohort's commuting area.
Concentrations and sources	Outdoor concentration determination method	SHEDS requires user to enter distributions for concentrations in exposure media. Distributions for outdoor concentrations can be derived from measurements or from fate and transport models.
	Indoor concentration determination method	SHEDS-Pesticides requires user to enter distributions for concentrations in exposure media. Distributions for indoor concentrations can be derived from measurements or from fate and transport models.  SHEDS-PM uses a physical or empirical mass balance model to estimate indoor concentrations.
	In-vehicle concentration estimation	SHEDS requires user to enter distributions for concentrations in exposure media. In-vehicle air concentrations are modeled using available measurements.
	Passive smoking	Indoor PM passive smoking concentrations are modeled using a mass balance model.

Attribute	Component	Remarks
	Other indoor sources	<p>Other indoor sources (e.g., tracked-in soil, stripping of chemicals via household water use, pesticide application rates) are not explicitly included in SHEDS-Pesticides, but are implicitly included through user-specified concentrations for indoor air and surfaces.</p> <p>SHEDS-PM includes cooking and resuspension as other indoor sources of particles.</p>
Extrapolation to study population	Method of allocating estimated exposures to study population	Daily exposures and doses are simulated for individuals in the specified cohort by combining actual macro-level and micro-level activity data with residues or concentrations in exposure media and exposure and dose factors. 2-stage Monte Carlo sampling is applied to simulate population distributions.

## APPENDIX C List of TRIM.Expo Input Parameters

**Table C-1<sup>1</sup>**  
**Example Input Parameters for Calculating Inhalation Exposures**

Parameter by Category	Units	Distribution Type	Reference/Source
<b>Building Parameters (for use in mass balance model)</b>			
Air exchange rates (ACH), residences – windows closed	1/time	Lognormal	Murray and Burmaster 1995
ACH, residences – windows open	1/time	Lognormal	Johnson et al. 1998
ACH, non-residential, enclosed microenvironments, filtered air	1/time		
ACH, non-residential, enclosed microenvironments, unfiltered air	1/time		
Efficiency of air cleaning device (F)	dimensionless fraction		
Flow rate through air cleaning device (q)	volume/time		
Fraction of outdoor pollutant intercepted by enclosure ( $F_B$ )	dimensionless fraction		
Indoor generation rate (S)	mass/time		
Indoor building volume (V)	volume		
Mixing factor (m)	dimensionless		
Pollutant decay coefficient ( $F_d$ )	1/time		
<b>Demographic Parameters</b>			
Age			Census data, Comprehensive Human Activity Database (CHAD)
Gender			Census data, Comprehensive Human Activity Database (CHAD)

<sup>1</sup> The input parameters and distribution types reflect the current initial choices that EPA is planning on using in developing the initial TRIM.Expo inhalation Prototype and are subject to change.



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LIST OF TRIM.EXPO INPUT PARAMETERS

Parameter by Category	Units	Distribution Type	Reference/Source
<b>Environmental Parameters</b>			
Temperature	degrees		National Climatic Data Center
<b>Physiological Parameters (for calculating ventilation rate)</b>			
Body mass (BM)	kilograms (kg)		Brainard and Burmaster 1992, Burmaster and Crouch 1997
Metabolic equivalence (MET)	dimensionless		
Oxygen uptake rate (VO <sub>2</sub> )	liters/min		Åstrand 1960, Mercier et al. 1991, Katch and Park 1975, Heil et al. 1995, Mermier et al. 1993, Rowland et al. 1987
Normalized oxygen uptake rate (NVO <sub>2</sub> )	ml/min/kg		Åstrand 1960, Mercier et al. 1991, Katch and Park 1975, Heil et al. 1995, Mermier et al. 1993, Rowland et al. 1987
Resting metabolic rate (RMR)	kcal/min	From regression fit specific to age and gender	Schofield 1985
<b>Pollutant Parameters</b>			
Ambient pollutant concentrations	mass/volume		Aerometric Information Retrieval System (AIRS), dispersion model, TRIM.FaTE
Microenvironmental concentrations	mass/volume		Mass balance model, direct measurement, intermedia transfer factors

**Table C-2<sup>2</sup>**  
**Example Input Parameters for Calculating Ingestion Exposures**

Parameter by Category	Units	Distribution Type	Reference/Source
<b>Demographic Parameters</b>			
Age			Census data, Comprehensive Human Activity Database (CHAD)
Gender			Census data, Comprehensive Human Activity Database (CHAD)
Body mass (BM)	kg		Brainard and Burmaster 1992, Burmaster and Crouch 1997
<b>Parameters Specific to Ground Water and Surface Water Intake</b>			
Concentration in tap water ( $C_{tw}$ )	mg/L		
Concentration in ground water or surface water ( $C_{gw/sw}$ )	mg/L		
Exposure duration (ED)	time		
Exposure frequency ( $EF_{z,tw}$ )	d/month (or equivalent)		
Rate of intake of tap water ( $I_{z,tw}$ )	L/kg/d		EPA Exposure Factors Handbook 1997b, Ershow and Cantor 1989, Canadian Ministry of Health and Welfare 1981
<b>Parameters Specific to Soil (Outdoors) Intake</b>			
Pollutant concentration in surface soil ( $C_{ss}$ )	mg/kg		
Exposure frequency ( $EF_{z,ss}$ )	d/month (or equivalent)		
Annually averaged daily rate of intake of soil ( $I_{z,ss}$ )	kg/kg/d		
<b>Parameters Specific to Dust (Indoors) Intake</b>			
Pollutant concentration in house dust [ $C_{hd}(i,t)$ ] ( <i>for exposure district, i, during time step t</i> )	mg/kg		
Pollutant concentration in surface soil [ $C_{ss}(i,t)$ ]	mg/kg		
Pollutant concentration of air particles [ $C_{ap}(i,t)$ ]	mg/m <sup>3</sup>		
Exposure frequency ( $EF_{z,hd}$ )	d/month (or equivalent)		
Annually averaged daily rate of intake of soil ( $I_{z,ss}$ )	kg/kg/d		
Fraction of indoor dust that originates from outdoor soil ( $f_{hds}$ )	dimensionless		

<sup>2</sup> The input parameters and distribution types reflect the current initial choices that EPA is planning on using in developing the initial TRIM.Expo ingestion Prototype and are subject to change.

APPENDIX C  
LIST OF TRIM.EXPO INPUT PARAMETERS

Parameter by Category	Units	Distribution Type	Reference/Source
<b>Parameters Specific to Home-grown Vegetables, Fruits, and Grains Intake</b>			
Pollutant concentration – air [C <sub>a</sub> (i,t)]	mg/m <sup>3</sup>		
Pollutant concentration in root zone soil (C <sub>rs</sub> )	mg/kg		
Pollutant concentration in: 1) grains [C <sub>g</sub> (i,t)], 2) exposed fruits and vegetables [C <sub>efv</sub> (i,t)], 3) protected fruits and vegetables [C <sub>pfv</sub> (i,t)]	mg/kg		
Exposure frequency (number of days per month equivalent, that individual z consumes homegrown foods in exposure district in): 1) grains [EF <sub>z,g</sub> (i,t)], 2) exposed fruits and vegetables [EF <sub>z,efv</sub> (i,t)], 3) protected fruits and vegetables [EF <sub>z,pfv</sub> (i,t)]	d/month (or equivalent)		
Annually averaged daily rate of intake of grains (I <sub>z,g</sub> )	kg/kg/d		
Annually averaged daily rate of intake of exposed fruits and vegetables (I <sub>z,efg</sub> )	kg/kg/d		
Annually averaged daily rate of intake of protected fruits and vegetables (I <sub>z,pfg</sub> )	kg/kg/d		
<b>Parameters Specific to Home-grown Dairy Product Intake</b>			
Pollutant concentration in dairy products of exposure district, i at time step, t [C <sub>k</sub> (i,t)]	mg/kg		
Pollutant concentration in pasture [C <sub>p</sub> (i,t)]	mg/kg		
Pollutant concentration in surface soil [C <sub>s</sub> (i,t)]	mg/kg		
Pollutant concentration in the water [C <sub>w</sub> (i,t)]	mg/kg		
Biotransfer factor from cattle diet to dairy products [C <sub>k</sub> (i,t)/I <sub>n<sub>dc</sub></sub> ]	d/kg		
Exposure frequency [EF <sub>z,k</sub> (i,t)]	d/month (or equivalent)		
Annually averaged daily rate of intake of dairy products (I <sub>z,k</sub> )	kg/kg/d		
Ingestion rate of pasture by dairy cattle (I <sub>p<sub>dc</sub></sub> )	kg/d		
Ingestion rate of soil by dairy cattle (I <sub>s<sub>dc</sub></sub> )	kg/d		

Parameter by Category	Units	Distribution Type	Reference/Source
Ingestion rate of water by dairy cattle ( $I_{w_{dc}}$ )	kg/d		
<b>Parameters Specific to Home-grown Egg Intake</b>			
Pollutant concentration of exposure district i, at time step, t [ $C_e(i,t)$ ]	mg/kg		
Pollutant concentration in pasture [ $C_p(i,t)$ ]	mg/kg		
Pollutant concentration in surface soil [ $C_s(i,t)$ ]	mg/kg		
Pollutant concentration in the water [ $C_w(i,t)$ ]	mg/kg		
Biotransfer factor from hen diet to eggs [ $C_e(i,t)/I_{hn}$ ]	d/kg		
Exposure frequency [ $EF_{z,e}(i,t)$ ]	d/month (or equivalent)		
Annually averaged daily rate of intake of eggs ( $I_{z,e}$ )	kg/kg/d		
Ingestion rate of pasture by chickens ( $I_{p_{hn}}$ )	kg/d		
Ingestion rate of soil by chickens ( $I_{s_{hn}}$ )	kg/d		
Ingestion rate of water by chickens ( $I_{w_{dc}}$ )	kg/d		
<b>Parameters Specific to Home-grown Meat and Poultry Intake</b>			
Pollutant concentration of exposure district, i at time step, t [ $C_k(i,t)$ ]	mg/kg		
Pollutant concentration in pasture [ $C_p(i,t)$ ]	mg/kg		
Pollutant concentration in surface soil [ $C_s(i,t)$ ]	mg/kg		
Pollutant concentration in the water [ $C_w(i,t)$ ]	mg/kg		
Biotransfer factor from cattle diet to meat [ $C_i(i,t)/I_{bc}$ ]	d/kg		
Exposure frequency [ $EF_{z,k}(i,t)$ ]	d/month (or equivalent)		
Annually averaged daily rate of intake of meat ( $I_{z,t}$ )	kg/kg/d		
Ingestion rate of pasture by beef cattle ( $I_{p_{bc}}$ )	kg/d		
Ingestion rate of soil by beef cattle ( $I_{s_{bc}}$ )	kg/d		
Ingestion rate of water by beef cattle ( $I_{w_{bc}}$ )	kg/d		

Parameter by Category	Units	Distribution Type	Reference/Source
<b>Parameters Specific to Locally-grown Vegetables, Fruits, and Grains Intake<sup>3</sup></b>			
Spatially-averaged pollutant concentration – air [ $C_a(\text{avg},t)$ ]	mg/m <sup>3</sup>		
<i>Spatially-averaged pollutant concentration in:</i> 1) grains [ $C_g(\text{avg},t)$ ], 2) exposed fruits and vegetables [ $C_{efv}(\text{avg},t)$ ], 3) protected fruits and vegetables [ $C_{pfv}(\text{avg},t)$ ]	mg/kg		
<i>Exposure frequency</i> (number of days per month equivalent, that individual z consumes locally-produced foods in exposure district in): 1) grains [ $EF_{z,g}(i,t)$ ], 2) exposed fruits and vegetables [ $EF_{z,efv}(i,t)$ ], 3) protected fruits and vegetables [ $EF_{z,pfv}(i,t)$ ]	d/month (or equivalent)		
<b>Parameters Specific to Locally-grown Dairy Product Intake<sup>4</sup></b>			
<i>Spatially-averaged pollutant concentration</i> – in the pastures of all suburban and rural exposure districts where local dairy products are produced during the time step, t [ $C_p(\text{avg},t)$ ]	mg/kg		
<i>Exposure frequency</i> (number of days per month equivalent, that individual z consumes locally-produced dairy products in exposure district in): [ $EF_{z,k}(i,t)$ ]	d/month (or equivalent)		
<b>Parameters Specific to Locally-grown Egg Intake<sup>5</sup></b>			
<i>Spatially-averaged pollutant concentration</i> – in the pastures of all suburban and rural exposure districts where local eggs are produced during the time step, t [ $C_p(\text{avg},t)$ ].	mg/kg		

<sup>3</sup> The parameters used to calculate the intake of pollutants for locally-grown vegetables, fruits, and grains are the same as those for home-grown with the following replacements.

<sup>4</sup> The parameters used to calculate the intake of pollutants for locally-grown dairy products are the same as those for home-grown with the following replacements.

<sup>5</sup> The parameters used to calculate the intake of pollutants for locally-grown egg products are the same as those for home-grown with the following replacements.

Parameter by Category	Units	Distribution Type	Reference/Source
<i>Exposure frequency</i> (number of days per month equivalent, that individual z consumes locally-produced eggs in exposure district i): $[EF_{z,e}(i,t)]$	d/month (or equivalent)		
<b>Parameters Specific to Locally-grown Meat and Poultry Intake<sup>6</sup></b>			
<i>Spatially-averaged pollutant concentration</i> – in the pastures of all suburban and rural exposure districts where local meat products are produced during the time step, t $[C_p(\text{avg},t)]$	mg/kg		
<i>Exposure frequency</i> (number of days per month equivalent, that individual z consumes locally-produced meat products in exposure district i): $[EF_{z,i}(i,t)]$	d/month (or equivalent)		
<b>Parameters Specific to Local Fish Intake</b>			
<i>Spatially-averaged pollutant concentration</i> – in the water of all exposure districts in the air shed being considered during the time step, t $[C_r(\text{avg},t)]$	mg/L		
Biotransfer factor from water to fish (BCF)	L/kg		
<i>Exposure frequency</i> (number of days per month equivalent, that individual z, in exposure district i, consumes locally caught fish): $[EF_{z,k}(i,t)]$	d/month (or equivalent)		
Annually-averaged daily rate of intake of fish ( $I_{z,f}$ )	kg/kg/d		

<sup>6</sup> The parameters used to calculate the intake of pollutants for locally-grown meat and poultry products are the same as those for home-grown with the following replacements.

APPENDIX C  
 LIST OF TRIM.EXPO INPUT PARAMETERS

Parameter by Category	Units	Distribution Type	Reference/Source
<b>Parameters Specific to Recreational Sport Meat (Hunting)</b>			
<i>Spatially-averaged pollutant concentration</i> – in the meat of game animals residing in the air shed being considered during the time step, $t$ [ $C_{sm}(avg,t)$ ]	mg/kg		
Time step averaged daily rate of intake of sport meat ( $I_{z,sm}$ )	kg/kg/d		