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CHAPTER 3

An Overview of Exposure Assessment Models Used by the US Environmental Protection Agency

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3.1 INTRODUCTION

Models are often used in addition to or in lieu of monitoring data to estimate environmental concentrations and exposures for use in risk assessments or epidemiological studies, and to support regulatory standards and voluntary programmes (Jayjock *et al.*, 2007; US EPA, 1989, 1992). The purpose of this chapter is to provide an overview of 35 models currently supported and used by the US EPA to assess exposures to human or ecological receptors (see Table 3.1 for a list of abbreviations). These models differ in regard to their purpose, and level and scope of analysis. For example, some of the exposure assessment models refer to a single pollutant or exposure pathway, while others assess multiple pollutants and pathways. Additionally, most of these models pertain to either human or ecological receptors, although a few are applicable to both receptor groups. These models may target the general population, subgroups within the population, or individuals (e.g., workers, consumers). In regard to temporal and spatial scale, some of these models predict acute, subchronic and/or chronic exposures at the local, urban, regional and/or national level. These models are frequently used by, and have sometimes been developed in collaboration with, researchers and practitioners in academia, consulting, private industry, state and local governments, and internationally.

The models included in this chapter can be used during different stages of the exposure assessment process. Specifically, these models represent the first half of the

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Table 3.1: List of abbreviations.[a]

Abbreviation	Full spelling
ARS	Agricultural Research Service
ADD	average daily dose
BART	best available retrofit technology
CO	carbon monoxide
CEAM	Center for Exposure Assessment Modeling
CAMR	Clean Air Mercury Rule
CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act
CHAD	Consolidated Human Activity Database
CSFII	Continuing Survey of Food Intakes by Individuals
CASAC	Clean Air Scientific Advisory Committee
CREM	Council for Regulatory Environmental Modeling
EEC	estimated environmental concentration
FIFRA	Federal Insecticide, Fungicide, and Rodenticide Act
FQPA	Food Quality Protection Act
GIS	geographical information system
HAP	hazardous air pollutant
HWIR	Hazardous Waste Identification Rule
LADD	lifetime average daily dose
MOE	margin of exposure
MSAT	Mobile Source Air Toxics
NAS	National Academy of Sciences
NAAQS	National Ambient Air Quality Standards
NERL	National Exposure Research Laboratory
NHANES	National Health and Nutrition Examination Survey
NATA	National-Scale Air Toxics Assessment
NSR	New Source Review
OAQPS	Office of Air Quality Planning and Standards
OAR	Office of Air and Radiation
OPP	Office of Pesticide Program
OPPT	Office of Pollution Prevention and Toxics
ORD	Office of Research and Development
OSWER	Office of Solid Waste and Emergency Response
OW	Office of Water
OP	organophosphate pesticide
PM	particulate matter
PCA	percent crop area
PBPK	physiologically based pharmacokinetic
PMN	pre-manufacturing notification
PSD	prevention of significant deterioration
RfD	reference dose
Reg Reviews	Registration Reviews
REDs	re-registration eligibility decisions
RTP	Research Triangle Park
RCRA	Resource Conservation and Recovery Act

(*continued*)

Table 3.1: (*continued*)

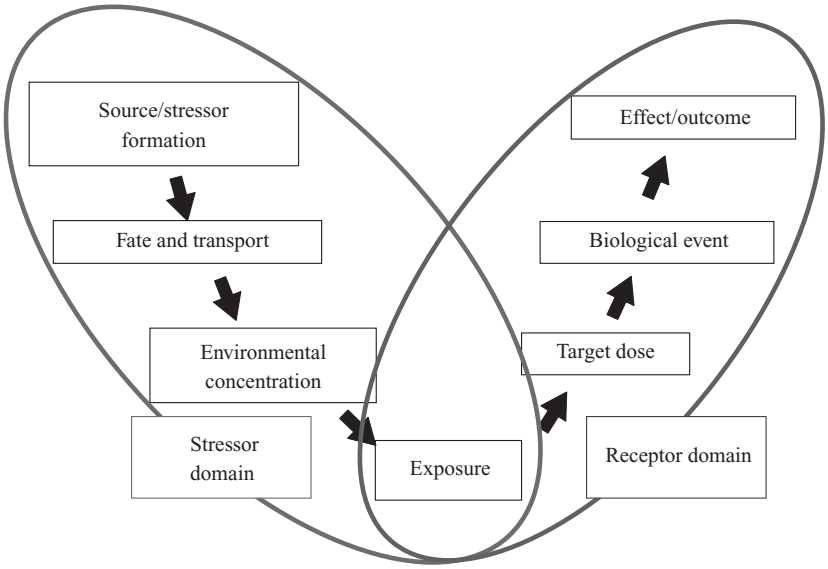
Abbreviation	Full spelling
SAB	Science Advisory Board
SAP	Science Advisory Panel
SOPs	standard operating procedures
SCRAM	Support Center for Regulatory Atmospheric Modeling
TMDL	Total Maximum Daily Load
TSCA	Toxic Substances Control Act
USDA	United States Department of Agriculture
US EPA	United States Environmental Protection Agency
VCCEP	Voluntary Children's Chemical Evaluation Program
WMU	Waste Management Unit

[a]Does not include acronyms for exposure assessment models (see Table 3.2).

source-to-outcome continuum (see Figure 3.1), and include selected fate/transport models, exposure models, and integrated fate/transport and exposure models. According to the literature, exposure is defined as contact between an agent and a target that takes place at an exposure surface over an exposure period, whereas dose is defined as the amount of an agent that enters a target after crossing a contact boundary (WHO, 2004; Zartarian *et al.*, 1997, 2005a). In general, the fate/transport models assess the movement and transformation of pollutants in the environment, and yield predicted ambient pollutant concentrations (in units of $mg\,m^{-3}$, $mg\,L^{-1}$ or $mg\,kg^{-1}$) in different environmental media (e.g., air, water, soil, food). The outputs of these models therefore represent concentrations to which receptors have the *potential* for exposure, although these estimates are often used as a proxy or surrogate for actual exposure, or can serve as an input to exposure models. The exposure models incorporate information on exposure factors and time activity patterns, and yield predicted exposures or doses (in units of $mg\,m^{-3}$ or $mg\,kg^{-1}\,day^{-1}$) based on actual (or assumed) contact between a receptor and the general environment or specific microenvironments. The outputs of these models are therefore the most representative of *actual* human or ecological exposures.

For the purposes of this chapter, the integrated fate/transport and exposure models include those models that yield both predicted ambient pollutant concentrations (based on algorithms for assessing a pollutant's fate and transport in the environment) and predicted exposures or doses (based on exposure factor information). However, these models do not incorporate information on time–activity patterns: model outputs are therefore based on *assumed* contact between a receptor and an agent. Note that although many of the exposure assessment models provide estimates of potential or absorbed dose, the primary focus of these models is on using algorithms and data to assess human or ecological exposures (i.e., the dose estimates from these models are based on simple calculations and assumptions about absorption rates, rather than kinetic or PBPK modelling). A review of stand-alone or more sophisticated PBPK dose models is outside the scope of this assessment.

Figure 3.1: Source-to-outcome continuum.



An important distinction among the various exposure assessment models used by the US EPA is that they are typically used for either "screening-level" or "higher-tiered" applications. Screening-level models included in this chapter do not incorporate time–activity patterns, and generally overpredict receptor exposures, because they are based on conservative (e.g., high-end) default scenarios and assumptions. These models are frequently used to obtain a first approximation, or to screen out exposures that are not likely to be of concern (US EPA, 1992). However, the default values in these models can sometimes be modified or changed if other values are deemed more suitable for the specific exposure scenario being evaluated. A small number of models used by the US EPA (which are highlighted below) are also sometimes referred to as "screening-level" because of their limited spatial and temporal scope, rather than because they are based on conservative exposure assumptions. On the other hand, higher-tiered models used by the US EPA typically include time–activity patterns, are based on more realistic scenarios and assumptions, and have broader spatial and temporal resolution. These models require much more data of higher quality than the screening-level models, and are intended to produce more refined estimates of exposure (US EPA, 1992).

Although all of the exposure assessment models included here have been internally peer-reviewed to ensure consistency with Agency-wide policies and procedures, many of these models have also undergone independent external peer review by outside experts. In this context, external peer review can take several different forms, depending on the intended use and complexity of the model. For example, models developed for basic research, planning or screening purposes will often undergo external letter peer reviews. For these types of review, four or five outside experts

provide an independent review of the model and prepare a written response to a set of specific charge questions. Other models, such as those designed for regulatory or advanced research purposes, may undergo more extensive external peer reviews by the US EPA's scientific advisory boards, panels or committees (e.g., SAB, SAP, CASAC). During these reviews, a panel of experts holds one or more meetings to discuss and evaluate the model structure and predictions, and the panel prepares a group report that attempts to reach consensus in response to a set of specific charge questions. Many of the models included here have also been published in the peer-reviewed literature in regard to their structure, potential applications and evaluation. These internal and external peer review efforts have resulted in continuous updates and improvements to the exposure assessment models used by the US EPA.

The models included in this chapter have also undergone varying degrees of model evaluation. The NAS (2007) defines model evaluation as the process of deciding whether and when a model is suitable for its intended purpose, and makes it clear that this process is not a strict validation or verification procedure, but rather one that builds confidence in model applications, and increases the understanding of model strengths and limitations. Similarly, the US EPA (2008a) defines model evaluation as the process used to generate information to determine whether a model and its analytical results are of a quality sufficient to serve as the basis for a decision. Model evaluation is a multifaceted activity involving peer review, corroboration of results with data and other information, quality assurance and quality control checks, uncertainty and sensitivity analyses, and other activities (NAS, 2007). Some of the approaches that have been used to evaluate the exposure assessment models used by the US EPA include comparing the structure, model inputs, and results of one model to another (i.e., model-to-model comparisons); comparing modelled estimates with measured or field data; and comparing modelled estimates with biomonitoring data (e.g., urine, blood).

Our overview of exposure assessment models currently supported and used by the US EPA complements and expands prior efforts to identify and summarise exposure assessment tools and models used by selected US EPA programme offices (Furtaw, 2001; Daniels *et al.*, 2003). This work also supports recent and ongoing efforts at the US EPA to characterise and evaluate its models (see Section 3.2 below). The current chapter serves as a readily available, concise reference that should provide a useful resource for modellers and practitioners of exposure and risk, as well as experimental scientists, regulators and other professionals responsible for addressing the implications of the use of these models.

3.2 BACKGROUND INFORMATION

A number of Agency guidelines, programmes and policies have shaped or provided the underlying basis for the development and refinement of the exposure assessment models used by the US EPA. For example, the US EPA's (1992) *Guidelines for Exposure Assessment* provides a broad discussion of the use of mathematical modelling in the absence of field data when evaluating human exposures. Specifically, the following five general aspects of a modelling strategy are discussed in the 1992 *Guidelines*:

- setting objectives;
- model selection;
- obtaining and installing the code;
- calibrating and running the computer model, and
- validation and verification.

In a subsequent consultation by the US EPA's SAB (2006a), it was recommended that the 1992 *Guidelines* be updated to cover advances and changes in the theory and practice of exposure assessment (e.g., in areas such as probabilistic analyses, exposure factors, aggregate exposure and cumulative risk, community-based research, and consideration for susceptible populations and life stages), and include a greater emphasis on specific issues related to exposure modelling, such as model evaluation, spatial aspects, and timing. Efforts to update the 1992 *Guidelines* are currently under way within the US EPA's Risk Assessment Forum (expected to be completed in 2009), and will include an expanded discussion of the role of mathematical modelling in conducting exposure assessments, as well as some specific examples of the US EPA's exposure models (Bangs, 2008, personal communication).[1]

The US EPA also established CREM in 2000 to promote consistency and consensus among environmental model developers and users, with a focus on establishing, documenting and implementing criteria and best management practices within the US EPA. In their initial efforts, CREM developed a preliminary online database, called the Models Knowledge Base, that includes an inventory and descriptions of more than 100 environmental models currently used by the US EPA. A report entitled *Draft Guidance on the Development, Evaluation, and Application of Regulatory Environmental Models* was also prepared by CREM: this discusses the role of modelling in the public policy process, and provides guidance to those who develop, evaluate and apply environmental models (Pascual *et al.* 2003). This report recommended that best practices be used to help determine when a model (despite its uncertainties) can be appropriately used to inform a decision, such as subjecting the model to peer review, assessing the quality of the data used, corroborating the model with reality, and performing sensitivity and uncertainty analyses.

In its external peer review of CREM's draft report, the US EPA's SAB (2006b) concluded that it provides a comprehensive overview of modelling principles and best practices, but recommended a number of ways in which the report and the Models Knowledge Base could be improved, including the need to gather or develop additional information about the framework and limitations of various models. The NAS also reviewed evolving scientific and technical issues related to the development, selection and use of computational and statistical models in the regulatory process at the US EPA. In its report *Models in Environmental Regulatory Decision Making*, the NAS (2007) recommended the following 10 principles to improve the US EPA's model development and evaluation process:

- evaluate a model through its entire life cycle;
- ensure appropriate peer review of a model;
- perform an adequate (quantitative) uncertainty analysis;
- use adaptive strategies to coordinate data collection and modelling efforts;

- conduct retrospective reviews of regulatory models;
- ensure model parsimony;
- carefully extrapolate from models;
- create an open evaluation process during rule-making;
- document the origin and history of each model; and
- improve model accessibility to stakeholders and others.

Efforts are currently under way by CREM to update the Models Knowledge Base and to respond to the NAS's recommendations to perform life cycle evaluations and retrospective analyses of existing US EPA models (Gaber, 2008, personal communication).[2] CREM also recently updated its draft guidance document in response to comments and recommendations from the SAB and NAS (US EPA, 2008a).

A number of generic Agency-wide guidance documents and policies have also influenced the US EPA's modelling efforts and underlying databases. For example, the US EPA's (2002a) *Guidelines for Ensuring and Maximizing the Quality, Objectivity, Utility, and Integrity of Information Disseminated by the Environmental Protection Agency* contains policy and procedural guidance related to the quality of information that is used and disseminated by the US EPA. The mandatory Agency-wide Quality System also provides policy and programme requirements that help ensure that the US EPA organisations maximise the quality of environmental information by using a graded approach to establish quality criteria that are appropriate for the intended use of the information and resources available (US EPA, 2000a). Similarly, the US EPA's (2006a) *System Life Cycle Management Policy* helps to ensure continued enhancements and improvements to the life cycle management of the US EPA's data and databases. Additionally, the US EPA's Peer Review Policy and accompanying *Peer Review Handbook* encourage the peer review of all scientific and technical information and work products intended to inform or support Agency decisions, including technical and regulatory models published by the Agency (US EPA, 2006b). These and other ongoing activities support the Agency's continued efforts to ensure the quality, transparency and reproducibility of the information in underlying databases and models used and disseminated by the US EPA.

3.3 METHODS

The models included in this chapter were identified primarily by searching the US EPA's website (www.epa.gov) using search terms such as "exposure assessment", "exposure model" and "environmental modelling". Materials contained within individual web pages developed by selected US EPA programme offices and research laboratories and centres related to exposure modelling and tools were also reviewed, including those by OPPT,[3] OAR's Technology Transfer Network SCRAM,[4] ORD's CEAM[5] and ORD's NERL.[6] Additionally, all of the entries listed in the CREM Models Knowledge Base were reviewed and used to identify relevant exposure assessment models. Finally, scientists and managers within different US EPA pro-

gramme offices, including ORD, OAR, OPPT, OPP, OW and OSWER, were contacted about their knowledge of other relevant models not already identified.

Several criteria were used to determine which models were ultimately included in or excluded from our overview. First, any model identified whose primary purpose is to estimate human or ecological exposures, and where the model outputs are expressed in units of exposure or dose, was included, as this was the primary focus of our review. These models were later categorised as either exposure models or integrated fate/transport and exposure models. One exception was the All-Ages Lead Model, which was excluded from this chapter because it was developed for a specific purpose (i.e., risk assessment for lead NAAQS), and is not readily transferable to other applications. Second, only a subset of those models whose primary purpose is to assess the fate and transport of pollutants in the environment, and where the modelled outputs are expressed in units of ambient media concentration, were included, with an emphasis on those fate/transport models that are the most frequently used by the US EPA for conducting exposure assessments, or which have linkages to the other exposure models included here. A complete listing of all fate/transport models was therefore considered to be outside the scope of the current assessment. Third, exposure assessment models no longer actively supported by the US EPA (i.e., the US EPA no longer provides technical support related to these models, and these models have not been updated) were excluded, although these models may still be acceptable for use outside the Agency and continue to be made available to the public. Finally, a detailed characterisation of broader modelling frameworks (i.e., computerised modelling systems that integrate or allow for interchanging various models and model components) was outside the scope of this chapter.

Information about each of the exposure assessment models was obtained from several sources. First, the available user and technical manuals, website summaries, workshop or technical presentations, Federal register notices, US EPA staff papers, external peer-reviewed reports, and published papers were reviewed. Second, extensive discussions and interviews were conducted with each of the model developers or project managers at the US EPA in order to fill in information gaps and obtain a better perspective on the history, development, applications, and strengths and limitations of each model. Third, a number of the models were run using real or hypothetical data by at least one of the co-authors (either prior to or during this review) to obtain a better understanding of the model inputs and outputs, key assumptions, default options, and interactions with other models. Fourth, a search of the published literature, selected journals and recent conference proceedings was conducted to help identify peer-reviewed publications and presentations that discuss how these models have been evaluated or applied in different settings.

3.4 RESULTS

A total of 35 exposure assessment models that are currently supported and used by the US EPA were identified for inclusion in this chapter. These include selected fate/transport models ($N = 12$), exposure models ($N = 15$) and integrated fate/transport

Table 3.2: Exposure assessment models currently used by the US EPA, by model category.

Model	Full model name	Supporting programme office	Website URL
Fate/transport models			
ISC	Industrial Source Complex	OAQPS	http://www.epa.gov/scram001/dispersion_alt.htm#isc3
AERMOD	AMS/EPA Regulatory Model	OAQPS	http://www.epa.gov/scram001/dispersion_prefrec.htm#aermod
ASPEN	Assessment System for Population Exposure	OAQPS	http://www.epa.gov/ttn/atw/nata1999/aspen99.html
CMAQ	Community Multiscale Air Quality	NERL	http://www.epa.gov/AMD/CMAQ/cmaq_model.html
CAMx	Comprehensive Air quality Model with extensions	OAQPS	http://www.camx.com
FIRST	FQPA Index Reservoir Screening Tool	OPP	http://www.epa.gov/oppefed1/models/water/first_description.htm
GENEEC	GENeric Estimated Environmental Concentration	OPP	http://www.epa.gov/oppefed1/models/water/geneec2_description.htm
SCIGROW	Screening Concentration in GROund Water	OPP	http://www.epa.gov/oppefed1/models/water/scigrow_description.htm
PRZM	Pesticide Root Zone Model	NERL	http://www.epa.gov/ceampubl/gwater/przm3
EXAMS	Exposure Analysis Modeling System	NERL	http://www.epa.gov/ceampubl/swater/exams/index.htm
WASP	Water Quality Analysis Simulation Program	NERL	http://www.epa.gov/athens/wwqtsc/html/wasp.html
EPANET		NRMRL	http://www.epa.gov/nrmrl/wswrd/dw/epanet.html

(*continued*)

Table 3.2: (*continued*)

Model	Full model name	Supporting programme office	Website URL
Exposure models			
HAPEM	Hazardous Air Pollutant Exposure Model	OAQPS	http://www.epa.gov/ttn/fera/human_hapem.html
APEX	Air Pollutants Exposure Model	OAQPS	http://www.epa.gov/ttn/fera/human_apex.html
SHEDS-Air Toxics	Stochastic Human Exposure and Dose Simulation for Air Toxics	NERL	http://www.epa.gov/AMD/AirToxics/humanExposure.html
SHEDS-PM	Stochastic Human Exposure and Dose Simulation for Particulate Matter	NERL	http://www.epa.gov/heasd
MCCEM	Multi-Chamber Concentration and Exposure Model	OPPT	http://www.epa.gov/oppt/exposure/pubs/mccem.htm
WPEM	Wall Paint Exposure Assessment Model	OPPT	http://www.epa.gov/oppt/exposure/pubs/wpem.htm
IAQX	Indoor Air Quality and Inhalation Exposure – Simulation Tool Kit	NRMRL	http://www.epa.gov/appcdwww/iemb/iaqx.htm
SWIMODEL	Swimmer Exposure Assessment Model	OPP	http://www.epa.gov/oppad001/swimodel.htm
PIRAT	Pesticide Inert Risk Assessment Tool	OPP	http://www.epa.gov/oppt/exposure/pubs/pirat.htm
DEEM™	Dietary Exposure Evaluation Model	OPP	http://www.exponent.com/deem_software
Calendex™	Calendex™	OPP	http://www.exponent.com/calendex_software/#tab_overview
CARES™	Cumulative and Aggregate Risk Evaluation	OPP	http://cares.ilsi.org
LifeLine™	LifeLine™	OPP	http://www.thelifelinegroup.org
SHEDS-Multimedia	Stochastic Human Exposure and Dose Simulation Model for Multimedia, Multi-pathway Chemicals	NERL	http://www.epa.gov/scipoly/sap/meetings/2007/081407_mtg.htm
SHEDS-Wood	Stochastic Human Exposure and Dose Simulation for Wood Preservatives	NERL	http://www.epa.gov/heasd/sheds/cca_treated.htm

(*continued*)

Table 3.2: (*continued*)

Model	Full model name	Supporting programme office	Website URL
Integrated fate/transport and exposure models			
HEM3	Human Exposure Model	OAQPS	http://www.epa.gov/ttn/fera/human_hem.html
PERFUM	Probabilistic Exposure and Risk Model for FUMigants	OPP	http://www.exponent.com/ProjectDetail.aspx?project = 450
EPA's Vapor Intrusion Model	EPA's Johnson and Ettinger (1991) Model for Subsurface Vapor Intrusion into Buildings	OSWER	http://www.epa.gov/oswer/riskassessment/airmodel/johnson_ettinger.htm
ChemSTEER	Chemical Screening Tool for Exposures & Environmental Releases	OPPT	http://www.epa.gov/oppt/exposure/pubs/chemsteer.htm
E-FAST	Exposure and Fate Assessment Screening Tool Version 2.0	OPPT	http://www.epa.gov/oppt/exposure/pubs/efast.htm
IGEMS	Internet Geographical Exposure Modeling System	OPPT	http://www.epa.gov/oppt/exposure/pubs/gems.htm
TRIM	Total Risk Integrated Methodology	OAQPS	http://www.epa.gov/ttn/fera/trim_gen.html
3MRA	Multimedia, Multi-pathway, Multi-receptor Exposure and Risk Assessment	NERL	http://www.epa.gov/ceampubl/mmedia/3mra/index.htm

and exposure models ($N = 8$). Table 3.2 provides a complete listing of these models, including the full model name, the supporting US EPA programme office, and the website URL.

3.4.1 Fate/transport models

The fate/transport models included here are all media-specific, and include selected air quality and dispersion models, and surface water and drinking water models (see Table 3.3). These models are discussed in more detail in the subsections below.

Air quality and dispersion models

The identified air quality and dispersion models are similar in that they predict ambient air concentrations of a pollutant at a given location for a specified duration of time. However, these models differ in regard to their complexity, and their spatial and temporal level of analysis. These models are currently used by the US EPA and other stakeholders in a variety of applications, and many were originally developed to meet statutory requirements, such as for attainment demonstrations or to satisfy permitting requirements. Recommended or preferred air quality and dispersion models are listed in the US EPA's (2005a) *Guideline on Air Quality Models*, which was first published in 1978 to provide guidance on model use, and ensure consistency and standardisation of model applications.

ISC (US EPA, 1995) and AERMOD (US EPA, 2004a, 2008b) represent steady-state Gaussian plume dispersion models (i.e., source-based dispersion models) that simulate the fate of chemically stable airborne pollutants based on local emission sources, and estimate airborne concentrations at different grid locations (Isakov *et al.*, 2006). ISC (long-term, ISCLT, or short-term, ISCST) is a long-standing US EPA model that was historically the preferred point source model for use in simple terrain owing to its past use, public familiarity and availability. This model has been used extensively to analyse impacts from a single or a few facilities, as well as for urban-wide air quality modelling of air toxic pollutants. However, the US EPA recently recommended that AERMOD be used as a replacement for ISC because of its more advanced technical formulation, and this model is now the preferred Agency model for assessing compliance with regulatory requirements such as NSR/PSD regulations. Both ISC and AERMOD are currently used as the atmospheric dispersion model in a number of other exposure assessment models. ASPEN (US EPA, 2000b) is a population-based air dispersion model that couples receptor point concentrations (estimated from ISCLT) with a GIS application to yield average airborne concentration at the census tract (block) level. This model has historically been used to evaluate ambient air concentrations of HAPs under the US EPA's (2006c) NATA programme.

CMAQ (Byun and Ching, 1999; US EPA, 2007a) and CAMx (ENVIRON, 2006) represent dynamic photochemical air quality dispersion models (i.e., grid-based chemical transport models) that incorporate complex atmospheric chemistry to simulate the fate of chemically reactive airborne pollutants in the general background on a regional scale (Isakov *et al.*, 2006). CMAQ is an advanced model that can be used to assess multiple air quality issues, including tropospheric ozone, fine particles,

toxics, acid deposition and visibility degradation. It has been used to support various Agency regulations, such as the US EPA's (2005b) CAMR. CAMx is another advanced model that is typically used to evaluate gases and particulates (e.g., ozone, PM, air toxics, mercury). This model has been widely used by the US EPA (2006d) to support assessments related to the NAAQS for ozone.

Typical inputs to the air quality and dispersion models include source data (e.g., emission rates, stack parameters), meteorological data (e.g., temperature, wind speed and direction, atmospheric stability class), physical and chemical properties (e.g., reactive decay, deposition, secondary transformations), and receptor data (e.g., grid coordinates, census track locations). Outputs to these models include estimates of maximum or average airborne concentrations (e.g., ppm or $mg\,m^{-3}$) over a certain duration (e.g., hourly, daily, annually) at a specified receptor level (e.g., grid, census tract). All of the air quality and dispersion models included here are deterministic models that rely on a single value for each input parameter, and yield point estimates for predicted concentrations. Although none of these models contain stochastic processes to address variability or uncertainty, some of them allow the user to vary specific input parameter values, such as source emission rates. AERMOD also has the ability to perform source contribution analyses. All of the identified models are considered to be higher-tiered models, because they provide average or best estimates of ambient pollutant concentrations. ISC and AERMOD also have screening-level versions that can be used to produce conservative (upper-bound) estimates.

The models included here have undergone extensive internal peer reviews (e.g., quality assurance and quality control checks of model code, databases) and varying degrees of external peer review. In particular, the ISC models have been extensively reviewed, updated and replaced, and revised over time (e.g., the ISC2 models were developed as replacements for previous model versions, and ISC3 models were based on revisions to algorithms contained in ISC2 models). AERMOD also underwent an external peer review of its formulation, documentation, and evaluation and performance in 1998 (US EPA, 2002b), and was found to be an appropriate replacement for ISC3 for regulatory modelling applications in 2005. ASPEN has been peer-reviewed by the US EPA's SAB as part of the peer review process for the Cumulative Exposure Project (SAB, 1996) and the 1996 NATA programme (SAB, 2001). CMAQ also underwent three formal external peer reviews from 2003 to 2007 (Aiyyer *et al.*, 2007; Amar *et al.*, 2004, 2005), and CAMx underwent an external peer review in 1997 (Kumar and Lurmann 1997).

A number of efforts have also been made to try to evaluate the air quality and dispersion models. For example, model inter-comparisons have been conducted between ISC and AERMOD (Silverman *et al.*, 2007). AERMOD was also chosen as a replacement for ISC3 for regulatory modelling applications, in part because its model performance was found to be better than that of ISC3 (Paine *et al.*, 1998). The performance of AERMOD has been extensively evaluated by using one set of databases during model formulation and development and another set of databases during final evaluation, which included four short-term tracer studies and six conventional long-term SO_2 monitoring databases in a variety of settings (Paine *et al.*, 1998). Evaluations of the ASPEN model have also included assessing how well ambient

Table 3.3: Selected fate/transport models used by the US EPA.

Model	Model purpose	Model type	Model inputs	Model outputs
ISC[a]	Estimates airborne pollutant concentrations from multiple sources (point, volume, area, or open pit) at urban or rural level (distances less than 50 km).	Steady-state Gaussian plume dispersion model.	Source data (emission rate, stack parameters), meteorological data (temperature, wind speed, wind direction, stability), receptor data (height, grid locations), building downwash parameters, terrain parameters (complex, simple), settling and removal processes (dry and wet deposition, precipitation scavenging – short-term model only).	Maximum concentration ($mg\,m^{-3}$), annual (or seasonal) average concentrations ($mg\,m^{-3}$).
AERMOD[a]	Estimates airborne pollutant concentrations from multiple sources (point, volume, area, line) at urban or rural level (distances less than 50 km).	Steady-state Gaussian or non-Gaussian plume dispersion model.	Source data (emission rate, stack parameters), meteorological data (temperature, wind speed, wind direction, stability), receptor data (height, grid locations), building downwash parameters, terrain parameters (complex, simple; hill and point elevation).	Maximum concentration ($mg\,m^{-3}$), annual (or seasonal) average concentrations ($mg\,m^{-3}$).
ASPEN	Estimates toxic air pollutant concentrations and population-weighted pollutant concentrations for a large number of sources (HAPs) at national level.	Steady-state, population-based Gaussian plume dispersion model.	Air dispersion model, meteorological data (wind speed, wind direction), settling, breakdown, and transformation processes (reactive decay, deposition, secondary formations), census track population data.	Annual average concentrations ($mg\,m^{-3}$).

Model characterisation	Model peer review and evaluation	Links to other models
Higher-tiered (allows for varying of source emission rates; can perform source contribution analyses; does not have stochastic process to address variability or uncertainty).	Prior external peer reviews of model (ISC2 models were developed as replacements for previous model version, ISC3 models were based on revisions to algorithms contained in ISC2 models); model inter-comparisons with AERMOD have been conducted.	Includes a long-term (ISCLT) and short-term (ISCST) component; SCREEN3 is a screening-level version of ISC3; used as atmospheric dispersion model in ASPEN (ISCLT2), IGEMS (ISCLT/ISCST), PERFUM (ISCST3), and 3MRA (ISCST3).
Higher-tiered (allows for varying of source emission rates, can perform source contribution analyses; does not have stochastic process to address variability or uncertainty).	External panel peer review of model formulation, documentation, and evaluation and performance in 1998; model has been tested in various types of environment, and modelling results have been compared with monitoring data and other air dispersion models.	AERSCREEN is a screening-level version of AERMOD; used as atmospheric dispersion model for HEM; predicted air concentrations used in APEX.
Higher-tiered (mapping module is used to interpolate estimated concentrations from the grid receptors to census tract centroids; does not have stochastic process to address variability or uncertainty).	External SAB peer review as part of the peer review of the Cumulative Exposure Project in 1996 and as part of the peer review of NATA in 2001; model results have been compared with monitoring data for HAPs in Texas.	Uses ISCLT2 as atmospheric dispersion model; predicted air concentrations used in HAPEM.

(*continued*)

Table 3.3: (*continued*)

Model	Model purpose	Model type	Model inputs	Model outputs
CMAQ	Estimates airborne pollutant concentrations (or their precursors) for multiple air quality issues at multiple scales including urban and regional levels.	Grid-based, three-dimensional, dynamic, Eulerian photochemical air quality simulation and dispersion model.	Meteorological data, emissions data (processed using the SMOKE emissions processor), chemistry-transport data and models (atmospheric transport, deposition, transformation processes, aerosol dynamics and atmospheric chemistry).	Hourly, daily, weekly or monthly average concentrations ($mg\,m^{-3}$), annual or multiyear average concentrations ($mg\,m^{-3}$).
CAMx	Estimates airborne pollutant concentrations for gases and particulates (ozone, PM, air toxics, mercury) at suburban, urban, regional and continental levels.	Grid-based, three-dimensional, dynamic, Eulerian photochemical air quality simulation and dispersion model.	Photochemical conditions, surface conditions, initial/boundary conditions, emissions rates, meteorology.	Hourly, daily, or annual average concentrations ($mg\,m^{-3}$).
FIRST	Estimates pesticide concentrations in untreated drinking water derived from surface water from non-point sources and aerial drift at watershed level.	Single-event process model.	Chemical properties (basic), pesticide application rate and frequency (maximum assumed), method of application (aerial, air blast, ground spray), environmental fate data (deposition, adsorption/desorption, degradation), PCA.	Daily peak concentration ($mg\,L^{-1}$), 1- and 10-year annual average concentration ($mg\,L^{-1}$).

Model characterisation	Model peer review and evaluation	Links to other models
Higher-tiered (simulates all atmospheric and land processes that affect the transport, transformation, and deposition of atmospheric pollutants; does not have stochastic process to address variability or uncertainty).	Model has undergone three formal external peer reviews from 2003 to 2007 (this is a community-supported model that undergoes continuous upgrades and improvements); modelling results have been compared with other atmospheric chemistry models (this is a community-supported model that has a formal process for model evaluation).	Used as air quality model for APEX (alone and combined with AERMOD); additional efforts under way to link with other models.
Higher-tiered (simulates the emission, dispersion, chemical reaction, and removal of pollutants in the troposphere; does not have stochastic process to address variability or uncertainty).	External peer review in 1997; model has been evaluated against observed ozone and PM concentrations in a number of studies.	Input/output file formats are based on the Urban Airshed Model; model has been used to provide inputs to the MENTOR/ SHEDS system.
Conservative (Tier I) screening level (assumes maximum application rates and highest exposure scenario; does not have stochastic process to address variability or uncertainty).	External SAP review of index reservoir scenario in 1998 and PCA methodology in 1999; limited model evaluation.	Designed to mimic a PRZM/EXAMS simulation (with fewer inputs).

(*continued*)

Table 3.3: (*continued*)

Model	Model purpose	Model type	Model inputs	Model outputs
GENEEC	Estimates pesticide concentrations in surface water (aquatic organisms) from non-point sources and aerial drift at farm pond level.	Single-event process model.	Chemical properties (basic), pesticide application rate and frequency (maximum assumed), method of application (aerial, air blast, ground spray), environmental fate data (deposition, adsorption/desorption, degradation).	Daily peak concentration ($mg\,L^{-1}$), 4-, 21-, 60- and 90-day average concentration ($mg\,L^{-1}$).
SCIGROW	Estimates pesticide concentrations in vulnerable groundwater (shallow aquifers, sandy, permeable soils, substantial rainfall/irrigation) from non-point sources at local level.	Regression model.	Chemical properties (basic), pesticide application rate and frequency (maximum assumed), environmental fate data (adsorption/desorption, degradation), groundwater monitoring data.	Highest average concentration ($mg\,L^{-1}$).
PRZM	Estimates pesticide and organic chemical loadings to surface water or groundwater from point or non-point sources, dry fallout or aerial drift, atmospheric washout, or groundwater seepage at local or regional level.	Dynamic, one-dimensional, finite-difference, compartmental (box) model.	Chemical and soil properties, pesticide application rate and frequency (maximum assumed), method of application (aerial, air blast, ground spray), environmental fate data (deposition, adsorption/desorption, degradation), PCA, site-specific information (daily weather patterns, rainfall, hydrology, management practices).	Daily loadings over 36-year period ($mg\,L^{-1}$).

Model characterisation	Model peer review and evaluation	Links to other models
Conservative (Tier I) screening level (assumes maximum application rates and highest exposure scenario; does not have stochastic process to address variability or uncertainty).	No external peer review; limited model evaluation.	Designed to mimic a PRZM/EXAMS simulation (with fewer inputs).
Conservative (Tier I) screening level (assumes maximum application rates and based on vulnerable groundwater sites; does not have stochastic process to address variability or uncertainty).	External SAP review in 1997; modelled estimates have been compared with groundwater monitoring datasets and other models (PRZM).	
Higher-tiered (Tier II) screening level (accounts for impact of daily weather, but uses maximum pesticide application rates and frequencies; stochastic processes address the variability in natural systems, populations, and processes as well as the uncertainty in input parameters using one-stage Monte Carlo).	External FIFRA SAP peer review; components of model have been evaluated (e.g., performance of soil temperature simulation algorithms); model calibration using sensitivity analyses and comparisons with other models.	Links subordinate PRZM and VADOFT models; receives data from and inputs data to EXPRESS; can be linked with other models.

(*continued*)

Table 3.3: (*continued*)

Model	Model purpose	Model type	Model inputs	Model outputs
EXAMS	Estimates pesticide and organic chemical concentrations in surface water or groundwater from point or non-point sources, dry fallout or aerial drift, atmospheric washout, or groundwater seepage at local or regional level.	Steady-state, one-dimensional, compartmental (box) model.	Chemical loadings (runoff, spray drift), chemical properties, transport and transformation processes (volatilisation, sorption, hydrolysis, biodegradation, oxidation, photolysis), system geometry and hydrology (volumes, areas, depths, rainfall, evaporation rates, groundwater flows).	Annual daily peak concentration ($mg\,L^{-1}$), maximum annual 96-hour, 21-day and 60-day average concentration ($mg\,L^{-1}$), annual average concentration ($mg\,L^{-1}$).
WASP	Estimates chemical concentrations (organics, simple metals, mercury) in surface water from point and non-point sources and loadings from runoff, atmosphere, or groundwater for complex water bodies at regional level.	Dynamic, three-dimensional, compartmental (box) model.	Chemical loadings (runoff, deposition, reaeration), chemical properties, flows (tributary, wastewater, watershed runoff, evaporation), transport and transformation processes (dispersion, advection, volatilisation).	Average concentration per water segment ($mg\,L^{-1}$).

Model characterisation	Model peer review and evaluation	Links to other models
Higher-tiered (Tier II) screening level (accounts for impact of daily weather, but uses maximum pesticide application rates and frequencies; problem-specific sensitivity analysis is provided as a standard model output).	External FIFRA SAP peer review; model system evaluation tests have compared model performance against measured data in either a calibration or validation mode.	Used as surface water quality model in 3MRA; includes file-transfer interfaces to PRZM3 terrestrial model and FGETS and BASS bioaccumulation models.
Higher-tiered (generates predicted best estimate values for each segment/time period; does not have stochastic process to address variability or uncertainty).	No formal peer review, but model application has been published in peer-reviewed literature; model components are published in peer-reviewed literature.	Uses chemical fate processes from EXAMS; can be linked with loading models, hydrodynamic and sediment transport models, and bioaccumulation models; can be linked to FRAMES; under development for inclusion within BASINS framework.

(*continued*)

Table 3.3: (*continued*)

Model	Model purpose	Model type	Model inputs	Model outputs
EPANET	Estimates chemical concentrations in treated drinking water delivered to consumers throughout a water distribution piping system over an extended period of time.	Dynamic, Lagrangian transport model with chemical reactions both in the bulk water and at the pipe wall.	Pipe network characteristics (network topology; pipe sizes, lengths, and roughness; storage tank dimensions; pump characteristics), water usage rates, source locations, chemical input rates, and chemical reaction coefficients.	Chemical concentration ($mg\,L^{-1}$) at each time step and water withdrawal point within the piping network (also estimates water age and source contribution).

[a]AERMOD was promulgated as a replacement to ISC3 on 9 November 2005.

modelling compares with central site monitoring. For example, a recent study found the ASPEN model results to be in substantial agreement with monitored ambient HAP concentrations in a large heterogeneous area in Texas, although poor agreement was found among a few HAPs that were not as well characterised (Lupo and Symanski, 2008). CMAQ has also been compared with other atmospheric chemistry models in a recent study assessing trends in atmospheric mercury deposition (Sunderland *et al.*, 2008), and CAMx modelling results have been evaluated against observed ozone and PM concentrations in a number of studies (Emery *et al.*, 2004; Morris *et al.*, 2004, Wagstrom *et al.*, 2008).

Surface water and drinking water models

The identified surface water and drinking water models also share some similarities and differences. For example, these models simulate the fate and transport of contaminants in the environment in order to ultimately predict loadings to or ambient concentrations in sediment, surface water bodies, ambient groundwater, or drinking water. However, these models differ in regard to relevant pollutants, receptors, and spatial and temporal scales. These models are currently used by the US EPA or other stakeholders in a variety of applications, including aquatic, drinking water and community exposure assessments. Unlike the air quality and dispersion models, the US EPA has not published any recent guidance on recommended or preferred water quality models for use in different applications.

FIRST (US EPA, 2001a) and GENEEC (US EPA, 2001b) are screening-level models that estimate pesticide concentrations in simple surface water bodies for use in drinking water exposure assessments and aquatic exposure assessments, respectively.

Model characterisation	Model peer review and evaluation	Links to other models
Higher-tiered (generates predicted best estimate values for each distribution point/time period; does not have stochastic process to address variability or uncertainty, although other researchers have added Monte Carlo extensions to this model).	Model structure and equations have been published in peer-reviewed literature; decay kinetics have been tested and evaluated with data collected from multiple water distribution systems; model predictions have been compared with field studies.	EPANET-MSX is an extensible, multispecies chemical reaction modelling system that has been linked to EPANET; EPANET-DPX is a distributed processing version of EPANET; the EPANET engine has been incorporated into several commercial software packages that are widely used by water utilities.

Both of these models are single-event models: i.e., they assume that one single large rainfall/runoff event occurs and removes a large quantity of pesticide from the field to the water at one time. FIRST is based on a relatively large (172.8 ha) index reservoir watershed that was selected to be representative of a number of reservoirs in the central Midwest that are known to be vulnerable to pesticide contamination. This model also accounts for the percentage of a watershed that is planted with specific crops (PCA), the adsorption of pesticides to soil and sediment, pesticide degradation in soil and water, and flow through the reservoir. GENEEC is based on a much smaller (10 ha) standard agricultural field-farm pond scenario that assumes a static water body. Both of these models were derived from higher-tiered (Tier II) models (see below), but they are simpler in design, and require fewer inputs and less time and effort to use. SCIGROW (US EPA, 2001c) is another screening-level model that estimates pesticide concentrations in shallow, vulnerable groundwater for use in drinking water exposure assessments. FIRST, GENEEC and SCIGROW are all used by OPP's Environmental Fate and Effects Division to provide conservative, screening-level (Tier I) predictions of pesticide concentrations (i.e., EECs) in order to assess human or ecological risks during the registration or re-registration process for a pesticide.

PRZM (Suarez, 2006) and EXAMS (Burns, 2000), which were developed within ORD's CEAM, are also screening-level models that provide more refined (Tier II) estimates of pesticide concentrations in simple surface water bodies for use in aquatic or drinking water exposure assessments. These models account for chemical-specific characteristics, and include more site-specific information regarding application methods and the impact of daily weather patterns on a treated field over time. These models also assume that a pesticide is washed off the field into a water body by 20–40

rainfall/runoff events per year. However, like the Tier I models, PRZM and EXAMS assume maximum pesticide application rates and frequencies for a vulnerable drinking water reservoir. PRZM is a dynamic, one-dimensional, finite-difference compartmental model that estimates pesticide and organic chemical loadings to surface water by simulating how a contaminant that leaches into soil (e.g., pesticide applied to a crop) is transported and transformed down through the crop root and unsaturated zone and reaches a surface water body. EXAMS then simulates the movement of the pesticide or organic chemical in surface water under either steady-state or dynamic conditions based on loadings from point or non-point sources, dry fallout or aerial drift, atmospheric washout, or groundwater seepage. PRZM and EXAMS have historically been used by OPP to assess agricultural pesticide runoff in water bodies where the pattern and volume of use are known (Tier II assessments). However, EXAMS has also been used by the US EPA to evaluate the behaviour of relatively field-persistent herbicides and to evaluate dioxin contamination downstream from paper mills, and by manufacturing firms for environmental evaluations of newly synthesised materials. EXPRESS (Burns, 2006) is a separate software system that is sometimes used to link the PRZM and EXAMS models together.

WASP (Ambrose *et al.*, 2006; Wool *et al.*, 2001) is a higher-tiered, dynamic, three-dimensional compartmental model that simulates pollutant concentrations in the sediment and surface water (by depth and space) in water bodies of different complexity on a regional level. WASP assesses transport and kinetic processes separately, and includes two types of module: water quality modules (eutrophication, heat) and toxicant modules (simple toxicants, non-ionising toxicants, organic toxicants, mercury). This model is applicable primarily to small rivers, lakes and reservoirs. However, because WASP can evaluate very complex water bodies, and integrates spatially across large networks, it is generally used for more detailed or specialised applications. For example, the US EPA's OW has used WASP to study the effects of phosphorus loading, heavy metal pollution and organic chemical pollution, including kepones, PCBs and volatile organics, on a number of aquatic ecosystems. BASINS (US EPA, 2001d) is a separate multipurpose environmental analysis and decision support system that integrates (using a GIS framework) environmental data, analytical tools and modelling programs. This system was designed for use by regional, state and local agencies in performing watershed and water quality-based studies, and is also used by the US EPA's OW to support the development of TDMLs. WASP is currently under development for inclusion within the BASINS system.

EPANET is a hydraulic and water quality model developed within ORD's NRMRL that tracks the flow of drinking water and its constituent concentrations throughout a water distribution piping system (US EPA, 2000c). EPANET can simulate the behaviour of different chemical species, such as chlorine, trihalomethane and fluoride, within pressurised pipe networks over extended periods. This model can also evaluate a wide range of chemical reactions, including the movement and fate of a reactive material as it grows or decays over time (e.g., using *n*th order kinetics to model reactions in the bulk flow, and zero- or first-order kinetics to model reactions at the pipe wall). EPANET was developed primarily as a research tool to help water utilities maintain and improve the quality of water delivered to consumers, but it can also be used to design water sampling

programmes (e.g., select compliance monitoring locations under the US EPA's Stage 2 Disinfectants and Disinfection Byproducts Rule), perform hydraulic model calibration, and conduct consumer exposure assessments. For example, the US EPA's National Homeland Security Research Center is currently using EPANET to predict the effects of contaminant incidents at specific locations over time within distribution systems (Morley *et al.*, 2007). This model has also been used in various epidemiological investigations, such as to estimate the contribution of contaminated groundwater from various points of entry of the distribution system to specific residences in Toms River, New Jersey (Maslia *et al.*, 2000), and to estimate the flow and mass of tetrachloroethylene in drinking water through a town's network to specific residences in Cape Cod, Massachusetts (Aschengrau *et al.*, 2008).

Primary inputs to the surface water and drinking water models include pesticide application rates and methods, physical and chemical properties, pollutant loadings, hydrology and flows, soil properties and topography, and environmental fate data and transport and transformation processes (e.g., soil degradation, hydrolysis, ionisation and sorption, advective and dispersive movement, volatilisation). EPANET also includes inputs related to the layout and characteristics of the piping system throughout a drinking water distribution network. Outputs to these models include short-term (e.g., daily peak) or longer-term (e.g., annual average) ambient concentrations in the sediment, surface water column, groundwater or drinking water, or time-varying concentrations at specific locations (e.g., distribution point). Most of these models are deterministic, and report either maximum or average values. The Tier I screening-level models are also expected to overestimate pesticide concentrations in water. Although few of these models contain stochastic processes to address variability or uncertainty, PRZM uses one-stage Monte Carlo techniques to address the variability in natural systems, populations and processes, as well as the uncertainty in input parameters. A problem-specific sensitivity analysis is provided as a standard model output for EXAMS. Additionally, although the current version of EPANET does not provide probabilistic estimates, other researchers have developed extensions of this model that have Monte Carlo capabilities (Morley *et al.*, 2007).

Each of the identified fate/transport models has been peer-reviewed internally, and many have undergone external peer reviews. For example, aspects of the FIRST and SCIGROW models underwent external FIFRA SAP reviews in the late 1990s, which included a review of the US EPA's index reservoir scenario and PCA methodology. PRZM and EXAMS have also been subjected to an external peer review by the FIFRA SAP. WASP has not had a formal external peer review, but has been heavily cited in the peer-reviewed literature for its application in water quality and eutrophication assessments (Tufford *et al.*, 1999; Wool *et al.*, 2003). The model structure and equations for EPANET have also been published in the peer-reviewed literature (Rossman *et al.*, 1994; Rossman and Boulos, 1996).

Although the screening-level surface water and drinking water models have undergone limited model evaluation, components of some of the other models have been evaluated. For example, the performance of soil temperature simulation algorithms was evaluated for PRZM, in which model results were compared and evaluated based on the ability to predict *in situ* measured soil temperature profiles in an

experimental plot during a 3-year monitoring study (Tsiros and Dimopoulos, 2007). Additionally, a sensitivity analysis of PRZM and three other pesticide leaching models was performed using a one-at-a-time approach of varying input parameters, in which it was found that parameters that had the largest influence on pesticide loss were generally those predicting the extent of soil sorption (Dubus *et al.*, 2003). The model performance of EXAMS has also been compared against measured data in a number of model system evaluation tests for different chemicals (e.g., dyes, herbicides, insecticides, phenols, other organic chemicals) and environments (e.g., small streams, rivers, ponds, rice paddies, bays). EPANET's decay kinetics have been tested and evaluated with data collected from multiple water distribution systems, and model simulation results have been compared with field data, other dynamic water quality models, and analytical solutions (Rossman *et al.*, 1994; Rossman and Boulos, 1996). This model also contains a calibration option that allows the user to compare the results of a simulation against measured field data if such data exist for a particular period of time within a distribution system.

3.4.2 Exposure models

The exposure models included here generally focus on either inhalation or multimedia exposures for human receptors at the individual and/or population level (see Table 3.4). HAPEM (Rosenbaum, 2005; Rosenbaum and Huang, 2007) and APEX (US EPA, 2006e) were developed primarily to support Agency regulations on criteria air pollutants (e.g., CO, PM, ozone) and air toxics (e.g., benzene) from mobile or stationary sources at local, urban or national scales. For example, HAPEM was used as the primary exposure model for assessing inhalation exposures to HAPs under the 2007 MSAT rule (US EPA, 2007b). APEX (formerly called the probabilistic NAAQS Exposure Model for Carbon Monoxide, pNEM/CO) was used to estimate inhalation exposures as part of the ozone NAAQS (US EPA, 2007c). HAPEM has historically been used more often than APEX for regulatory purposes, because it relies on relatively few inputs and is easy to use, but this model is better suited for assessing long-term exposures to pollutants on a national scale (e.g. air toxics) rather than shorter-term exposures to pollutants on a local scale (e.g., criteria pollutants). These models have also been used within and outside the Agency for various applications, such as determining priority pollutants under the US EPA's (2006c) NATA programme, and estimating NO_2 exposures from various emission sources, such as on-road vehicles and indoor gas cooking (Rosenbaum *et al.*, 2008). Although TRIM-Expo (US EPA, 2003a) was developed as the "next generation" multimedia exposure model to support these same types of regulations, to date, this model has relied on APEX only for assessing inhalation exposures (i.e., the ingestion exposure module has not yet been completed).

SHEDS-Air Toxics (Isakov *et al.*, 2006; Stallings *et al.*, 2008) and SHEDS-PM (Burke, 2005; Burke *et al.*, 2001) were developed by ORD primarily as internal research models to provide state-of-the-art research tools for evaluating inhalation exposures to toxic and particulate air pollutants, respectively. SHEDS-Air Toxics has been used to assess benzene exposures in case studies linking air quality and exposure

models (Isakov *et al.*, 2006), and SHEDS-PM has been used in case studies to evaluate $PM_{2.5}$ exposures in Philadelphia (Burke *et al.*, 2001). A number of algorithms and improvements developed for inhalation exposure in these two SHEDS models have also been incorporated into the regulatory models, such as HAPEM and APEX.

MCCEM (US EPA, 2007d) and WPEM (US EPA, 2001e, 2007e) represent indoor exposure models that were developed by OPPTS to provide more detailed exposure assessments of indoor air pollutants from sources such as carpeting and wall paint. Although these models could potentially be used for assessing exposures to new chemicals, the level of specificity provided by these models is typically not required for making routine decisions under Section 5 of TSCA. Currently, these models are being used internally by OPP to assess antimicrobial exposures, and in instances where there is a potential concern about a major commodity chemical that requires a more detailed or accurate assessment of potential consumer uses and exposures (e.g., formaldehyde in homes). The WPEM model was also designed as a support tool for industry to assist in the early design of safer new painting products (i.e., products that would not result in exposures of concern). These models have many potential external applications and users, including states, academic researchers, consulting firms, and other governments. For example, MCCEM has been used to perform chemical-specific indoor air exposure assessments for benzene and toluene under the US EPA's VCCEP (ACC, 2006a, 2006b). IAQX (Guo, 2000a, 2000b) is a similar type of indoor exposure model that was developed within ORD primarily for external users conducting high-end exposure research (not for regulatory or internal research purposes). The IAQX model implements over 30 source models and five sink models, and is often used as a teaching tool by various universities (Guo, 2008, personal communication).[7] This model has also been used to perform chemical-specific indoor air exposure assessments for acetone (i.e., to estimate exposure concentrations for the nail tip removal scenario) under VCCEP (ACC, 2003).

The SWIMODEL was developed by OPP's Antimicrobial Division as a screening tool to assess exposures to pool chemicals and breakdown products found in swimming pools and spas (US EPA, 2003b). This model is typically used to assess three primary exposure routes (incidental ingestion, dermal absorption, and inhalation), but can also be used to assess other less significant exposure routes. The SWIMODEL generally relies on conservative equations and default input parameter values to calculate worst-case exposures for either competitive or non-competitive swimmers. Although this model can be used to assess exposures in either indoor or outdoor settings, predicted outdoor exposures will tend to be more conservative than predicted indoor exposures. OPP is in the process of updating some of the model input parameters (e.g., recreational exposure time and frequency), but these updates have not yet been incorporated into the model itself. This model is used primarily by OPP to support the registration and re-registration of pesticides, and has been used by pesticide registrants and researchers to assess potential swimmer exposures.

PIRAT (US EPA, 2007f) is another common screening-level exposure model used internally by OPP to support the US EPA's evaluation of new inert ingredients as part of the pesticide risk assessment process. This model generally relies on conservative assumptions, default scenarios and model equations that are codified in the

Table 3.4: Selected exposure models used by the US EPA.

Model	Model purpose	Exposure routes	Model inputs	Model outputs
HAPEM	Estimates population-level exposures to criteria pollutants (CO, PM) and air toxics (HAPs) for general population or subgroups at urban and national levels.	Inhalation (indoors, outdoors, in-vehicle commuting).	Ambient air concentrations (measured or modelled) based on mobile, area or point sources, near road factor, indoor/outdoor data (ratio), census tract population and demographic data, commuting data, exposure factors, activity patterns.	Monthly, seasonal or annual average concentrations ($mg\,m^{-3}$).
APEX	Estimates population-level exposures and doses to criteria pollutants (CO, ozone) and air toxics (benzene, chromium) for general population or subgroups at local, urban and consolidated metropolitan levels.	Inhalation (indoors, outdoors, in-vehicle commuting).	Ambient air concentrations (measured or modelled) based on mobile, area or point sources, indoor/outdoor data (ratio or mass balance model), census tract population and demographic data, commuting data, exposure factors, activity patterns.	1-hour, 8-hour, daily, monthly or annual average concentrations (ppm or $mg\,m^{-3}$); delivered doses ($mg\,kg^{-1}\,day^{-1}$) for CO only.

Model characterisation	Model peer review and evaluation	Links to other models
Screening level (appropriate for assessing average long-term exposures at urban/national scale; stochastic process addresses variability in activity patterns and behaviours using one-stage Monte Carlo).	External SAB peer review of model in 2001 as part of evaluating NATA 1996 data, and model reviewed as part of 2007 MSAT rule; some model components (activity data, microenvironmental factors, commuting data) have been evaluated; model results compared with ASPEN (>30 HAPs) and APEX (benzene).	Uses predicted air concentrations from ASPEN, AERMOD or CMAQ.
Higher-tiered (stochastic process addresses variability in population, and accounts for spatial and temporal variability of microenvironmental parameters using one-stage Monte Carlo; new version will also address uncertainty in input parameters using two-stage Monte Carlo).	External CASAC peer review in 2006 as part of evaluating ozone NAAQS; extensive evaluation of computer code; some model components (activity data, microenvironmental factors, commuting data) have been evaluated; model results compared with HAPEM (benzene).	Uses predicted air concentrations from AERMOD or CMAQ; serves as inhalation exposure module for TRIM.[a]

(*continued*)

Table 3.4: (*continued*)

Model	Model purpose	Exposure routes	Model inputs	Model outputs
SHEDS-Air Toxics	Estimates individual or population-level exposures and doses to air toxics (benzene, formaldehyde) for general population or subgroups at local and urban levels.	Inhalation (indoors, outdoors, in-vehicle commuting), dermal (showering/bathing and residues/spillage during refuelling), and ingestion (dietary).	Ambient air concentrations (measured or modelled) based on ambient (outdoor) and non-ambient (indoor) sources, indoor/outdoor data (ratio, mass balance model, or regression equation), residue data and dietary diaries, census tract population and demographic data, commuting data, exposure factors, activity patterns.	Daily average concentrations ($mg\,m^{-3}$); total daily average exposure ($mg\,m^{-3}$), and total daily intake dose ($mg\,kg^{-1}\,day^{-1}$); contribution of ambient and non-ambient sources to each.
SHEDS-PM[b]	Estimates individual or population-level exposures and doses to particulate matter for different size fractions (fine, coarse, ultrafine) and species (ions, metals) for general population or subgroups at local and urban levels.	Inhalation (indoors, outdoors, in-vehicle commuting).	Ambient air concentrations (measured or modelled) based on ambient (outdoor) and non-ambient (indoor) sources, indoor/outdoor data (ratio, mass balance model, or regression equation), census tract population and demographic data, commuting data, exposure factors, activity patterns.	Daily average concentrations ($mg\,m^{-3}$); total daily average exposure ($mg\,m^{-3}$), total daily intake dose (mg), and total daily deposited dose (mg); contribution of ambient and non-ambient sources to each.

Model characterisation	Model peer review and evaluation	Links to other models
Higher-tiered simulation model (stochastic process addresses variability within and between individuals in a population, and uncertainty in input parameters at event level, using two-stage Monte Carlo).	Model has not been externally peer-reviewed because it is an internal research model that is continually modified (but peer-reviewed publications related to its application are expected); model has not been evaluated because of limited access to good air toxics data (but NERL's recently completed exposure study in Detroit will be used to evaluate this model).	Some algorithms have been incorporated into HAPEM and APEX; model combines SHEDS-PM approach for air pollutants with SHEDS-Multimedia algorithms for dietary and dermal exposures; case study applications with CMAQ, AERMOD modelled concentrations.
Higher-tiered (stochastic process addresses variability across population in exposure factors and uncertainty in input parameters using two-stage Monte Carlo).	External peer review is currently under way; model predictions were compared with exposure field studies (community and personal exposures), including data from the NERL PM Panel Study in RTP (new project will compare current model version with same data).	Some algorithms have been incorporated into HAPEM and APEX; model capable of using predicted PM air concentrations from AERMOD or CMAQ.

(*continued*)

Table 3.4: (*continued*)

Model	Model purpose	Exposure routes	Model inputs	Model outputs
MCCEM	Estimates individual-level exposures and doses to chemicals released from consumer products or materials in residential setting.	Inhalation (indoors).	Indoor environment (e.g., type of residence, zone volumes, interzonal air flows, air exchange rate), pollutant emission rate (as a function of time), exposure factors, occupant activity patterns.	Single-event dose (mg); 15-min, 1-hour, and daily average concentration ($mg\,m^{-3}$); ADD, LADD and acute peak dose ($mg\,kg^{-1}\,day^{-1}$).
WPEM	Estimates individual-level exposures and doses to chemicals released from wall paint (latex, oil based) applied using a roller or brush for residents or workers in residential setting.	Inhalation (indoors).	Chemical and paint-specific data (e.g., type of paint, chemical weight fraction), painting scenario (e.g., room size, building type, air exchange rate), exposure factors, occupancy and activity patterns (e.g., weekdays/ weekends, during painting event).	Highest instantaneous, 15-min, 8-hour, and lifetime average daily concentration ($mg\,m^{-3}$); LADD ($mg\,kg^{-1}\,day^{-1}$).
IAQX	Estimates individual-level exposures to chemicals in residential setting (general simulation program and specific programs for indoor paint, indoor spills, particles, and flooring/ carpeting).	Inhalation (indoors).	Pollutant sources (e.g., number), building features (e.g., volume of zone, air flow rates, number of interior surface types), ventilation systems and interior sinks (adsorption and desorption rates), exposure factors, emission rate.	Concentration ($mg\,m^{-3}$) or exposure ($mg\,m^{-3} \times$ time) – based only on breathing rate, not body weight.

Model characterisation	Model peer review and evaluation	Links to other models
Higher-tiered (stochastic process addresses uncertainty in input parameters using one-stage Monte Carlo).	External letter peer review in 1998; model published in peer-reviewed literature; model was evaluated using data from test house and through comparisons against other models (model compared well with monitoring data and other models).	Uses WPEM for paint scenarios.
Higher-tiered (does not have stochastic process to address variability or uncertainty).	External letter peer review in 1998; model was evaluated extensively by creating emission rate algorithms based on small-chamber studies and comparing modelled estimates with measured data in the US EPA test home (results were comparable).	Model is subset of MCCEM (i.e., engine and mathematics are from MCCEM, but tailored for specific application of wall paint); model is based on data generated from IAQX.
Higher-tiered (designed mainly for advanced users; requires more knowledge to use than other indoor air quality models; does not have stochastic process to address variability or uncertainty).	External peer review via published papers; limited model evaluation (except for paint model) because model based on existing models.	Model implements over 30 source models and five sink models; complements and supplements existing IAQ simulation programs (e.g., RISK, MCCEM, CONTAMW); data generated from model is used in WPEM.

(*continued*)

Table 3.4: (*continued*)

Model	Model purpose	Exposure routes	Model inputs	Model outputs
SWIMODEL	Estimates individual-level exposures and doses to pool chemicals and breakdown products in swimming pools and spas.	Inhalation (indoor, outdoor), dermal, incidental ingestion (other routes include buccal/ sublingual, nasal/orbital, aural).	Physico-chemical data, water concentration (expected mean and maximum at the maximum label use rate), air concentration (empirically measured or estimated using Henry's law or Raoult's law), exposure factors, dermal permeability values, absorption rates.	Potential dose rate or intake ($mg\ event^{-1}$), ADD ($mg\ kg^{-1}\ day^{-1}$), LADD ($mg\ kg^{-1}\ day^{-1}$).
PIRAT	Estimates individual-level exposures and doses to pesticide inert ingredients in residential setting.	Inhalation (indoor, outdoor), dermal (product, pets, dust, surface), incidental ingestion (hand, toy, grass, dirt).	Type of product, product formulation, function of inert, application technique and rate, exposure factors, use patterns.	ADD, LADD and acute potential dose ($mg\ kg^{-1}\ day^{-1}$); MOE.
DEEM^{TM}	Estimates individual or population-level dietary exposures and doses to pesticides for the general population or subgroups in residential settings.	Dietary ingestion (food, water).	Residues (pesticides and analytes), consumption data, CSFII population data, exposure factors, toxicity data rates.	Average daily intake ($mg\ kg^{-1}$); acute dose, ADD and LADD ($mg\ kg^{-1}\ day^{-1}$); MOE and % RfD.

Model characterisation	Model peer review and evaluation	Links to other models
Conservative screening level (uses default equations and parameter values, and assumes worst-case exposures; does not have stochastic process to address variability or uncertainty).	Limited external peer review (data on exposure duration and frequency published in peer-reviewed literature); limited model evaluation (indirect validation by comparing model results with biomonitoring studies bridged using PBPK models).	Used, along with other OPP models, in support of pesticide registration and re-registration decisions.
Conservative screening level (uses default assumptions and scenarios, and assumes continuous exposures to predicted concentrations; does not have stochastic process to address variability or uncertainty).	External letter (modified) peer review in 2004 (residential SOPs were previously reviewed by an SAP); limited model evaluation because based on default residential SOPs.	Relies on same assumptions and SOPs as active ingredients.
Higher-tiered (stochastic process addresses variability in residue values using one-stage Monte Carlo).	External SAP peer review in 1998; validation of model outputs using other Monte Carlo software when using same inputs; modelling results compared with other dietary and aggregate exposure models (SHEDS-Multimedia) and with biomonitoring data.	Used as dietary exposure model in Calendex.

(*continued*)

Table 3.4: (*continued*)

Model	Model purpose	Exposure routes	Model inputs	Model outputs
Calendex™	Estimates individual or population-level dietary and residential exposures and doses to pesticides for the general population or subgroups in residential setting.	Inhalation, dermal, dietary ingestion (food, water), and incidental ingestion (dust, surfaces).	Product use, residues and concentrations, consumption data, contact probabilities, degradation rates, CSFII population data, activity patterns, exposure factors, toxicity data.	Average daily intake ($mg\,kg^{-1}$); acute dose, 21-day average dose, ADD and LADD ($mg\,kg^{-1}\,day^{-1}$); MOE and % RfD.
CARES™	Estimates individual or population-level dietary and residential exposures and doses to pesticides for the general population or subgroups in residential settings.	Inhalation, dermal, dietary ingestion (food, water), and incidental ingestion (dust, surfaces).	Product use, residues and concentrations, consumption data, contact probabilities, degradation rates, US Census (PUMS) population data, activity patterns, exposure factors, toxicity data.	Daily, short-term or intermediate (2–30 days or 1–3 months), and 1-year average dose and toxic equivalent dose ($mg\,kg^{-1}\,day^{-1}$); MOE, hazard index, or toxicity equivalence factor.
LifeLine™	Estimates individual or population-level dietary and residential exposures and doses to pesticides for the general population or subgroups in residential settings.	Inhalation (shower/bath), dermal (shower/bath), dietary ingestion (food, water), and incidental ingestion (dust, surfaces, soil, pets, hand-to-mouth).	Product use, residues and concentrations, consumption data, contact probabilities, degradation rates, NCHS Natality population data, activity patterns, exposure factors, absorption.	Maximum daily absorbed dose, average daily absorbed dose, average seasonal absorbed dose, and 1-year average absorbed dose ($mg\,kg^{-1}\,day^{-1}$); MOE, % RfD, or toxicity equivalence factor.

Model characterisation	Model peer review and evaluation	Links to other models
Higher-tiered (stochastic process addresses variability in residue values and contact levels using one-stage Monte Carlo).	External SAP review in 2000, and high level of external review by stakeholders; extensive QA/QC testing and verification of processes; modelling results compared with other dietary and aggregate exposure models (CARES, LifeLine) and with biomonitoring data for chlorpyrifos.	Uses DEEM as dietary exposure model; uses PRZM/EXAMS to estimate drinking water concentrations.
Higher-tiered (stochastic process addresses variability in residue levels, consumption, and activity patterns using one-stage Monte Carlo; contribution analysis function can be used to conduct sensitivity analyses).	External SAP review in 2002; modelling results compared with other dietary and aggregate exposure models (Calendex, LifeLine) and with biomonitoring data for carbaryl; acute dietary exposure values compared with residue data (monitoring and market survey data) for chlorpyrifos.	Builds off former REX model.
Higher-tiered (stochastic process addresses variability in population by age and season using one-stage Monte Carlo).	External SAP review in 1999 and 2000; modelling results compared with other dietary and aggregate exposure models (Calendex, CARES).	Software probabilistic methodologies and basic approaches used in Tribal LifeLine™ model.[c]

(*continued*)

Table 3.4: (*continued*)

Model	Model purpose	Exposure routes	Model inputs	Model outputs
SHEDS-Multimedia[d]	Estimates individual or population-level exposures and doses to pesticides and other chemicals (metals, persistent bioaccumulative toxins) for the general population or subgroups in residential settings.	Inhalation, dermal, dietary ingestion (food, water), and incidental hand-to-mouth and object-to-mouth ingestion (dust, soil, surface residues).	Product use (optional), residues and concentrations (modelled or measured), application/decay rates (optional), consumption data, media contact probabilities, US Census population data (built in), activity patterns (CHAD data built in), exposure factors, absorption rates.	Average daily exposure ($mg\,kg^{-1}$), average daily absorbed dose ($mg\,kg^{-1}\,day^{-1}$).
SHEDS-Wood	Estimates individual or population-level exposures and doses to wood preservatives (arsenic, chromium) for children in frequent contact with CCA-treated decks and playsets.	Dermal and incidental hand-to-mouth ingestion (soil, wood residue).	Residues and concentrations, contact probabilities, transfer efficiencies, US Census population data, activity patterns (longitudinal), exposure factors, absorption rates.	15-day and 90-day average absorbed doses, average daily absorbed dose, and lifetime average daily absorbed dose ($mg\,kg^{-1}\,day^{-1}$).

[a]Although there is a TRIM-Expo module within the TRIM Framework, it currently relies solely on APEX for evaluating inhalation exposures.
[b]SHEDS-ozone model is currently under development.
[c]New version has been developed for tribal communities and other focused populations (Tribal LifeLine™) that relies on the same probabilistic methodologies and basic approaches as existing software (changes made to some software operational functions, exposure opportunity modules, and knowledgebases).
[d]SHEDS-dietary module is currently being incorporated into SHEDS-Multimedia (version 4); additional enhancements will include cumulative algorithms and other changes to address 2007 SAP comments.

US EPA's (1997a) residential SOPs to assess aggregate residential exposures to pesticide inert ingredients. Prior to August 2006 these residential SOPs were also used by OPP for screening purposes to assess REDs for active pesticides. Reg Reviews have replaced the former RED process, and OPP is in the process of upgrading the

Model characterisation	Model peer review and evaluation	Links to other models
Higher-tiered (stochastic process addresses variability in population and uncertainty in input parameters using bootstrap method and two-stage Monte Carlo; several sensitivity analysis methods applied separately).	External SAP peer review in 2002, 2003 and 2007; model results compared with other dietary and aggregate exposure models (DEEM, CARES, Calendex, LifeLine) and with data collected from NHEXAS, NHANES, US EPA/ORD/ NERL and other field measurement studies.	Can be linked with air quality and PBPK models (used in MENTOR Framework; interfaces with ORD's ERDEM).
Higher-tiered (stochastic process addresses variability in population and uncertainty in input parameters using bootstrap method and two-stage Monte Carlo; sensitivity analysis option).	External SAP peer review in 2002 and 2003; two published papers; US EPA reports; model results compared with other CCA exposure models (produced similar mean estimates).	Uses modified version of LifeLine to calculate body weight and surface area for children.

residential SOPs (e.g., to include distributions) for use in future Reg Reviews. Other models that are used by OPP to support Reg Reviews, and which predict dietary and/ or residential aggregate pesticide exposures, include DEEM^{TM} (Kidwell *et al.* 2000), Calendex^{TM} (Peterson *et al.*, 2000), CARES^{TM} (Farrier and Pandian, 2002; Young *et*

al., 2006) and LifeLine™ (LifeLine Group, Inc., 2000; Price *et al.*, 2001). These models were designed in response to the 1996 FQPA to assess multimedia pesticide exposures in residential settings, although they can also be used for other chemicals and institutions (e.g., school, office). DEEM™ is the most frequently used by OPP to assess exposures, because many pesticides require refinement only in dietary assessments. Calendex™ is another model that is often used by OPP to assess both dietary exposures (based on DEEM™) and multi-pathway residential exposures to pesticides in support of FQPA. For example, Calendex™ was the primary model used to evaluate the 31 OP pesticides under the OP cumulative risk assessment (US EPA, 2006f) and the 10 NMC pesticides under the NMC cumulative risk assessment (US EPA, 2007g). CARES™, which began as a spreadsheet model called Residential Exposure Assessment (REX), was developed by industry in consultation with the US EPA as a publicly available alternative to Calendex™ that is free of charge (i.e., DEEM™ and Calendex™ have a licensing fee). LifeLine™ was also developed as a publicly accessible model as part of a cooperative effort between the US EPA and external researchers to assess aggregate exposures in support of pesticide registration under FQPA. In addition to their regulatory applications, all of these models have been (or can be) used by external users such as academics or communities for broader research purposes (e.g., to determine important exposure pathways and risk drivers).

SHEDS-Multimedia (Stallings *et al.*, 2007), formerly called SHEDS-Pesticides, is ORD's state-of-the-science aggregate and cumulative exposure model. This model is similar to OPP's dietary and residential aggregate exposure models, and is also intended to support OPP's exposure and risk assessments under FQPA. However, SHEDS-Multimedia has some unique capabilities, such as using a microenvironmental approach to track the movement of individuals throughout the day; relying on a within-day (1–60 min) time step (rather than a daily time step); simulating hand-to-mouth residue ingestion as a function of dermal exposure; accounting for dermal loading and removal processes (e.g., washing, bathing); and using a more sophisticated algorithm for constructing longitudinal activity patterns of simulated individuals. To date, this model has been used to provide supplemental information on children's exposure (via hand-to-mouth contact) in OPP's NMC cumulative risk assessment (US EPA, 2007g), was used in OPP's aldicarb and methomyl RED assessments (US EPA, 2007h), and is being used in OPP's upcoming pyrethroids cumulative risk assessment. SHEDS-Multimedia has also been applied by various academic institutions and other government agencies for research and regulatory purposes. SHEDS-Wood (Zartarian *et al.*, 2005b, 2006) is a scenario-specific version of SHEDS-Multimedia developed by ORD specifically to assess children's exposures to wood preservatives from decks and playsets. This model was used in OPP's children's risk assessment for chromated copper arsenate (CCA) (US EPA, 2008c). SHEDS-Wood has also been used outside the Agency by industry and state agencies for CCA and other wood preservative assessments.

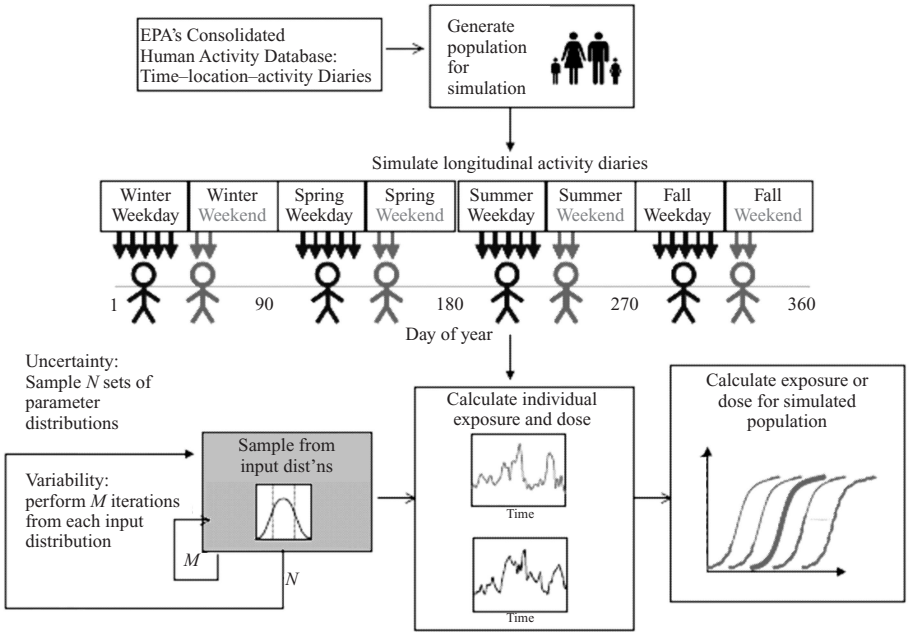
All of the identified exposure models couple environmental pollutant concentrations in specific environmental media or microenvironments with estimates of the actual or assumed amount of time individuals spend in contact with these media or microenvironments to provide the most robust characterisation of exposure. These

models simulate and track an individual's movements through time and space (i.e., microenvironmental approach) and/or apportion the time of day spent in various activities or locations in order to yield a time series or estimate of daily exposure to a pollutant. Similar steps among these models include:

- simulating an individual and their activity patterns (and in some cases simulating longitudinal activity patterns);
- combining activity information, environmental media concentrations, and exposure factors in exposure algorithms; and
- simulating population estimates using probabilistic sampling (see Figure 3.2).

However, specific aspects of these models may differ for each step, such as using different datasets and information sources for demographic characteristics, environmental media concentrations, activity patterns, and other exposure factors. Assumptions about longitudinal activities – i.e., simulating a person's activity pattern over a year or longer based on diary data for one day or a few days – can also differ among the models (e.g., models may assume a person has the same activity pattern every day, can draw a random activity pattern each day, or can account for correlated activities from one day to the next). Additionally, exposure algorithms and underlying fate/transport models can differ across the models (e.g., some models track dermal hand

Figure 3.2: General SHEDS model approach.



loading together with body hand loading, whereas others track these separately, and do not use dermal hand loading as an input to hand-to-mouth ingestion). MCCEM and WPEM differ from the population-based simulation models in that they represent steady-state, box models that rely on mass balance equations to estimate airborne exposures in different locations (i.e., zones) by distributing air within a home or other indoor setting, and apportion the amount of time individuals spend each day within each zone based on published time–activity patterns. IAQX is also an individual-level model, but it is not a steady-state box model (i.e., it calculates the time history of indoor air concentrations or personal exposures). The SWIMODEL also relies on a series of equations that calculate route-specific exposures based on chemical concentrations, physiochemical data, and exposure times assumed for selected swimmers. With the exception of MCCEM, WPEM, IAQX, SWIMODEL and PIRAT, all of the exposure models summarised here are designed primarily to characterise exposures at the population level (although the SHEDS and OPP models can also be used to characterise exposures at the individual level by using exposure time profiles).

Common inputs to the exposure models include product use, physico-chemical data, residue and concentration data (measured or modelled), consumption data, commuting data, indoor/outdoor relationships (e.g., using a factors or mass balance approach), indoor environment data, degradation and transfer rates, contact probabilities, population and demographic data, activity patterns, and other microenvironment data or exposure factors. Population and demographic data are typically based on the US Census or the USDA's CSFII, while activity patterns and scenarios are typically based on CHAD (McCurdy *et al.*, 2000; Stallings *et al.*, 2002) and the US EPA's (1997a) residential SOPs. Other exposure factors, such as intake rates and body weight, are generally based on the US EPA's (1997b) *Exposure Factors Handbook*, CSFII, or NHANES III for specified population or subpopulation groups. Outputs to these models generally include distributions of ambient concentrations (ppm or $mg\,m^{-3}$), average daily intake or exposure ($mg\,kg^{-1}$), and potential or absorbed doses ($mg\,kg^{-1}day^{-1}$) averaged over the short-term (e.g., 15 min, 1 hour, 8 hour, 1 day), intermediate (e.g., annual average concentration or ADD), or longer-term (e.g., lifetime average concentration or LADD) durations. However, because many of these models either generate time-series (hour by hour) exposure profiles over the course of a day, or use the calendar day as the basic unit of time for calculating exposures, estimated exposures can be averaged over any specified duration or number of days. Some of these models also compare estimated exposure or dose levels to existing toxicity criteria to evaluate potential human risks (e.g., MOE, % of RfD, hazard index, toxicity equivalence factor).

With the exception of several models used to assess individual and/or screening-level exposures (i.e., MCCEM, WPEM, IAQX, SWIMODEL and PIRAT), all of the exposure models reviewed are probabilistic models that utilise stochastic processes to address the variability and/or uncertainty in population estimates or model input parameters. For these models, the variability in population exposures is generally accounted for by running simulations for many individuals and then aggregating across all individuals. Uncertainty (and sometimes intra- and inter-subject variability) is typically addressed by defining various input variables using a distribution rather

than a point estimate. For example, some of the exposure models specify a probability distribution for the following model input parameters to address uncertainty and/or variability: ambient air concentrations; pesticide residue values in food; consumption rates; microenvironment factors; and different activity patterns or durations. Most of the exposure models rely on one-stage Monte Carlo techniques to address either variability or uncertainty (or both combined). Among the models reviewed here, the SHEDS models are the only exposure models that currently use two-stage Monte Carlo techniques to address both the variability in input parameters and the uncertainty of the mean of the first distribution (this feature will soon be available for APEX). SHEDS-Multimedia and SHEDS-Wood also rely on a bootstrap method for addressing uncertainty (i.e., so that fewer data result in more uncertainty and more data result in less uncertainty) (Xue *et al.*, 2006), and SHEDS-Wood includes an additional sensitivity analysis feature that uses a percentile scaling approach or multiple stepwise regression (this feature will soon be available for SHEDS-Multimedia). CARES^{TM} also includes a contribution analysis function that can be used to conduct sensitivity analyses. Of these models, SWIMODEL and PIRAT are the only screening-level models intentionally designed to perhaps overestimate exposures, but any of the exposure models can be modified to use conservative input parameters to produce high-end or bounding estimates. Although HAPEM is sometimes referred to as a "screening-level" model, this is due solely to its limited spatial and temporal abilities (i.e., it is most appropriate for assessing average long-term exposures at the national scale).

Because most of the exposure models included here are designed to support higher-tiered assessments, these models have generally undergone extensive internal review by the US EPA, and many have also been externally peer-reviewed. For example, HAPEM underwent an external SAB (2001) peer review as part of the evaluation of the 1996 NATA programme, and was externally reviewed as part of the 2007 MSAT rule (US EPA, 2007b). APEX also underwent an external peer review by CASAC (2006) as part of its evaluation of the ozone NAAQS. SHEDS-PM is currently being peer-reviewed, prior to its public release in 2009, but SHEDS-Air Toxics has not been externally peer-reviewed, because this model was developed primarily as an internal research model, and is continually being modified as part of NERL's ongoing research projects (although it will be described in subsequent peer-reviewed publications related to various application projects). MCCEM and WPEM both had external letter peer reviews in 1998, and MCCEM was patterned after an earlier DOS version that has been described in the peer-reviewed literature (Koontz and Nagda, 1991). IAQX has also been published in the peer-reviewed literature (Guo, 2002a, 2002b), but has not had a separate external letter peer review. The SWIMODEL has not undergone a formal external peer review, but components of this model (e.g., exposure duration and frequency for competitive swimmers) have been published in the peer-reviewed literature (Reiss *et al.*, 2006). PIRAT underwent a modified external letter peer review in 2004, and the residential SOPs have been reviewed previously by the US EPA's SAP. Because the US EPA's OPP requires that their FIFRA SAP review any model being used in exposure assessment for regulatory purposes, all of the OPP and SHEDS models developed to assess dietary and residential aggregate exposures have

undergone such peer reviews, including DEEM™ (SAP, 2000a), Calendex™ (SAP, 2000b), CARES™ (SAP, 2002a), LifeLine™ (SAP, 2001), SHEDS-Multimedia (SAP, 2007) and SHEDS-Wood (SAP, 2002b).

Although it is difficult to evaluate the results of some of these models in their entirety, most of the exposure models reviewed have undergone some degree of model evaluation. For example, despite the limited availability of personal monitoring data to perform direct comparisons with HAPEM, many of the key components of this model (e.g., activity data, microenvironment factors, and commuting data) have been evaluated in the peer-reviewed literature (Özkaynak *et al.*, 2008). HAPEM has also been evaluated relative to ASPEN by comparing modelling results for more than 30 HAPs, which illustrated the importance of accounting for time–activity patterns, commuting patterns, and other factors that can result in lower or higher estimated exposures (Özkaynak *et al.*, 2008). Attempts to evaluate APEX include comparisons of model results with personal ozone concentration measurements as part of the NAAQS assessment for ozone, in which model results were found to predict average personal exposure concentrations reasonably well, but to underestimate the variability in these estimates (US EPA, 2007c). In another study, APEX was found to under-predict personal ozone exposure measurements in indoor and in-vehicle microenvironments when windows were open, and to overpredict concentrations when windows were closed (Long *et al.*, 2008).

The results of APEX were also compared with HAPEM in a case study of benzene emissions in Houston, in which these models were found to provide similar estimated distributions for population exposures (Rosenbaum *et al.*, 2002). SHEDS-PM model predictions have been compared with some community and personal exposure field studies (Burke *et al.*, 2001), including data from the NERL's PM Panel Study in RTP (Burke *et al.*, 2002), and a new project is under way that will compare the current version of this model with these same PM data. However, personal exposure studies with appropriate study designs and sufficient measurements for a thorough evaluation of the SHEDS-PM model are limited (Burke *et al.*, 2001) and, to date, there has been limited access to a good air toxics dataset for evaluation of the SHEDS-Air Toxics model (although NERL's recently completed exposure study in Detroit will be used to evaluate the SHEDS models for air toxics species, and PM mass and components).

The prior (DOS) version of MCCEM was extensively evaluated, and included comparisons of model predictions with outputs from two other well-recognised indoor air models (CONTAM and INDOOR). Model outputs from the current (Windows) version of MCCEM have also been compared with the prior version using equivalent inputs. In addition, measured indoor air concentrations of toluene from an adhesive used in installing floor tiles have been compared with MCCEM model predictions based on small-chamber and research house testing (Nagda *et al.*, 1995). Similarly, WPEM has been extensively evaluated using data generated from small-chamber testing to develop emission rate algorithms, and by comparing model predictions with measured data collected in a US EPA research test home in North Carolina involving alkyd and latex primer and paint. In general, the comparisons for MCCEM and WPEM have shown a high degree of correspondence between modelled and measured

values. The IAQX model has undergone only limited evaluation (except for the paint module, which was based on test house and small-chamber data), because this model is based on a number of existing models.

The SWIMODEL has undergone limited evaluation using a PBPK model to bridge the output of published biomonitoring data to compare with model predictions in an effort to provide an indirect validation of or "reality check" on the modelling outputs (US EPA, 1999). PIRAT has also undergone little evaluation, because it is based on the US EPA's default residential SOPs. However, a comparison of measured insecticide (chlorpyrifos) exposure estimates from contact with turf based on urine biomonitoring with exposure estimates calculated using the US EPA's residential SOPs revealed that the measured residue transfers were well below the SOP estimates (Bernard *et al.*, 2001). Similarly, former exposure assessments performed under OPP's REDs process for OPs were found to overestimate human exposures when compared with biomonitoring data (Duggan *et al.*, 2003). Other analyses presented by the US EPA (2004b) to the FIFRA SAP have also suggested that the use of pharmacokinetic and biomonitoring data provides more refined estimates of carbaryl exposures than estimates based on the US EPA's residential SOPs. Calendex™, CARES™ and LifeLine™ have also been evaluated by comparing modelling results with other dietary and residential aggregate exposure models, as well as with biomonitoring and environmental monitoring or market survey data (Duggan *et al.*, 2003; Shurdut *et al.*, 1998; Wright *et al.*, 2002). In addition, model-to-model comparisons have shown that the dietary and residential aggregate exposure models can produce varying results, because of differences in methodologies (Young *et al.*, 2008). However, the US EPA's FIFRA SAP has recommended that the US EPA continue to use all of these models as a means of incorporating model uncertainty into an assessment, because each model possesses unique features that will prove useful in looking at different issues and more complex questions (SAP, 2004).

Additionally, a number of initial efforts have been made to evaluate the SHEDS-Multimedia model, including comparing the results of this model with those of other dietary or aggregate exposure models (Price and Zartarian, 2001; Xue *et al.*, 2004, 2008), comparing individual model predictions with available field measurements and biomonitoring data (Hore *et al.* 2005; Zartarian *et al.* 2000), and performing pathway-specific comparisons (Driver and Zartarian, 2008; Price and Zartarian, 2001). In general, the SHEDS-Multimedia predictions have compared reasonably well with biomonitoring data and other models, especially when evaluating the dietary module. However, the model was found to underpredict aggregate exposure results for chlorpyrifos based on a National Human Exposure Assessment Survey (NHEXAS) Minnesota biomonitoring study, most likely because it did not include a pathway for ingestion of environmental degradate (3,5,6-trichloro-2-pyridinol) residues. Efforts are currently under way within ORD's NERL to address this pathway, and additional evaluations will be performed using data from NHANES and NERL's Measurement Study in Jacksonville for metals and pyrethroid pesticides. More research is needed to obtain - data for critical model inputs (e.g., dermal transfer coefficient, longitudinal activity data), and to conduct model evaluations for different chemical classes. The results of SHEDS-Wood have also compared well with other models (Xue *et al.*, 2006).

3.4.3 Integrated fate/transport and exposure models

The integrated fate/transport and exposure models included here represent a combination of screening-level and higher-tiered models that are focused on either inhalation or multimedia exposures for human and/or ecological receptors (see Table 3.5). HEM (US EPA 2007i) represents a population-based air dispersion modelling system that couples estimated ambient concentrations from an air dispersion model (AERMOD) with information on US Census block locations to predict potential population-level inhalation exposures and risks. HEM is often referred to as a screening-level model that provides surrogate exposure estimates, because human receptors are assumed to be continuously exposed at the census tract concentration over a lifetime. HEM was developed as a risk assessment tool in the early 1990s to support the US EPA's Residual Risk Program, and to calculate industry sector risks for stationary sources. PERFUM (Reiss and Griffin, 2008) is a similar type of inhalation exposure model that integrates computer code from an atmospheric dispersion model (ISCST3) with some modifications to calculate downwind concentrations and potential acute exposures to nearby residents and other bystanders from fields treated with soil fumigants. This model was developed by industry in consultation with OPP to perform realistic and accurate buffer zone calculations, and to support the US EPA's registration of soil fumigants, such as iodomethane.

The US EPA's (2002c, 2004c) Johnson and Ettinger (1991) Model for Subsurface Vapor Intrusion into Buildings estimates indoor air concentrations of pollutants and incremental cancer risks based on subsurface vapour intrusion from contaminated groundwater and soils. This model predicts the volatilisation of contaminants located in the subsurface soil or water (e.g., chemical fate/transport within soils) and subsequent mass transport of vapours into indoor spaces (e.g., chemical fate/transport between soil column and enclosed spaces) by relating the vapour concentration at the source of the contaminant to the vapour concentration in the indoor space. This model can be used to evaluate steady-state (infinite or non-diminishing source) as well as quasi-steady-state (finite or diminishing source) vapour transport. The US EPA's vapour intrusion model is based on several modifications to the Johnson and Ettinger (1991) model, which relied on a number of simplifying assumptions and was developed for use as a screening-level (fate/transport) model. Specifically, the US EPA has developed a series of spreadsheets that allow for site-specific application of the Johnson and Ettinger (1991) model. Depending on the source characteristics, and on whether default or site-specific data are used, the US EPA's modified vapour intrusion model can be used for either screening-level or more advanced exposure and risk applications. Potential applications for this model include RCRA Corrective Action sites, CERCLA Superfund sites, and voluntary clean-up sites (but this model does not account for contaminant attenuation, and should not be used for sites contaminated with petroleum products from leaking underground storage tanks).

ChemSTEER (US EPA 2004d, 2007j), E-FAST (US EPA, 2007k) and IGEMS (US EPA, 2007l) represent multimedia models that were developed to support OPPT's new and existing chemical programmes, such as new chemicals submitted for PMN review under TSCA Section 5 and existing chemicals evaluated under TSCA Section

6. Specifically, ChemSTEER was designed to assess potential human (worker) exposures to and environmental releases of chemicals during manufacturing, processing and use operations, while E-FAST was developed to assess potential human and environmental exposures from consumer products and industrial releases (see Figure 3.3). Both of these models, which are used to assess a few thousand new and existing chemicals each year, are considered to be conservative screening-level models that generally overpredict receptor exposures by using conservative (e.g., high-end) default assumptions and scenarios. However, the default values in these models can be modified, and should be changed if other values are deemed more suitable for the specific exposure scenario being evaluated. IGEMS, which was also developed to assess potential human and environmental exposures from fugitive and industrial releases, is characterised as a higher-tiered model, because it provides more details at the receptor level than E-FAST (e.g., users can change any parameter and select receptors to run ISC air models). This model is therefore typically reserved for those chemicals where a more accurate assessment of exposure is needed, or where a screening-level model is not applicable. Although all three of these models are routinely used by the US EPA for regulatory review of new and existing chemicals, they also serve as "all purpose" models because of their broad potential applications, and have been widely used outside the Agency by consultants, academics, communities, local and state governments, and internationally.

Figure 3.3: General E-FAST model approach.

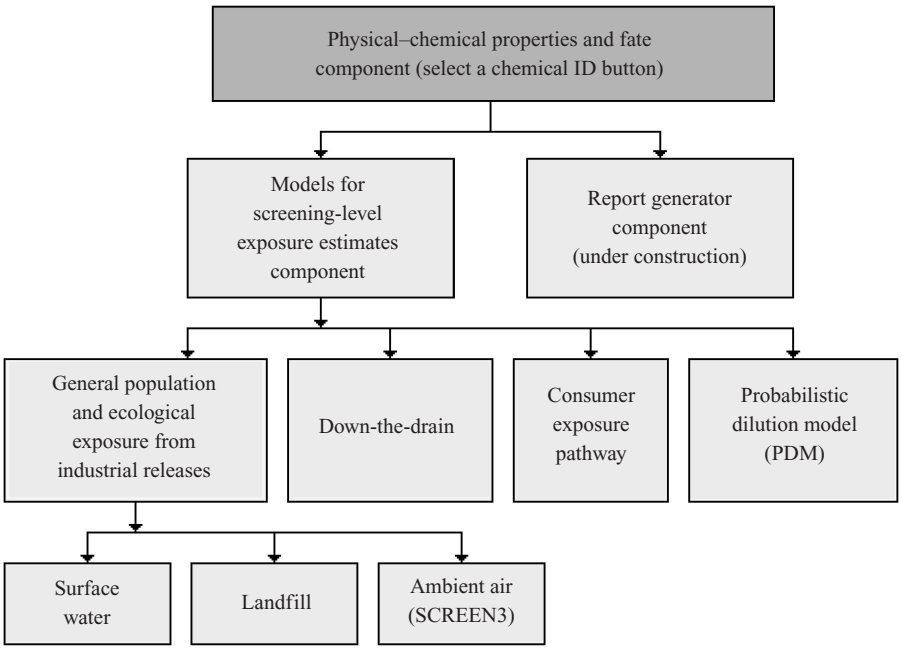


Table 3.5: Selected integrated fate/transport and exposure models used by the US EPA.

Model	Model purpose	Exposure routes	Model inputs	Model outputs
HEM[a]	Estimates population-level exposures to air toxics (HAPs) for general population or subgroups at urban and national levels.	Inhalation (outdoor).	Ambient air concentrations (modelled) based on point sources, census tract population and demographic data, exposure factors.	Maximum and annual average concentrations ($mg\,m^{-3}$); hazard index; risk (per million).
PERFUM	Estimates individual-level (acute) exposures to fumigants and degradation products for nearby residents and other bystanders near fields treated with soil fumigants.	Inhalation (outdoor).	ISCST3 computer code, field emissions or flux data, meteorological data, exposure factors.	Distribution of average daily concentrations ($mg\,m^{-3}$); MOE.
EPA's Vapor Intrusion Model[b]	Estimates indoor air pollutant concentrations and risk levels due to subsurface vapour intrusion from contaminated groundwater and soils.	Inhalation (indoor).	Chemical properties, saturated and unsaturated soil properties (soil type, porosity, soil gas flow), chemical concentrations (groundwater, soil vapour), building properties (air exchange rate, building area and mixing height, crack width).	Steady-state or time-averaged concentration ($mg\,m^{-3}$ per $mg\,kg^{-1}$ soil or per $mg\,L^{-1}$ water), risk-based media concentration ($mg\,kg^{-1}$ soil or $mg\,L^{-1}$ water), incremental cancer risk.

Model characterisation	Model peer review and evaluation	Links to other models
Conservative screening level (assumes continuous exposure at census tract over lifetime; does not have stochastic process to address variability or uncertainty).	Model components have been peer-reviewed (e.g., AERMOD), and the model itself underwent a SAB consultation in December 2007 as part of the US EPA's Risk and Technology Review Assessment Plan; an application using this model is currently undergoing a formal SAB review.	Uses AERMOD as atmospheric dispersion model.
Higher-tiered (estimates based on variability in meteorological conditions; prior version accounted for uncertainty in flux rates).	External SAP peer review of model in 2004; model published in peer-reviewed literature; limited model evaluation (flux rates back calculated based on multiple field measurements).	Uses ISCST3 as atmospheric dispersion model (AERMOD is being considered for future versions).
Conservative screening level (infinite source) or higher-tiered (finite source) (conservative default or site-specific data can be used; does not have stochastic process to address variability or uncertainty).	Original model published in peer-reviewed literature; limited model evaluation (few empirical data for either bench-scale or field-scale calibration or verification).	Based on Johnson and Ettinger model; modified by the US EPA in 1998, 2001, 2002 and 2004.

(*continued*)

Table 3.5: (*continued*)

Model	Model purpose	Exposure routes	Model inputs	Model outputs
ChemSTEER	Estimates environmental releases and individual or population-level exposures and doses to chemicals for workers during manufacturing, processing and use operations.	Inhalation (indoor, outdoor), dermal (product).	Physico-chemical properties, production/use volume, case-specific parameters (e.g., operating days, batch amounts, container type), release sources, exposure factors, worker activities.	Potential dose rates (mg day^{-1}); ADD, LADD and acute potential dose (mg kg^{-1} day^{-1}); releases (kg $site^{-1}$ day or kg yr^{-1} all sites).
E-FAST	Estimates population-level exposures and doses to chemicals for humans and ecological receptors from industrial releases and consumer products.	Inhalation (indoor, outdoor), dermal (consumer product), ingestion (drinking water, fish).	Physico-chemical properties, chemical release information (e.g., amount, media, days, location), fate information, air dispersion model, type of consumer product, exposure factors, and use patterns.	Lifetime average daily or acute concentrations (e.g., mg L^{-1}, mg m^{-3}); LADD (mg kg^{-1} day^{-1}); percentage exceedances.
IGEMS	Estimates population-level exposures and doses to chemicals for humans and ecological receptors from industrial releases.	Inhalation (outdoor), dermal (water), ingestion (drinking water).	Physico-chemical properties, chemical release information (e.g., amount, media, days, location), fate information, air dispersion model, surface water and groundwater models, exposure factors, and use patterns.	Lifetime average daily concentrations (e.g., mg L^{-1}, mg m^{-3}); LADD (mg kg^{-1} day^{-1}).

Model characterisation	Model peer review and evaluation	Links to other models
Conservative screening level (uses default parameter values and calculations; assumes worst-case scenarios for each source and worker activity; does not have stochastic process to address variability or uncertainty).	Components of ChemSTEER have been externally peer-reviewed (and any models or scenarios incorporated into ChemSTEER would have gone through an external peer review process); modelling results compared with monitoring data.	Uses several dozen release and exposure models; selected model outputs (environmental releases) are used as inputs to E-FAST.
Conservative screening level (uses default parameter values and high-end assumptions; assumes continuous exposures to predicted concentrations; does not have stochastic process to address variability or uncertainty).	External letter peer review of consumer exposure module in 1998 and the general population, down-the-drain, and probabilistic dilution model modules in 2001; limited model evaluation except for the consumer paint module.	Uses SCREEN3 as atmospheric dispersion model and WPEM emission algorithm for consumer latex paint exposures; other consumer emissions based on Chinn algorithm; in OPPT New Chemical Program, EPI-Suite provides fate information and ChemSTEER provides release information.
Higher-tiered, screening level (assumes continuous exposures to predicted concentrations, but is more detailed at the receptor level than E-FAST; does not have stochastic process to address variability or uncertainty).	Components of IGEMS have been peer-reviewed and evaluated because it is based on existing models.	Uses other environmental models for air (ISC), soil and groundwater (CSOIL, AP123D), and surface water (PRout).

(*continued*)

Table 3.5: (*continued*)

Model	Model purpose	Exposure routes	Model inputs	Model outputs
TRIM	Estimates fate and transport, environmental media concentrations, and population-level exposures and doses for human and ecological receptors from pollutants.	Inhalation, ingestion (ecological), dermal (ecological).	Physico-chemical properties, chemical release information (e.g., amount, media, days, location), fate information, air dispersion model, surface water and groundwater models, exposure factors, and use patterns.	Mass concentration in media and biota (g); biota and pollutant intakes ($mg\,kg^{-1}\,day^{-1}$); exposure concentrations (ppm or $mg\,m^{-3}$); delivered doses ($mg\,kg^{-1}\,day^{-1}$).
3MRA	Estimates population-level exposures and doses to chemicals for human and ecological receptors from land-based WMU releases.	Inhalation (outdoor, indoor), ingestion (drinking water, garden and farm products, fish), dermal.	Physico-chemical properties and fate information for air, surface water and groundwater models, human and ecological exposure (doses).	Annual average daily concentrations (e.g., $mg\,L^{-1}$, $mg\,m^{-3}$) and applied dose ($mg\,kg^{-1}\,day^{-1}$); cancer risk, hazard quotient, MOE.

[a]HEMScreen, which contained the ISCLT air dispersion model, is no longer used or supported by the US EPA.
[b]EPA's Johnson and Ettinger (1991) model for subsurface vapour intrusion into buildings.

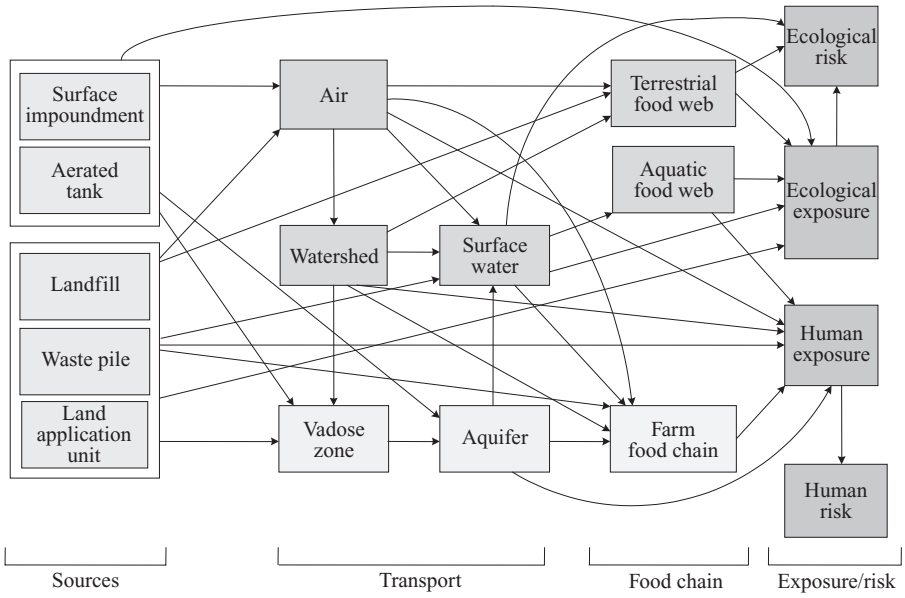
TRIM (US EPA, 2003c, 2006e) and 3MRA (US EPA, 2003d) potentially represent the "next generation" of highly integrated multimedia models that can support various regulatory and research efforts. The TRIM framework, which was developed by the US EPA's OAQPS, contains three modules that assess the fate and transport of pollutants in the environment (TRIM-FaTE), potential multimedia exposures to human receptors (TRIM-Expo), and potential noncancer and cancer risks to human or ecological receptors (TRIM-RISK). This model framework is expected to support Agency activities such as the Residual Risk Program, the Integrated Urban Air Toxics Strategy, petitions to delist individual HAPs and/or source categories, the review and setting of NAAQS, and regulatory impact analyses for air toxics regulations. 3MRA is a similar type of multimedia model that operates within the broader FRAMES framework. This model, which was originally developed by ORD to support OSW's HWIR for conducting risk assessments around hazardous waste sites, simulates

Model characterisation	Model peer review and evaluation	Links to other models
Higher-tiered (stochastic process addresses variability and uncertainty in input parameters using two-stage Monte Carlo; sensitivity analysis option).	External SAB peer review of conceptual approach and TRIM.FaTE in 1998 and second review in 1999; several peer-reviewed publications, verification of model approach and performance, benchmarking results against other models, and comparisons with field data.	Modules include TRIM-FaTE, TRIM-Expo, and Trim-Risk; uses APEX to estimate inhalation exposures.
Higher-tiered (stochastic process addresses variability and uncertainty in input parameters using two-stage Monte Carlo).	External SAB peer review of the complete model system in 2004; verification of model approach and performance, benchmarking results against other models, and comparisons with other analytical solutions, numerical models, and field data.	Uses other environmental models for air (ISCST3), subsurface transport (EPACMTP), surface water transport (EXAMS), and groundwater (MULTIMED).

potential population-level exposures and risks for human or ecological receptors from land-based WMU releases (see Figure 3.4). This model can also be used to assess a wide range of multimedia risk assessment problems including national and site-specific applications, such as evaluations of remedial actions at hazardous, toxic and radioactive waste sites.

All of the identified integrated fate/transport and exposure models include algorithms for assessing a pollutant's fate and transport in the environment; yield ambient pollutant concentrations in different environmental media; and estimate potential exposures, doses or risks for human and/or ecological receptors. However, modelled exposures do not account for actual time–activity patterns, and are generally based on the assumption that an individual or population has daily or continuous contact with predicted environmental media concentrations. For example, HEM, E-FAST and 3MRA predict outdoor ambient air concentrations, and assume that

Figure 3.4: General 3MRA model approach.



receptors are stationary and remain exposed to this concentration for 24 hours per day (even when indoors or at another location). E-FAST and 3MRA also calculate pollutant concentrations in ground and surface water, and assume that receptors consume this water (untreated) as their sole drinking water source on a daily basis (even if this water is not known to be used for consumption). ChemSTEER utilises a somewhat different approach in which generic scenarios that combine sources and worker activities for a given operation are used to yield conservative (reasonable worst-case) results based on several dozen release and exposure models (see Table 3.6). For example, common worker activities with the potential for inhalation exposures include sampling, drumming, and clean-up of equipment (Matthiessen, 1986). Because the integrated fate/transport and exposure models are based on assumed rather than actual contact with a contaminant, they are more relevant for characterising *potential* (rather than actual) exposures to human or ecological receptors. It is noteworthy that the primary use of some of these models (e.g., E-FAST) is to provide a quick turnaround, first-tiered analysis for evaluating a large number of chemicals in a short time period in order to screen out those that are not likely to be of concern. Chemicals or facilities that do not pass this initial screen will generally undergo more refined analyses by substituting default assumptions with more accurate or site-specific data, or by using a higher-tiered model.

General inputs to these models include chemical or product-specific information (e.g., product type, formulation, chemical and physical properties), product use patterns (e.g., volume, rate, technique), chemical release information (e.g., amount, media), site-specific information (e.g., operations, releases, location, land use, build-

ing-related parameters), pollutant concentrations in a given waste stream or medium (e.g., soil gas), and other exposure factors (e.g., intake rates, body weight). These latter values are generally based on the US EPA's (1997b) *Exposure Factors Handbook* for model default (or user-defined) populations or subpopulation groups. These models also typically incorporate other fate/transport models, or rely on simple algorithms or standard mass balance equations. The US EPA's (2009) EPI Suite™ model is also sometimes used to provide estimates of physical/chemical and environmental fate and transport properties that can be used as inputs to screening-level exposure models in the absence of reliable measured data. Outputs to these models generally include environmental media concentrations (e.g., $mg\,m^{-3}$, $mg\,kg^{-1}$, $mg\,L^{-1}$) and potential exposures or doses ($mg\,kg^{-1}\,day^{-1}$) averaged over longer-term (e.g., LADD), intermediate (e.g., ADD) and short-term (e.g., acute potential dose) durations. Some of these models also compare estimated exposure or dose levels with existing toxicity criteria to calculate potential human or ecological risks (e.g., MOE, cancer risk, fraction of exceedance).

With the exception of PERFUM, TRIM and 3MRA, none of the identified integrated fate/transport and exposure models attempt to address the variability or uncertainty in model input parameters or exposure estimates. This is not surprising for screening-level models such as ChemSTEER and E-FAST, which are designed to provide upper-bound estimates of exposure. PERFUM accounts for daily and seasonal variability in meteorological conditions by calculating a distribution of average daily soil fumigant concentrations at each receptor point around the field. TRIM is a probabilistic model that includes features for performing sensitivity analyses as well as two-stage Monte Carlo analyses that can address both the variability and uncertainty in selected input parameters. 3MRA has a similar two-stage Monte Carlo analysis function that operates through a separate parallel computing model called SuperMUSE (Babendreier and Castleton, 2005). Although TRIM and 3MRA are considered to be higher-tiered models, both of these models can be used to perform simple deterministic screening-level analyses using conservative default parameters. Like HAPEM, 3MRA is also sometimes referred to as a screening-level model because of its limited spatial and temporal scope (i.e., it was originally designed for national-level and chronic health assessments, although it can be adapted to site-specific and regional scales).

All of the integrated fate/transport and exposure models included here have been internally reviewed in accordance with Agency-wide policies and procedures, and these models have undergone varying degrees of external peer review. Although HEM itself has not undergone a formal peer review, because it comprises a regulatory default model (i.e., its air dispersion model, AERMOD, has been peer reviewed), it underwent an SAB consultation in December 2007 as part of the US EPA's Risk and Technology Review Assessment Plan. An application using HEM is also currently undergoing a formal SAB review. PERFUM underwent an external SAP peer review in 2004, and its conceptual approach and methodology have been published in the peer-reviewed literature (Reiss and Griffin 2006). The US EPA's modified vapour intrusion model is based on fate/transport equations that have been published in the peer-reviewed literature (Johnson and Ettinger, 1991). Components

Table 3.6: Examples of default models included in ChemSTEER screening-level model.

Model	Model description	Default sources/activities
AP-42 Loading Model	Estimates releases to air from displacement of air containing chemical vapour as a container or vessel is filled with liquid.	Loading or unloading of liquids into transport container or vessels.
Mass Transfer Coefficient Model	Estimates releases to air from evaporation of a chemical from an open, exposed liquid surface (outdoor sources of release).	Cleaning liquid residues from tank trucks or rail cars used to transport raw material or products or equipment cleaning losses of liquids.
Penetration Model	Estimates releases to air from evaporation of a chemical from an open, exposed liquid surface (indoor sources of release).	Cleaning liquid residues from bottles, small containers, drums, and totes used to transport raw material or products; cleaning liquid residuals from storage or transport vessels; sampling liquids.
Automobile Finish Coating Overspray Loss Model	Estimates releases of overspray of non-volatile chemicals in coatings during their application to refinished automobiles using spray guns within a spray booth with controls to capture overspray from the exhaust.	Default for calculating multimedia releases of a chemical to air, as well as water, incineration, or landfill for the Automobile Refinish Spray Coating Application source/activity.
Cooling Tower Blowdown Loss Model	Estimates releases of a volatile cooling tower additive chemical as a result of evaporation of the recirculating fluid (e.g., water).	Conditional default model for estimating releases to air from the Recirculating Water-Cooling Tower Additive Releases source/activity.
Mass Balance Inhalation Model	Estimates the amount of chemical inhaled by a worker (typical and worst case) during an activity in which chemical vapour is generated.	Default for calculating worker inhalation exposures to a volatile chemical while performing the following sources/activities: cleaning liquid residuals or loading and unloading of liquids into transport containers/vessels, sampling of liquids, vapour release from open liquid surfaces.

(*continued*)

Table 3.6: (*continued*)

Model	Model description	Default sources/activities
UV Roll-Coating Inhalation Model	Estimates the amount of chemical inhaled by a worker who conducts activities near roll coater(s) using coatings or inks.	Default for calculating worker inhalation exposures to a chemical while performing the roll coating source/activity.
Small Volume Handling Model	Utilises worst-case and typical exposure rates to estimate the amount of chemical inhaled by a worker during handling of "small volumes" (<54 kg/worker-shift) of solid/powdered materials.	Default for calculating worker inhalation exposures to a chemical while performing any source/activity for sampling solids (handling of these small volumes is presumed to be scooping, weighing and pouring of the solid materials).
1-Hand Dermal Contact with Liquid Model	Estimates dermal exposure to the chemical for one-hand contact with liquid containing the chemical.	Default for calculating worker dermal exposures to a liquid chemical while performing liquid sampling sources/activities.
2-Hand Dermal Immersion in Liquid Model	Estimates dermal exposure to the chemical for two-hand immersion in liquid containing the chemical .	Default for calculating worker dermal exposures to a liquid chemical while performing the following sources/activities: automobile spray coating, miscellaneous sources/activities related to liquid processing.

of ChemSTEER have been externally peer-reviewed, and because models in ChemSTEER have been extensively used in Agency assessments for over 10 years, any models or scenarios incorporated into ChemSTEER would have gone through an external peer review process. E-FAST had an external letter peer review of its consumer exposure module in 1998, and a review of its general population, down-the-drain and probabilistic dilution model modules in 2001. IGEMS has undergone limited external peer review, because it is based on existing models that have already been peer-reviewed, and it is still under development. TRIM and 3MRA have been extensively reviewed (internally and externally), although it has not been possible to assess these models in their entirety owing to their complexity. TRIM underwent two external US EPA SAB (1998, 2000) peer reviews, in which the development of TRIM and the TRIM-FaTE module was found to be conceptually sound and scientifically based. 3MRA also underwent an external US EPA SAB (2004) peer review, and its approach and equations have been published in the peer-reviewed literature (Marin *et al.*, 2003).

For most of the reviewed models, attempts have been made to evaluate them when data are available for such an evaluation, but it can be difficult to evaluate screening-level models designed to yield upper-bound or worst-case estimates. HEM, PERFUM and the US EPA's modified vapour intrusion model have undergone limited model evaluation, while ChemSTEER and E-FAST have been partially evaluated when data were available for this purpose. For example, the mass balance approach used by ChemSTEER has been evaluated by comparing model predicted exposures for specific operations with monitoring data reported in selected studies from the available literature (Fehrenbacher and Hummel, 1996). This evaluation illustrated that estimated exposures based on the midpoint of the range of default input values were well within one order of magnitude of the measured exposures, but that selection of more conservative model input values overestimated exposures by one or more orders of magnitude. The consumer paint module in E-FAST also underwent extensive evaluations as part of the WPEM model review, and components of IGEMS have been evaluated because it is based on existing models. A number of efforts have been made to evaluate TRIM (particularly the TRIM-FaTE module) and 3MRA by verifying the approach and performance of these models, including performing sensitivity analyses and benchmarking the results of these models against one another (US EPA, 2002d). The results of TRIM-FaTE have also been tested by the US EPA (2005c) using field data on organic and inorganic pollutants (e.g., PAHs and mercury), and the results of 3MRA have been compared with other analytical solutions, numerical models, and field data.

3.5 DISCUSSION

In this chapter, we have provided an overview of 35 exposure assessment models that are currently supported and used by the US EPA for regulatory, research, voluntary programme or other purposes. These include selected fate/transport models, exposure models, and integrated fate/transport and exposure models. We can draw a number of observations based on our review of these models.

First, this review included models that were developed for a specific purpose, route(s) of exposure, or category of pollutants, as well as those that were designed for more general applications. For example, most of the fate/transport models were developed as generic models to assess compliance with environmental standards or estimate media-specific chemical concentrations applicable to both human and ecological receptors. The exposure models, on the other hand, were typically developed to assess human exposures and risks due to either inhalation exposures from criteria and toxic air pollutants or aggregate multimedia exposures to pesticides or other chemicals in residential settings. The integrated fate/transport and exposure models were designed for either a specific purpose (e.g., human inhalation exposures from HAPs or fumigants) or to assess multimedia exposures for human or ecological receptors to many different chemicals from a variety of sources (e.g., industrial releases; manufacturing, processing and use operations; waste disposal sites; consumer products). Despite their original purpose, many of the exposure assessment models included here have evolved over time to include broader applications.

Second, many of the models we reviewed were found to rely on a common set of underlying inputs, databases, equations, or other models. For example, the air quality and dispersion models rely on similar sources of emissions and meteorological data, and the surface water and drinking water models rely on similar types of environmental fate and application rate data. For the exposure models, many use data collected from the US Census Bureau to define population characteristics (e.g., demographics) and receptor locations (e.g., census tracts). These models also typically use human exposure factors (e.g., body weight, intake rates) based on the US EPA's (1997b) *Exposure Factors Handbook*, and time–activity patterns (e.g., hand-to-mouth contacts) based on the US EPA's (1997a) CHAD. In addition, many of the default scenarios and equations included in the dietary and residential aggregate exposure models for pesticides and inert ingredients are based on the US EPA's residential SOPs, and food consumption data in these models are often based on the USDA's CSFII. A number of the exposure models and integrated fate/transport and exposure models also include modules for, or build off, the fate/transport models.

Third, an important distinction among the various models summarised here is their level of analysis and spatial and temporal resolution. For example, the fate/transport models generally represent either steady-state or dynamic conditions and predict ambient concentrations that are applicable to local, urban, regional or national scales for short- or longer-term time periods. The exposure models and integrated fate/transport and exposure models are also applicable for assessing exposures at the local, urban or national level. Most of these models allow for the estimation of acute (short-term, single-dose), subchronic and/or chronic (long-term, lifetime) potential or actual exposures or doses. Some of these models produce time-averaged or time-integrated exposure estimates, whereas others produce a time series or time profile of exposure estimates. In addition, these models are generally designed to assess exposures either to individuals (e.g., residents, consumers, workers) or to the general population or subgroups, although some models can be used to assess both individual-level and population-level exposures.

Fourth, the exposure assessment models evaluated here differ in regard to how to characterise their outputs and modelling results. That is, these models generally provide either conservative (e.g., upper-bound) estimates for screening-level applications, or more refined estimates for higher-tiered purposes. The US EPA relies on several conservative screening-level models to estimate potential exposures to human or ecological receptors, such as those that support OPP's registration and re-registration of pesticides and OPPT's new and existing chemical programmes in order to quickly screen and prioritize several thousand chemicals each year. As noted, a few of the US EPA's models are referred to as screening-level models because of their limited spatial or temporal resolution, rather than because they provide conservative estimates of exposure. The US EPA also relies on a number of higher-tiered models to provide best estimates or the most accurate characterisation of chemical concentrations or exposures.

Fifth, only a subset of the models that we reviewed had capabilities, such as stochastic processes, to assess the variability and/or uncertainty in modelled estimates and input parameters. These tended to be the higher-tiered exposure models and some of the integrated fate/transport and exposure models. For these models, such assessments were usually accomplished by performing one- or two-dimensional Monte Carlo analyses, sensitivity analyses, and/or contribution analyses. Time–activity patterns and chemical or pesticide residue values in different environmental media were the most common model input parameters that were varied in order to address variability or uncertainty. Because the screening-level models are generally designed to produce overestimates of exposure, they typically do not address variability or uncertainty, and instead use deterministic methods to produce point estimates of concentration or exposure.

Sixth, all of the exposure assessment models supported and used by the US EPA have been internally peer-reviewed to ensure consistency with Agency-wide policies and procedures, and many of these models have undergone external peer review by independent outside experts. External peer reviews can consist of letter peer reviews, panel reviews, reviews by scientific advisory boards, and/or publication in the peer-reviewed literature. These rigorous internal and external peer review efforts have resulted in continuous updates and improvements to the US EPA's models.

Seventh, the models included in this chapter have undergone varying degrees of model evaluation. Although complex computational models can never be truly validated (NAS, 2007), and it has been difficult to evaluate many of the US EPA's models in their entirety owing to limitations in analytical monitoring technologies and other factors (e.g., personal monitors are usually passive devices that yield time-averaged rather than time-series results), some of the key components of the US EPA's exposure assessment models have been evaluated using different approaches. For example, detailed studies have been undertaken in order to obtain real-world activity and commuting data and information on microenvironmental factors for use in some of the exposure models. Many of these models have also compared modelling outputs with actual air measurements or field data, and some of the dietary and residential aggregate exposure models have compared modelled estimates with biomonitoring data. Additionally, a large number of these models have compared their results with

those of other models. Such "model to model" comparisons are considered to be a useful way to assess or corroborate a model's performance, and to address model uncertainty (NAS, 2007).

Eighth, in many cases there is not a single "right" or "best" model, and several models may be used to estimate environmental concentrations or exposures (US EPA, 1992). This finding was apparent in our review of the various models included in this paper, in which several models were sometimes available for the same or similar purpose, although the methodologies and outputs of these models might differ. For example, more than one fate/transport model is available to assess outdoor ambient pollutant concentrations at different receptors, and multiple exposure models are available for assessing inhalation exposures to criteria and toxic air pollutant and other indoor pollutants. Several exposure models are also available to assess dietary and residential aggregate exposures to pesticides. Although improved coordination among and within the US EPA's programme offices may be warranted in order to avoid model duplicity, or to develop more uniform models, it may be advantageous to rely on multiple models for regulatory and research purposes. For example, the US EPA's FIFRA SAP has recommended that several complementary models continue to be used by OPP as a way to evaluate and address model uncertainties (SAP, 2004), and the NAS (2007) has stated that such "model to model" comparisons are a useful way to assess or corroborate a model's performance.

Ninth, although most of the US EPA's exposure models have been designed to be "stand-alone" models, recent and ongoing efforts in the US EPA have focused on developing integrated modelling approaches. For example, attempts have been made to conduct integrated air quality and exposure modelling in order to identify those sources and microenvironments that contribute to the greatest portion of personal or population exposures, and to determine optimum risk management strategies (Isakov *et al.*, 2006). Advanced approaches that can combine regional and local models have also been touted as a future direction for air quality modelling of HAPs in order to address the spatial variability of air concentrations and allow for better treatment for chemically reactive air toxics (Touma *et al.*, 2006). The US EPA's (2008d) draft White Paper on *Integrated Modeling for Integrated Environmental Decision Making* further recommends that the Agency adopt a "systems thinking approach" and consistently and systematically implement integrated modelling approaches and practices that inform Agency decision-making.

Tenth, each of the individual models and model categories contains various strengths and weaknesses. For example, many of the exposure assessment models have a wide range of applications and are used by a number of internal and external users. Most of these models are also self-contained, well documented, and relatively easy to use. However, a few of the exposure and integrated fate/transport and exposure models (particularly those that assess multiple pathways, scenarios or receptors) are complex, and require many data inputs or more advanced users. In addition, only a subset of the models reviewed consider multiple sources and pathways, with the remaining models addressing only a single route of exposure (e.g., inhalation). Some of these models are also limited in their spatial or temporal scope, their ability to address model variability and uncertainty, and the extent to which they have been externally peer-reviewed and

evaluated. The exposure assessment models also differ in regard to the accuracy and characterisation of their estimates, with the fate/transport and screening-level models providing "potential" or conservative estimates of exposure, and the higher-tiered exposure models providing the most accurate estimates of exposure.

In summary, this chapter provides an overview of 35 exposure assessment models that are currently supported and used by the US EPA. These models represent the first half of the source-to-outcome continuum, and include selected fate/transport, exposure, and integrated fate/transport and exposure models. Although our review does not include all of the US EPA's models, the information presented here should provide a useful up-to-date resource for exposure and risk modellers and practitioners. This work also supports recent and ongoing efforts at the US EPA, such as proposed strategies by the CREM, to further inventorise, characterise and evaluate its models.

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