PART I

Decision Support and Assessment Modelling

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CHAPTER 1

Environmental Fate and Bioaccumulation Modelling at the US Environmental Protection Agency: Applications to Inform Decision-Making

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1.1 INTRODUCTION

Environmental fate and bioaccumulation models provide a framework for understanding how biogeochemical processes affect pollutant transport and bioavailability in the atmosphere and aquatic and terrestrial systems. They provide a basis for predicting the impacts of human activities on natural ecosystems and biological exposures. Models can also be viewed as testable hypotheses of processes driving the fate and bioaccumulation of environmental contaminants. The overall hypothesis embodied by any given model is tested when the model is applied to a natural system and compared with observational data and/or other models with different functional forms. In this way, models are valuable tools for improving understanding of how ecosystems function, and for prioritizing areas for future research.

Environmental models are also used as applied tools for environmental management. The application of environmental models to inform policy is an iterative process where, despite pervasive scientific uncertainties, decisions must be made. Models assist in synthesising best-available scientific understanding to predict how different policy choices will affect environmental and human health risks. Given the diversity of environmental modelling applications across disciplines, defining a "regulatory environmental model" can be challenging. An expert panel convened by the US National Research Council (NRC) provides the following broad definition for a model (NRC, 2007): "a simplification of reality that is constructed to gain insights into select attributes of a particular physical, biological, economic, or social system".

Modelling of Pollutants in Complex Environmental Systems, Volume II, edited by Grady Hanrahan.

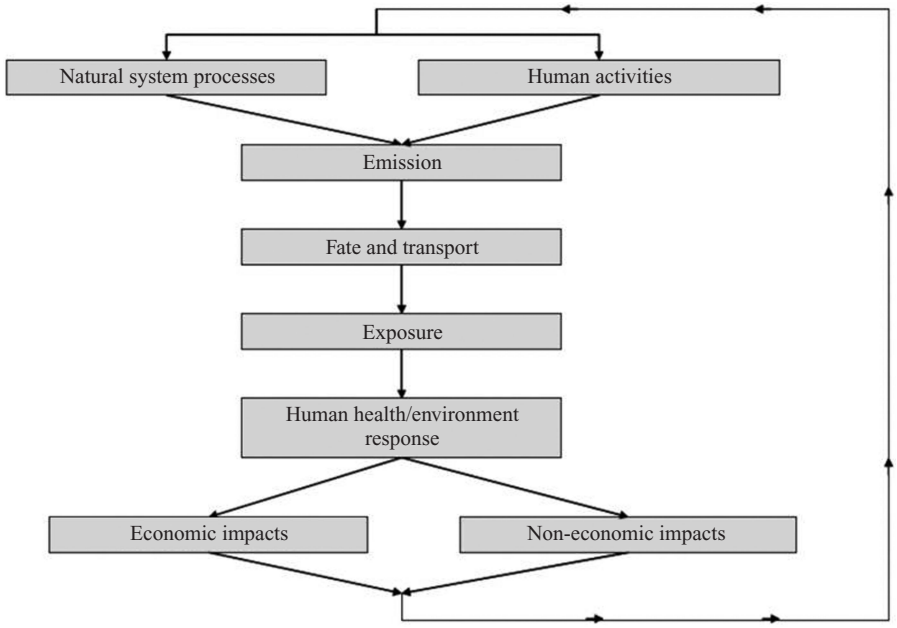
The subset of models most often used to provide information for policy determinations are computational models. The NRC panel defines these models as "those that express the relationships among components of a system using mathematical relationships" and use measurable variables, numerical inputs, and mathematical relationships to produce quantitative outputs (NRC, 2007). This definition of computational models is intentionally broad, to allow for the diversity of regulatory environmental models, which range from simple, site-specific, empirical relationships to computationally intensive, process-based simulations on the global scale (US EPA, 2009a).

The use of environmental models in the decision-making process has increased over the last several decades. In the 1970s, technology-based standards in the US dominated the laws governing air, surface and subsurface water, and drinking water protection (NRC, 2007). In 1980 a Supreme Court decision on workplace standards for benzene exposure catalysed a shift from technology-based standards to regulatory assessments that consider the nature and significance of risks posed by environmental contaminants. In this case, the Supreme Court struck down a standard that would have reduced benzene concentrations as far as technologically possible, because it did not consider whether existing concentrations posed a "significant risk of material health impairment" (448 USC § 607, 10 ELR, 20489). This decision implied that some form of quantitative assessment is needed to decide whether a risk is large enough to warrant regulation (Charnley and Eliott, 2002).

Another factor driving demand for quantitative model-based policy analysis in the US is the mandated development of regulatory impact assessments (RIAs). According to Executive Order 12866, issued in 1993, RIAs must include a formal cost–benefit analysis for any new regulation with costs exceeding $100 million, or with a significant impact on the economy and/or society (Exec. Order No. 12,866, 3 CFR § 638, 1993). Such an approach is meant to improve the efficiency of environmental regulations by showing when the benefits of a regulation are likely to exceed its costs, and whether alternatives to that regulation are more or less costly (Hahn *et al.*, 2000). The increasing prevalence of environmental modelling applications in policy analysis also reflects the need for decisions to keep pace with rapidly growing databases of environmental information from real-time monitoring systems and relatively new data collection methods using satellites and remote sensing. In addition, advances in computing over the past several decades according to Moore's law (Moore, 1965) have greatly enhanced capabilities for simulating complex environmental fate and transport processes over large spatial scales.

Figure 1.1 illustrates the role of fate and transport models in the integration of environmental and social/economic information needed for risk assessments and RIAs. Predicting how biogeochemical processes affect the fate and bioavailability of contaminants is a critical component of risk assessments that assess human exposures, health effects and ecosystem impacts. The purpose of risk assessments is to characterise potential adverse impacts associated with particular activities or events, where these impacts are evaluated based on both the *magnitude* of effects and the *likelihood* of their occurrence (Suter, 2007). The philosophy of protecting public health with an "adequate margin of safety" is specified in a variety of statutes, including the total

Figure 1.1: Basic modelling elements relating human activities and natural systems to environmental impacts.



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maximum daily load (TMDL) programme within the Clean Water Act (CWA section 303(d)(1)(C)) and the Clean Air Act (CAA section 109(b)(1)). This concept is now the primary objective of quantitative risk assessments, and also introduces the idea of uncertainty in modelling assessments. Risk assessments must recommend emissions limits within an adequate margin of safety for specific contaminants based on their environmental exposure pathways, bioaccumulation potential, and persistence in the environment. Findings need to stand up under the extensive scrutiny associated with judicial review in the US, which places a significant burden of proof on regulatory agencies for demonstrating the human health risks associated with exposures to environmental contaminants (Charnley and Eliott, 2002).

Models used in regulatory applications face more scrutiny than those used internally for screening level assessments and research models. For example, one senior agency official in the US EPA's Office of Water estimated that ~10% of the information compiled for regulatory actions is needed to make the decision, and the remaining 90% is needed to support the judicial review process and ensure that the decision stands up in court (Charnley and Eliott, 2002). All final agency actions are subject to judicial review (McGarity and Wagner, 2003). An action is normally not considered final until it has direct consequences for the person or entity attempting to

challenge that action in court, and thus many modelling applications at US EPA are not subject to this level of review.

This chapter reviews the regulatory background and policy applications driving the use of various types of environmental fate and bioaccumulation model at US EPA (air quality, surface water and watersheds, contaminated sites). Comparing current research frontiers with contemporary policy applications within each modelling area helps to illustrate the interactions between research fields and regulatory models intended for application by environmental practitioners. We highlight, in particular, the interrelationship between emerging research, ongoing data collection, and regulatory model improvement efforts. The chapter concludes with a summary of US EPA's recent efforts to enhance the quality and transparency of modelling applications used to inform environmental regulations.

1.2 ATMOSPHERIC FATE AND TRANSPORT MODELLING

National Ambient Air Quality Standards (NAAQS) for criteria pollutants must "protect public health" "allowing an adequate margin of safety".

Clean Air Act, 42 USC § 7409(b)(1)

1.2.1 Regulatory background: the Clean Air Act

Air quality models are used to calculate pollutant concentrations and deposition rates using information on emissions, transport, and atmospheric chemistry. Application of models during the regulatory process helps in identifying source contributions to air quality problems, and in evaluating the effectiveness of regulations in reducing human and ecological exposures. National standards for air quality were established in 1970 with the Clean Air Act (CAA). Title 1 of the CAA put in place the National Ambient Air Quality Standards (NAAQS) for area, emission and stationary sources of six "criteria pollutants" considered harmful to public health and the environment.[1] NAAQSs are promulgated at the Federal level and implemented by state implementation plans (SIPs) that are approved by US EPA. Generally, SIPs require states to model the impacts of proposed emissions reductions targets to determine whether reductions in ambient atmospheric concentrations are acceptable. These plans include detailed descriptions of how a proposed emission reduction programme will bring states into compliance with NAAQS. Regional-scale modelling has become an integral part of SIP development for ozone and fine particulate matter ($PM_{2.5}$), and these standards are reviewed every five years.

Other areas of the CAA also use information from air quality models to develop regulatory air-quality thresholds and implement standards. Title II of the CAA regulates mobile sources, and Title III requires that US EPA list hazardous air pollutants (HAPs) that could "cause, or contribute to, an increase in mortality or an increase in serious irreversible or incapacitating reversible illness". Title IV regulates acid deposition, and titles V and VI deal with permits and stratospheric ozone

protection. US EPA listed only eight HAPs in the first 18 years after the CAA was established, prompting Congress to identify an additional 188 with known adverse effects on human health that require regulation. Following the 1990 amendments to section 112 of the CAA, US EPA was required to list and regulate, on a prioritized schedule, "all categories and subcategories of major sources and area sources that emit one or more HAPs".

1.2.2 Model selection and evaluation criteria

Because of the widespread use of air-quality models for Federal and state-level regulatory activities, US EPA's Office of Air and Radiation (OAR) has developed extensive guidelines for model selection, application and evaluation.[2]

Three main types of modelling application support regulatory activities:

- *Dispersion models* are used in a state's permitting processes to determine compliance with NAAQS and other regulatory requirements. These models use emissions data and meteorological inputs to predict pollutant concentrations at downwind locations.
- *Photochemical models* are used to simulate pollutant concentrations and deposition resulting from multiple emissions sources at a variety of spatial scales. These models are widely used to determine the effectiveness of emissions control strategies at keeping pollution levels below regulatory thresholds, or reducing atmospheric deposition rates.
- *Receptor models* are used to identify the contribution of different emissions sources and source regions to deposition and ambient concentrations at a given receptor, based on the chemical and physical characteristics of gases and particles. Unlike photochemical and dispersion air quality models, receptor models use the chemical and physical characteristics of gases and particles measured at sources and receptors.

Table 1.1 provides a summary of some of the most frequently used models within each class. For dispersion-modelling applications US EPA lists preferred/recommended models that must be used by the state in the development of SIPs (Appendix W, 40 CFR Part 51, Vol. 70, No. 216, 68218–68261). Alternative models are also provided, but must be justified on a case-by-case basis.[3]

Photochemical models are needed to develop SIPs and determine the effectiveness of different regulatory strategies for pollutants such as O_3, which is a secondary product of other atmospheric precursors. Two major classes of photochemical models are:

- *Lagrangian trajectory models*, which simulate the emission, transport and expansion, chemistry, and deposition of individual parcels of pollutants moving through the atmosphere;
- *Eulerian models*, which simulate the emission, advective transport, diffusion, chemistry, and deposition of pollutants through a three-dimensional matrix of finite grid volumes (i.e., "boxes").

Table 1.1: Overview of frequently used air quality models at the US EPA. All information adapted from: http: //www.epa.gov/ttn/scram/aqmindex.htm.

	Preferred/recommended dispersion models
AERMOD	Steady-state plume model that incorporates air dispersion based on planetary boundary layer turbulence structure and scaling concepts, including vertical treatment of sources, and varied terrain. AERMOD was promulgated as a replacement to ISC3 in 2006.
CALPUFF	A non-steady-state puff dispersion model that simulates the effects of varying meteorological conditions on pollution transport, transformation, and removal. CALPUFF can be applied for long-range transport over complex terrain. It includes algorithms for subgrid scale effects such as terrain impingement, as well as pollutant removal due to wet and dry deposition, chemical transformations, and effects of particulate matter on visibility.
BLP	A Gaussian plume dispersion model designed to handle unique modelling problems associated with aluminium reduction plants, and other industrial sources where plume rise and downwash effects from stationary line sources are important.
CALINE3	CALINE3 is a steady-state Gaussian dispersion model designed to determine air pollution concentrations at receptor locations downwind of highways located in relatively homogeneous terrain. CALINE3 is incorporated into the more refined CAL3QHC and CAL3QHCR models.
CAL3QHC/ CAL3QHCR	A CALINE3 based CO model with queuing and hotspot calculations, and with a traffic model to calculate delays and queues that occur at signalised intersections; CAL3QHCR is a more refined version based on CAL3QHC that requires local meteorological data.
CTDMPLUS	Complex Terrain Dispersion Model Plus Algorithms for Unstable Situations (CTDMPLUS) is a refined point-source Gaussian air quality model for use in all stability conditions for complex terrain. The model contains, in its entirety, the technology of CTDM for stable and neutral conditions. CTSCREEN is the screening version of CTDMPLUS.
OCD	Offshore and Coastal Dispersion Model Version 5 (OCD) is a straight-line Gaussian model developed to determine the impact of offshore emissions from point, area or line sources on the air quality of coastal regions. OCD incorporates over-water plume transport and dispersion. as well as changes that occur as the plume crosses the shoreline. Hourly meteorological data are needed from both offshore and onshore locations.
	Examples of frequently used photochemical models
CMAQ	The Community Multiscale Air Quality (CMAQ) is a regional Eulerian model that includes capabilities for conducting urban- to regional-scale simulations of multiple air quality issues, including tropospheric ozone, fine particles, toxics, acid deposition, and visibility degradation.

(*continued*)

Table 1.1: (*continued*)

	Examples of frequently used photochemical models
CAMx	The Comprehensive Air quality Model with extensions (CAMx) is a Eulerian photochemical dispersion model that simulates air quality over many geographic scales. The model treats a wide variety of inert and chemically active pollutants, including ozone, particulate matter, inorganic and organic $PM_{2.5}/PM_{10}$, mercury and other toxics. CAMx also has plume-in-grid and source apportionment capabilities.
REMSAD	The Regional Modelling System for Aerosols and Deposition (REMSAD) was developed to understand distributions, sources and removal processes relevant to regional haze, particulate matter and other airborne pollutants, including soluble acidic components and toxics.
UAM-V®	The UAM-V Photochemical Modelling System has been used widely for air quality studies focusing on ozone. It is a three-dimensional photochemical grid model designed to calculate concentrations of both inert and chemically reactive pollutants by simulating physical and chemical processes in the atmosphere affecting pollutant concentrations. This model is typically applied to model air quality "episodes" – periods during which adverse meteorological conditions result in elevated ozone pollutant concentrations.
	Examples of frequently used receptor models
CMB	The Chemical Mass Balance (CMB) Model is based on an effective-variance least-squares method (EVLS). CMB requires speciated profiles of potentially contributing sources and the corresponding ambient data from analysed samples collected at a single receptor site. CMB is ideal for localised non-attainment problems, and has proven to be a useful tool in applications where steady-state Gaussian plume models are inappropriate, as well as for confirming or adjusting emissions inventories.
UNMIX	The US EPA UNMIX model "unmixes" the concentrations of chemical species measured in the ambient air to identify the contributing sources. Chemical profiles of the sources are not required, but instead are generated internally from the ambient data using a mathematical formulation based on a form of factor analysis. For a given selection of species, UNMIX estimates the number of sources, the source compositions, and source contributions to each sample.
PMF	The positive matrix factorisation (PMF) technique is a form of factor analysis where the underlying co-variability of many variables (e.g., sample-to-sample variation in PM species) is described by a smaller set of factors (e.g., PM sources) to which the original variables are related. The structure of PMF permits maximum use of available data and better treatment of missing and below-detection-limit values.

Eulerian models use a fixed spatial grid, whereas Lagrangian models have a moving frame of reference, and spatial scales depending on the sources and receptors of interest. Eulerian grid models solve numerical expressions describing vertical and horizontal transport, chemical, and emission processes by dividing the modelling domain into a large number of cells, which interact through advective and diffusive transport (Cooter and Hutzell, 2002). Photochemical air quality models often use a three-dimensional Eulerian grid to fully characterise physical processes in the atmosphere and predict the species concentrations throughout the entire model domain.

The community multiscale air quality model (CMAQ) (Byun and Ching, 1999) is one of US EPA's most widely used models. CMAQ is a regional-scale Eulerian model that combines current knowledge of atmospheric chemistry and meteorological processes affecting air quality to model the fate and transport of ozone, particulates, toxics, and acid deposition. CMAQ was originally developed for $PM_{2.5}$ and O_3 assessments, and has been extended for a range of other applications, including mercury (Bullock and Brehme, 2002), atrazine (Cooter and Hutzell, 2002), aerosols (Binkowski and Roselle, 2003; Nolte *et al.*, 2008), NO_x (Han *et al.*, 2009), ozone (Sahu *et al.*, 2009; Yu *et al.*, 2009), and many others.

The National Oceanic and Atmospheric Administration's (NOAA) Hybrid Single Particle Lagrangian Integrated Trajectory Model (HYSPLIT) (Draxier and Hess, 1998) is an example of a Lagrangian air quality model that calculates pollutant dispersion by assuming either puff or particle dispersion. In the puff model, puffs expand until they exceed the size of the meteorological grid cell (either horizontally or vertically) and then split into several new puffs, each with its share of the pollutant mass. In the particle model, a fixed number of initial particles are advected within the model domain by the mean wind field and a turbulent component. The NOAA HYSPLIT model is well suited for deriving source–receptor relationships for contaminants (Cohen *et al.*, 2002, 2004) and tracing plumes of emissions from wildfires and other sources.[4]

Receptor models (Table 1.1) are data-intensive methods used for identifying and quantifying contributions of pollutions to concentrations at different receptors, and for source apportionment. These models are therefore a natural complement to other air quality models, and are used in SIPs for identifying sources contributing to air quality problems. For example, the Chemical Mass Balance (CMB) model fully apportions receptor concentrations to chemically distinct sources, using a source profile database. UNMIX and PMF (Table 1.1) internally generate source profiles from the ambient data. Greater data abundance and quality (more species, stratified measurements by particle size, and shorter sampling intervals) therefore greatly improve the utility of receptor modelling. Receptor model algorithms are continuously improved to take advantage of new datasets.

1.2.3 Recent regulatory applications of air models

The Clean Air Interstate Rule (CAIR) and the Clean Air Mercury Rule (CAMR) are two recent examples of Federal rules (both promulgated in 2005) under the Clean Air Act (CAA) that extensively used results from air quality models (US EPA, 2005a,

2005b). CAIR proposed an overall cap for NO_x and SO_x emissions from electric utilities in the US, combined with a trading programme designed to optimise the economic efficiency of emissions reductions. CAMR was the first-ever rule in the US regulating mercury emissions from coal-fired utilities.

In 2008 the Court remanded CAIR owing to concerns about the implementation and effectiveness of the emissions trading programme, but left the rule in place until US EPA issues a replacement (United States Court of Appeals, 2008b). One of the Court's concerns related to an individual state's ability to achieve compliance with air quality standards when no set limits were enforced on individual point sources. Although modelling simulations performed as part of the rulemaking indicated that the cap and trade programme would be successful, the Court did not consider this evidence to be sufficient to meet regulatory requirements.

A review of previous legal challenges to the Agency's model-based decision-making (McGarity and Wagner, 2003) showed that, in prior rulings, science-based challenges to the Agency were generally unsuccessful unless they could demonstrate choices that were "arbitrary and capricious" (i.e., lacked a logical rationale), and that the underlying science of the Agency's modelling applications was rarely questioned. In the case of CAIR, the specific modelling application in question was the Integrated Planning Model (IPM). IPM provides 20–30 year forecasts of least-cost energy expansion, electricity dispatch, and emissions controls strategies based on extensive historical data representing the US electric power system. The model determines the least-cost method of meeting energy and peak demand requirements over a specified period (e.g., 2010 to 2030), and considers a number of key operating or regulatory constraints (e.g., emission limits, transmission capabilities, renewable generation requirements, fuel market constraints) that are placed on the power and fuel markets. The Court's concerns with IPM results thereby challenged US EPA's integrated modelling assessment that combined behavioural assumptions with air-quality simulations. Such a precedent may indicate that integrated modelling activities will face greater legal scrutiny than modelling within a single disciplinary domain, such as the air quality modelling performed using CMAQ and reported in the Technical Support Documents (TSD) of the final CAIR rule (US EPA, 2005b).

In 2008 the Court also remanded and vacated CAMR (United States Court of Appeals, 2008a) owing to what it deemed to be inappropriate regulation of mercury emissions sources under section 111 of the CAA (which allows an emissions trading programme) rather than section 112 intended for regulating HAPs. From a scientific perspective the RIA for the CAMR rule provides another example of an integrated modelling analysis for decision-making (US EPA, 2005c). Because mercury exposure is dominated by the consumption of marine and freshwater fish (Mahaffey *et al.*, 2004; Sunderland, 2007), analysing how emissions controls may reduce health impacts on wildlife and humans requires an understanding of atmospheric and aquatic fate and transport, bioaccumulation and human exposure pathways. Modelling conducted as part of the rule analysis therefore included: CMAQ model simulations that assessed the impact of emissions controls on deposition across the contiguous US (Figure 1.2 – see colour insert); water body fate, transport and bioaccumulation simulations based on the SERAFM (Knightes, 2008), WASP (Ambrose, 1988), and BASS (Barber,

2006) models for a variety of freshwater ecosystems; and human exposure analyses based on freshwater fish consumption rates and preferences (US EPA, 2005c).

Integrated environmental modelling applications, such as the example provided by the CAMR rule analysis, are needed to assess the effectiveness of regulations in terms of human health and ecological indicators. Demand for such modelling applications represents a shift towards outcome-oriented decision-making by government agencies. For example, the CAA also requires US EPA to assess relationships between exposure to other (i.e., in addition to NO_2 and SO_2) criteria air pollutants (ozone, particulate matter, carbon monoxide, lead) and human health impacts. To do this, US EPA must combine atmospheric transport and chemistry models with epidemiological models for morbidity and mortality.

Modelling performed as part of the CAMR analysis also illustrates some of the challenges associated with combining multiple models with differing spatial and temporal scales. Mercury deposition originates from both local and long-range sources. Relative contributions of sources within the regulatory domain (country, state, etc.) to deposition depend on the magnitude and composition of mercury released, and on physical and chemical factors that affect the transport and conversion of global atmospheric mercury sources to water soluble forms that deposit rapidly (Lin and Pehkonen, 1999). Across the entire US, a large fraction (70–80%) of the mercury deposited originates from natural and global sources (Seigneur *et al.*, 2004; Selin *et al.*, 2007). However, individual ecosystems in proximity to point sources may receive a much greater contribution from domestic sources that will be affected by emissions control. Because of the significance of global sources for mercury deposition, regional air-quality models such as CMAQ must use boundary conditions from global chemical transport models such as GEOS-Chem (Selin *et al.*, 2007). Differences in rate constants and underlying algorithms between regional and global modelling frameworks can result in erroneous results at the boundaries of the modelling domain. For example, the modelling simulation in Figure 1.2 erroneously shows enhanced mercury deposition at the eastern extreme of the CMAQ model over the Atlantic Ocean where it meets the boundary conditions provided by the global GEOS-Chem model. Finally, mercury is integrated globally both through the atmosphere and also in the human exposure pathway through commercial market fisheries (Sunderland, 2007). Analysis of the exposure pathway must therefore consider the effects of domestic emissions on global fisheries, in addition to domestic water bodies, greatly increasing the complexity of modelling analyses required (Sunderland and Mason, 2007).

Temporal lags in ecosystem responses to regulatory actions have a direct impact on cost–benefit analyses performed as part of RIAs. For example, in the case of mercury, freshwater ecosystems require anywhere from a few years to many decades to reach steady state with new atmospheric deposition levels (Knightes *et al.*, 2009). When translated into economic terms for policy analysis, discounting of regulatory benefits into net present values means that ecosystem lag times result in large declines in regulatory "benefits" (Knightes *et al.*, 2009).

In summary, regulatory assessments that use fate and transport models for pollutant dispersion are increasingly requiring information on the global scale to assess the effectiveness of domestic regulations at reducing human exposures and

associated health effects. Accordingly, modelling analyses supporting decision-making are required to integrate information across disciplines at multiple spatial and temporal scales.

1.2.4 Future directions in air quality modelling

Atmospheric fate and transport models used in policy analysis require an extensive history of past applications and substantial evaluation. Such models are often referred to as "validated and verified". However, model evaluation efforts should ideally continue throughout the entire life cycle of a model's use. Model parameters need to be continuously updated with new measurement data, and with improvements in scientific understanding of fate and transport processes (NRC, 2007). An example of this practice is provided by the exchange of information between US EPA's regulatory modelling division in the Office of Air and Radiation and the Atmospheric Modeling and Analysis Division (AMAD) in the National Exposure Research Laboratory of US EPA's Office of Research and Development. The research and development group tests new model developments or extensions to existing models such as CMAQ, to add or enhance existing modelling capabilities based on regulatory needs. Model development often includes adding new algorithms based on basic science research into atmospheric chemistry reaction rates and transport mechanisms. The credibility of new and enhanced models for regulatory applications is established by comparing simulated results with measurement data to develop performance indicators.

The GEOS-Chem global atmospheric chemical transport model (CTM) provides an example of the intersection between research and regulatory modelling applications. GEOS-Chem is used by over 50 research groups globally, and also for a variety of regulatory assessments performed by US EPA. One example, as mentioned above, was the use of GEOS-Chem to provide the global boundary conditions for the 2005 CAMR modelling simulations. Many atmospheric chemistry researchers are now focused on exploring the interactions between climate and air quality using CTM simulations (with models such as GEOS-Chem) driven by general circulation model (GCM) simulations of 21st century climate (Jacob and Winner, 2009). Such simulations, in combination with projections on future emissions levels, can help to plan for future changes in air quality (Wu *et al.*, 2008) and identify the most appropriate regulatory actions. In addition, growing recognition of the importance of air–sea and air–land exchange processes for global budgets (e.g., Figure 1.3 – see colour insert) emphasises the need for coupled biogeochemical models for mercury (Selin *et al.*, 2008; Sunderland and Mason, 2007), methanol (Millet *et al.*, 2008), nitrous oxide (Suntharalingam *et al.*, 2000), and carbon cycling (Suntharalingam *et al.*, 2003, 2008). Finally, much research is now focused on resolving uncertainty in emissions inventories and associated source contributions to atmospheric pollution through the use of inverse modelling of emissions source regions using CTMs (Kopacz *et al.*, 2009; Palmer *et al.*, 2006; Suntharalingam *et al.*, 2005).

1.3 SURFACE WATER QUALITY MODELLING

The objective of the Act is to "restore and maintain the chemical, physical and biological integrity of our Nation's waters." Water quality standards set by statute "shall be such as to protect the public health or welfare. . ."

Clean Water Act (CWA), 33 USC § 1313(c)(2)(A)

1.3.1 Regulatory background

The goal of the Clean Water Act (CWA) is "to restore and maintain the chemical, physical and biological integrity of the Nation's waters" (33 USC § 1251(a)). Under section 303(d), the CWA requires all states to submit a "303(d) list" of all impaired and threatened waters to US EPA for approval every two years. A state lists waters as impaired if current regulations and controls are not stringent enough to meet the water quality standards. The state must also establish priorities for the development of total maximum daily loads (TMDLs) based on severity of pollution and the sensitivity of the uses of the waters, among other factors (40 CFR §130.7(b)(4)), and provide a long-term plan for completing TMDLs within 8 to 13 years of a water being listed.

Water quality standards define protection goals by designating uses for a given water body, setting criteria to protect those uses, and establishing provisions to protect water quality from pollutants. A water quality standard consists of four basic elements:

- designated uses (e.g., recreation, water supply, aquatic life, agriculture);
- criteria to protect designated uses (numeric pollutant concentrations and narrative requirements);
- an antidegradation policy to maintain and protect existing uses and high-quality waters; and
- general policies addressing implementation issues (e.g., low flows, variances, mixing zones).

A TMDL calculates how much of a given pollutant can enter a water body before the water body exceeds quality standards. Models are used to quantify this "assimilative capacity", and for determining a waste load allocation that ensures that this capacity is not exceeded (DePinto *et al.*, 2004). TMDLs allocate inputs of pollutants to point sources (waste load allocation (WLA) through the National Pollutant Discharge Elimination System (NPDES) Program) and non-point sources (load allocation (LA)). A margin of safety (MOS) is required for numerical assessments to account for uncertainty in the load calculation. The TMDL consists of three parts, which all introduce uncertainty and variability into load assessments:

$$\text{TMDL} = \sum \text{WLA} + \sum \text{LA} + \text{MOS}$$

Waste loads and non-point sources are often temporally variable, and may undergo transformations, gains, or losses within the water body. The timing and location of critical conditions may be related to climate (e.g., precipitation, snow melt) or hydrology (e.g., high flow, low flow), or be event-based (e.g., discharge, spills). The

MOS is based on the desired level of protection that the TMDL will provide, which is subject to policy interpretations and subjective deliberations. The MOS may also include "implicit" and "explicit" components. The implicit MOS includes conservative assumptions on how the numeric target is derived, how the numeric model application is developed, and the feasibility of restoration activities. The explicit MOS includes uncertainties in the modelling system or water body response, such as setting numeric targets at more conservative levels than sampling results indicate, adding a safety factor to pollutant loading estimates, and/or setting aside a portion of the available loading capacity (US EPA, 1999).

TMDLs are developed using various techniques, ranging from simpler mass budget calculations to more complex chemical and hydrodynamic differential mass balance simulations. Water quality models allow the explicit representation of time-dependent transport and transformation processes that affect exposures. The Ecosystems Research Division in US EPA's National Exposure Research Laboratory has developed and applied a variety of water quality models for TMDL development and water quality protection. Examples of such models are described in more detail below.[5] US EPA provides assistance to the regional offices, state and local governments, and their contractors in implementing the CWA through the Watershed and Water Quality Modeling Technical Support Center.[6]

1.3.2 Examples of water quality models used in TMDLs and regulatory actions

WASP (Water Quality Analysis Simulation Program)

The Water Quality Analysis Simulation Program (WASP7) is an enhancement (version 7) of the original WASP (Di Toro *et al.*, 1983; Connolly and Winfield, 1984; Connolly and Thomann, 1985; Ambrose, 1988) that simulates water quality conditions and responses. WASP is a dynamic compartment-modelling framework for aquatic systems that includes water column segments and underlying benthic segments. The WASP modelling framework consists of a simple flow module (including net flows, gross flows, and kinematic wave propagation), several different kinetic modules, including heat (HEAT), toxicants (TOXI), nutrients (EUTRO) and mercury (MERCURY), and the time-varying processes of advection, dispersion, point and diffuse mass loading, and boundary exchange.

Examples of previous WASP applications include investigations of:

- eutrophication and phosphorus loading (James *et al.*, 1997; Tufford and McKellar, 1999; Wang *et al.*, 1999);
- kepone, a carcinogenic insecticide (O'Connor *et al.*, 1983);
- volatile organics (Ambrose, 1987; Zhang *et al.*, 2008);
- heavy metals (Caruso, 2003; Yang *et al.*, 2007); and
- mercury (US EPA, 2001b; 2004a, 2004b).

WASP has been used to develop TMDLs for the Neuse River Estuary, North Carolina (Wool *et al.*, 2003); Cape Fear River, North Carolina; Fenholloway River, Florida;

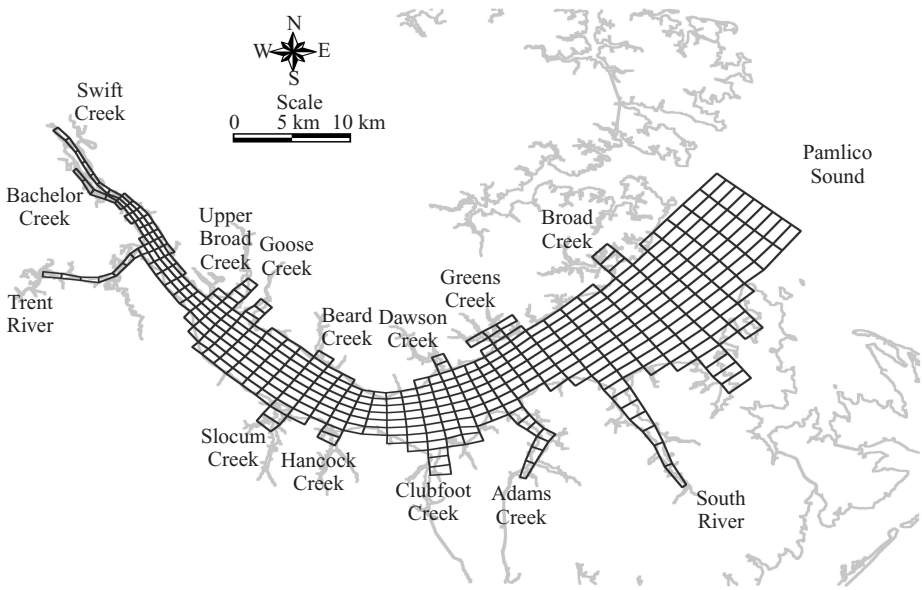
Mobile Bay, Alabama; Flint Creek, Alabama; Coosa Lakes, Alabama; Lake Allatoona, Georgia; and Alabama River, Alabama.[7] Figure 1.4 shows the WASP grid developed to simulate nutrient dynamics in the Neuse River, North Carolina.

Because WASP is primarily a fate and transport model, it has a relatively simple hydrodynamic component. The model uses known inflows and outflows for each WASP segment, or the kinematic wave formulation for flow routeing. For systems with more complex hydrodynamics EFDC or DYNHYD can be used, and then the hydrodynamic file can be linked into WASP. These models are described below.

Environmental Fluid Dynamics Code (EFDC) and DYNHYD

The Environmental Fluid Dynamics Code (EFDC) (Hamrick, 1996) is a multidimensional hydrodynamic model used to simulate flow and solids movement, and for solving three-dimensional, vertically hydrostatic, free surface, turbulent-averaged equations of motion for variably dense fluids. EFDC has been applied to over 100 water bodies, including rivers, lakes, reservoirs, wetlands, estuaries and coastal ocean regions in support of environmental assessment and regulatory investigations. DYNHYD is an enhancement of the Potomac Estuary hydrodynamic model, and employs

Figure 1.4: Example of Water Quality Simulation Program (WASP) grid developed to simulate nutrient dynamics in the Neuse River Estuary, NC.



Source: Wool, T.A., Davie, S.R. and Rodriquez, H.N. (2003). Development of 3-D hydrodynamic and water quality models to support total maximum daily load decision process for the Neuse River Estuary, North Carolina. *Journal of Water Resource Planning and Management*. 129: 295–306. (In the public domain.)

one-dimensional continuity and momentum equations for a branching network. DYNHYD can be used as an intermediary step between WASP's kinematic wave and EFDC.

River and Stream Water Quality Model (QUAL2K/QUAL2E)

The River and Stream Water Quality Model (QUAL2K or Q2K; Chapra *et al.*, 2007) is a modernized version of the QUAL2E (Q2E) model (Brown and Barnwell, 1987). QUAL2K is a branching, one-dimensional model, where the channel is well mixed vertically and laterally. QUAL2K models the diurnal heat budget and water-quality kinetics, and simulates carbonaceous biochemical oxygen demand (BOD), anoxia, sediment–water interactions, algal growth, pH, and pathogens. Collecting the appropriate data for model calibration can be a major problem for complex hydrodynamic models such as QUAL-2E. To help address some of these issues, QUAL2E-UNCAS provides a series of uncertainty analysis techniques, including sensitivity analysis, first-order error analysis, and Monte Carlo simulations. These techniques are described in detail elsewhere (Barnwell *et al.*, 2004).

BASINS

The Better Assessment Science Integrating point and Non-Point Sources (BASINS) software system is a multipurpose environmental analysis system designed for regional, state and local agencies that perform watershed and water-quality-based studies. The BASINS system was originally introduced in 1996, with improved versions in 1998, 2001 and 2004. The most recent development of BASINS 4.0 integrates an open-source geographic information system (GIS) architecture with national watershed data and modelling and assessment tools. BASINS integrates environmental data, analytical tools and modelling programs for management applications such as the development of TMDLs. BASINS provides a means to search the web for necessary GIS data layers, such as monitoring data, hydrography, land use, and digital elevation. These files are then pulled into a common layer data source that can be used to populate watershed and water quality models. A series of models have been housed within the BASINS framework, including PEST (the Parameter Estimation Tool), HSPF (Hydrological Simulation Program – FORTRAN), AQUATOX, and SWAT. Currently there is an effort to move WASP into BASINS.

EXAMS

The Exposure Analysis Modelling Systems (EXAMS) (Burns *et al.*, 1982; Burns, 2004) was developed to rapidly evaluate the fate and transport of synthetic organic chemicals such as pesticides, industrial materials and leachates from disposal sites, and resulting exposure levels. EXAMS analyses long-term (steady-state), chronic chemical discharges, and short-term acute chemical releases from episodic discharges or weather-driven runoff and erosion. EXAMS also performs full kinetic simulations that allow for monthly variation in the meterological parameters and alterations of chemical loadings on a daily timescale. EXAMS is generalisable in structure for different spatial dimensions, and in the number of contaminants and chemical

degradation by-products modelled. The user determines the level of complexity of the environmental description and the number of chemicals simulated.

Expected concentrations of synthetic contaminants and their by-products can be simulated using EXAMS. The user can specify the exposure interval so that EXAMS will report acute (e.g., 96 hours) or chronic (21 days or longer) exposures. Sensitivity analysis is included in EXAMS to present the relative importance of each transformation and transport process. The persistence of each chemical through transport of transformation after the source of contaminant has been removed can also be determined. EXAMS has also been linked to PRZM3 (the Pesticide Root Zone Model) and BASS (a food web bioaccumulation model). PRZM is a one-dimensional, dynamic, compartment model that simulates chemical movement in an unsaturated soil system around the plant root zone. PRZM3 includes both PRZM and VADOFT (Vadose Zone Flow and Transport Model) in its internal structure. VADOFT simulates moisture movement and solute transport in the vadose zone (the zone from the ground surface to the water table in terrestrial systems). Linking PRZM to VADOFT allows the fate and transport and exposures of nearby water bodies to be modelled following applications of agricultural pesticides.

1.3.3 Current and future directions for water quality modelling

US EPA's Office of Research and Development is currently working to improve both the underlying science and the physical simulation capabilities of its available water quality modelling tools. In WASP7, recent advances have increased the number of algal types in the eutrophication module. This allows for different physiological growth parameters for algae, which are important for accurately represent the timing of blooms and algal concentrations. Algorithms describing mercury kinetics are also being updated to reflect recent advances in understanding of environmental processes driving methylation, demethylation, oxidation and reduction reactions.

Current research projects involving WASP include simulating headwaters of watersheds, smaller stream and river systems, and complex hydrologic systems including reservoirs, impoundments and flood plains. To better represent the diversity of these systems, recent WASP developments have included the incorporation of the weir equations to handle flow routeing over dams/impoundments, and variable hydraulic geometry to handle systems with variable widths, depths and velocities as functions of volumetric flow rates. Future versions of the model will include DYNHYD algorithms for flow routeing, updated solids routines based on shear stress, process-based solids deposition, scour equations, and the introduction of a fourth solids type (cobbles) to represent solids that cannot resuspend or scour.

Better representation of watershed influences on receiving water quality is required for water quality modelling to include assessments of how smaller rivers and streams affect the dynamics of large water bodies. Recent mercury cycling research and TMDL development by US EPA reinforces the importance of the watershed as a loading source for most freshwater systems. TMDLs developed for Brier Creek and the Ocklocknee and Ogeechee watersheds in Georgia applied the Watershed Char-

acterisation System-Mercury Loading Model (WCS-MLM) to simulate mercury loadings into the river of interest. A spatially explicit watershed model for mercury (the Grid-Based Mercury Model, GBMM) has since been developed as an enhancement to initial work performed using WCS-MLM. GBMM uses GIS layers of digital elevation, land-use type, soil-use type and stream hydrography to simulate watershed soil mercury concentrations, runoff and erosion to nearby water bodies (streams and rivers) as a function of atmospheric deposition loading to watersheds.[8] As WASP is moved into BASINS, GBMM is similarly being incorporated into BASINS. GBMM was originally developed within ArcGIS, but the transition into BASINS will assist in pulling the necessary data layers for use in GBMM, as well as being constructed using an open-source, freely available GIS program.

Much of the present work enhancing modelling capabilities at US EPA is focused on combining multiple modelling tools to assess interactions among environmental media and human behaviour. For example, understanding the effectiveness of atmospheric mercury emissions controls requires the output of atmospheric models to be linked to watershed, water body and bioaccumulation models to simulate changes in fish mercury levels (Knightes *et al.*, 2009). The scales of modelling analysis are also growing beyond processes occurring within a single water body to include the interrelationships of ecosystems and account for environmental stressors that are typically not limited by political boundaries.

To enhance technological capabilities for integrated modelling analyses, US EPA has been applying specific tools such as the Framework for Risk Analysis of Multi-Media Environmental Systems (FRAMES). FRAMES enables complex environmental process simulations based on linked modelling applications by allowing different models to pass data efficiently. For example, US EPA has developed a pilot application for 53 twelve-digit hydrologic unit code (HUC) headwater watersheds within the Albermarle and Pamlico watersheds in North Carolina and Virginia. For this application, hydrologic, water quality and bioaccumulation models were linked in FRAMES, along with an ecological model for habitat suitability index and a companion mercury watershed tool. The coupled modelling application was used to simulate the fate of atmospherically deposited nitrogen and mercury through the watershed and into streams and rivers to predict impacts on fish communities. Linking systems within a single framework facilitated sensitivity and uncertainty analysis for the unified modelling system. Ongoing modelling of the effects of hydrology and erosion on nitrogen and mercury cycling in the Cape Fear River basin is also linking atmospheric, watershed and water body models for a complete analysis of ecosystem processes. However, linking models across different media can be challenging, owing to propagation of uncertainty. For example, closing the hydrological mass balance across linked atmospheric and aquatic models can be difficult, because atmospheric models typically use simulated precipitation for the deposition via rainfall, whereas watershed hydrology models have traditionally used observed rain gauge station data. Synchronised water mass balances require the precipitation rates to be identical, otherwise pollutants such as nitrogen, sulfur and mercury are lost from the atmosphere at rates different from those at which they are deposited on the land surface, resulting in mass balance errors. Differences in spatial and temporal resolution of simulations across

different media must also be reconciled in these types of application. Generally, the time steps used for atmospheric modelling simulations are small (seconds) compared with ecosystem models (days), while the spatial domain of atmospheric models tends to be much larger (grid sizes of the order of kilometres) than ecosystem models (grid sizes of the order of metres).

1.4 BIOACCUMULATION MODELLING

Regulatory action on existing toxic substances are authorized "if the Administrator finds that there is a reasonable basis to conclude that the manufacture, processing, distribution in commerce, use, or disposal of a chemical substance or mixture, or any combination of such activities, presents or will present unreasonable risk of injury to health or the environment".

Toxic Substances Control Act (TSCA), 15 USC § 2605(a)

A pesticide may be registered only if the Administrator finds that "when used in accordance with widespread and commonly recognized practice, it will not cause unreasonable adverse effects on the environment."

Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA), 7 USC § 136(c)(5)(D)

A protective standard for pesticide residues is rebutted only once "there is reasonable certainty that no harm will result from aggregate exposures to these residues".

Federal Food, Drug, and Cosmetic Act, 21 USC § 346a

1.4.1 Regulatory background

Chemical substances that achieve high concentrations in organisms relative to ambient environmental concentrations (air/water/sediments) can pose a variety of human and ecological health risks. Generally, those chemicals that are persistent, bioaccumulative, toxic, and subject to long-range transport have been the focus of chemical screening assessments and regulatory control strategies (Mackay and Fraser, 2000). Bioaccumulation of chemicals is generally quantified using either empirical data or mechanistic models. Empirical approaches use field data to derive a bioconcentration factor (BCF) or bioaccumulation factor (BAF), whereas mechanistic models use mass balance relationships to characterise biological uptake and loss processes (Mackay and Fraser, 2000). Organism/water concentration ratios measured in laboratory tests (BCFs) or in the field (BAFs) have limited predictive capability, and are subject to numerous errors, such as those caused by biological variability (Arnot and Gobas, 2006). Mechanistic models require more extensive data about chemical properties and food webs, but can provide insight into bioaccumulation phenomena, and have much greater predictive capability. Such models are used for a variety of applications, including screening of new and existing chemicals for their potential to bioaccumulate, developing environmental quality guidelines for water and sediments, and assessing exposure of biota to pollutants.

Bioaccumulation modelling is an integral part of several different regulatory programmes at US EPA, including water quality assessments, contaminated site clean-up, and screening of new chemicals. As discussed above, bioaccumulation modelling may also be used to inform risk and regulatory assessments for atmospherically deposited contaminants. Water quality standards as part of the CWA for bioaccumulative contaminants such as mercury are listed as fish tissue residue guidelines rather than as aqueous concentration thresholds (US EPA, 2008). These assessments require information on bioaccumulation that is derived from models on a site-specific basis, or is based on simplified bioaccumulation factors (BAFs) for different ecosystems. The Superfund programme also requires information on potential bioaccumulation of metals and organic contaminants to develop hazard indices for humans and wildlife that in turn guide remediation goals. Finally, US EPA's Office of Pollution Prevention and Toxic Substances (OPPTS) is tasked with screening new and existing chemicals used by industry for potentially harmful environmental effects, including bioaccumulation. For example, the new chemicals programme under the Toxic Substances Control Act (TSCA) requires US EPA to review approximately 2000 new chemicals per year, and to issue decisions on 20–30 chemicals per day (NRC, 2007).

1.4.2 Chemical screening

Screening-level models are useful for identifying chemicals that could potentially pose a threat to human or ecological health because of persistence in the environment, bioaccumulation potential, or toxicity. These models are not subject to the same rigorous review standards as other regulatory models, because they are meant to trigger further studies of investigations of potentially problematic chemicals. Physical chemical properties can be used as screening-level models to identify those chemicals most likely to pose environmental risks. Some of these screening-level models may be simplifications of more complex bioaccumulation models with simplifying assumptions.

For example, the BAF-QSAR model[9] is a generic tool that provides estimates of the bioaccumulation factor (BAF) of non-ionic organic chemicals in three general trophic levels of fish (i.e., lower, middle and upper). The BAF predictions are considered "generic" in that they are not considered to be for a particular species of fish. The model is essentially a quantitative structure–activity relationship (QSAR) requiring only the octanol–water partition coefficient (K_{ow}) of the chemical and the metabolic transformation rate constant (if available) as input parameters. BAF-QSAR v1.1 is derived from the parameterisation and calibration of a mechanistic bioaccumulation model to a large database of evaluated empirical BAFs from Canadian waters. The empirical BAFs are for chemicals that are poorly metabolised and are grouped into lower, middle and upper trophic levels of fish species. The model is calibrated to each trophic level of measured BAF values, thus providing estimates that are in agreement with empirical BAFs. The model can be used to predict dietary concentrations for higher trophic-level predators (e.g., birds and mammals), including human exposure concentrations from fish in their diet. When a contaminant is known to meet the criteria for bioaccumulation potential, persistence in the environment and toxicity,

additional more detailed modelling simulations are often focused on specific sites of interest where contamination is thought to be a problem. Simple BAF calculations may not accurately predict concentrations of extremely hydrophobic chemicals and metals such as mercury that are often the chemicals of greatest concern (Barber, 2003).

1.4.3 Examples of regulatory and research models commonly used by US EPA

AQUATOX

AQUATOX is a simulation model for aquatic ecosystems, predicting the fate of pollutants, nutrients and organic chemicals and their ecosystem effects on fish, invertebrates and aquatic plants (Rashleigh, 2003; US EPA, 2001a). AQUATOX can be used to develop numeric nutrient targets based on desired ecological endpoints, evaluate impacts of several stressors which may cause biological impairment, predict effects of pesticides, evaluate response to invasive species, and (when linked with the BASINS modelling system) determine effects of land-use change on aquatic life. Example applications of the model include periphyton response to nutrients, snail grazing and variable flow in Walker Branch, Tennessee (US EPA, 2001), eutrophication due to nutrient and organic matter loadings at Coralville Reservoir, Iowa, and computation of bioaccumulation of organic toxins in Lake Ontario (US EPA 2000b), among others (Bingli *et al.*, 2008; Park *et al.*, 2008; Rashleigh *et al.*, 2009).

BASS

The Bioaccumulation and Aquatic System Simulator (BASS) model is a physiological model that simulates the population and bioaccumulation dynamics of age-structured fish communities. BASS describes contaminant dynamics using algorithms that account for species-specific terms affecting uptake and elimination of mercury, such as diet composition and growth dilution among different age classes of fish (Barber, 2001, 2006). For example, fish mercury intake is modelled as a function of gill exchange and dietary ingestion, and the model partitions mercury internally to water, lipid and non-lipid organic material. The structure of BASS is generalised and flexible, allowing users to simulate both small, short-lived species (dace and minnow) and large, long-lived species (bass, perch, and trout) by specifying either monthly or yearly age classes for any given species. The community's food web is defined by identifying one or more foraging classes for each fish species, based on body weight, body length, or age. The dietary composition of each foraging class is then specified as a combination of benthos, incidental terrestrial insects, periphyton/attached algae, phytoplankton, zooplankton, and/or other fish species (Barber, 2006).

Although BASS was developed to investigate the bioaccumulation of chemical pollutants within a community or ecosystem context, it can also be used to explore population and community dynamics of fish assemblages that are exposed to a variety of non-chemical stressors such as altered thermal regimes associated with hydrological alterations or industrial activities, commercial or sports fisheries, and introductions of

non-native or exotic fish species. BASS can be used to evaluate various dimensions of fish health through its capability to simulate the growth and predator–prey dynamics for individual fish, and the productivity, recruitment/reproduction and mortalities of their associated populations. Process-based models such as BASS that simulate the toxicokinetic, physiological and ecological processes of fish provide scientifically defensible tools that can overcome many of the limitations and uncertainties associated with the use of BAF approaches (Barber, 2003).

AQUAWEB

AQUAWEB was developed by Arnot and Gobas (2004), and is a modified version of the Gobas 1993 food web model (Gobas, 1993) developed for assessing the degree of bioaccumulation of hydrophobic organic chemicals in aquatic ecosystems. AQUAWEB is a kinetically based model that provides site-specific estimates of chemical concentrations in organisms of aquatic food webs from chemical concentrations in water and sediments (Arnot and Gobas, 2004). For zooplankton, aquatic invertebrates and fish the model calculates rates of chemical uptake from the water and the diet, and rates of chemical elimination to the water, faeces and the "pseudo" loss mechanism of growth dilution. The model requires input data on chemical properties (K_{ow}), environmental conditions, species-specific characteristics, and food web structure. These data are used to develop rate constants for chemical uptake and elimination in fish through dietary intake, gill ventilation, metabolic transformation, faecal egestion, and growth dilution.

1.4.4 Future research and regulatory directions

In 2004 the Stockholm Convention on Persistent Organic Pollutants proposed to eliminate most globally persistent, bioaccumulative and toxic substances. Such assessments have traditionally relies on vakues of K_{ow} for different chemicals, or empirical BAF/BCF data when such information is not available. Generally, those chemicals with $K_{ow} > 10^5$ are considered bioaccumulative, and are screened for further study in regulatory assessments. However, a variety of studies have shown that terresterial food webs (air-breathing organisms) can bioaccumulate chemicals with low K_{ow} values but high octanol–air (K_{oa}) partition coefficients (K_{oa} range 10^6–10^{12}) (Kelly and Gobas, 2001; Kelly *et al.*, 2007). For example, Kelly *et al.* (2007) showed that although hydrophobic chemicals such as hexachlorocyclohexanes (HCHs, $K_{ow} = 10^{3.8}$), tetrachlorobenzenes ($K_{ow} = 10^{4.1}$) and ensdosulfans ($K_{ow} = 10^{3.7}$) do not biomagnify in piscivorous aquatic organisms, they accumulate to a significant degree in terrestrial food webs. The authors also found that two thirds of all chemicals used in commerce have $K_{ow} > 10^2$ and $K_{oa} > 10^6$, and could therefore accumulate in terrestrial food webs. This research strongly suggests that chemical screening models based on K_{ow} values that do not consider K_{oa} values for terrestrial food webs will miss a large number of bioaccumulative contaminants. Future research and regulatory work needs to consider the implications of these findings for current chemical screening methods in the US.

1.5 CONTAMINATED SITE REMEDIATION

Standards for treatment of hazardous wastes disposed onto land shall specify "those levels or methods of treatment, if any, which substantially diminish the toxicity of the waste or substantially reduce the likelihood of migration of hazardous constituents from the waste so that short-term and long-term threats to human health and the environment are minimized."

Resource Conservation and Recovery Act (RCRA), 42 US § 6924(m)

The President shall select a remedial action that is protective of human health and the environment, that is cost effective, and that utilises permanent solutions and alternative treatment technologies or resource recovery technologies to the maximum extent practicable.

Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA), 42 USC § 9621(b)

1.5.1 Regulatory background

Both Federal and state-level regulatory programmes oversee contaminated site remediation depending on the nature, extent and severity of contamination. Larger sites with multiple contaminants across environmental media and one or more potentially responsible parties (PRPs) that are listed as Superfund sites fall under the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) or the Resource Conservation and Recovery Act (RCRA). These are both Federal programmes that govern the way sites are characterised, assessed and remediated. In general, CERCLA and RCRA sites rely on risk-based approaches: that is, typically, human health and ecological risk assessments are conducted, and provide the basis for determining remedial standards or clean-up goals. State-level oversight tends to fall under Brownfields-type programmes or other environmental programmes (e.g., every state has a clean-up programme, typically invoked in the context of changes in land use or through real estate transactions). Again, as for the Federal programmes, state regulatory oversight typically involves developing a risk assessment to determine the potential for adverse effects, and generally clean-up levels and remediation goals are based on agreed regulatory thresholds for risk and hazard.

The Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA), commonly known as Superfund, was enacted by Congress on 11 December 1980. This law established a provision for taxing the chemical and petroleum industries, and provides broad Federal authority to respond directly to releases or threatened releases of hazardous substances that may endanger public health or the environment. CERCLA establishes prohibitions and requirements with respect to closed and abandoned hazardous waste sites, and provides for liability of parties responsible for releases of hazardous waste at these sites. Initially, it established a trust fund to provide for clean-up when no responsible party could be identified. However, the trust fund has been largely depleted in recent years.

CERCLA authorises both short- and long-term removal actions. Short-term responses are required when there is the threat of immediate danger to human health

and the environment, whereas longer-term responses are required for releases that are not immediately life-threatening, but which are serious with respect to potential effects as a result of exposure in humans and animals. The overall goal of any CERCLA remedy is to protect human health and the environment: thus, in virtually all cases, risk assessments are conducted to evaluate the potential for adverse effects.

RCRA is the law that governs disposal of all hazardous and non-hazardous solid waste. Facilities that generate, treat, store or dispose of hazardous waste are regulated under Subtitle C of RCRA. As with CERCLA, the overall mandate of the law is to protect human health and the environment. The two general approaches that RCRA takes are: preventing environmental problems by ensuring that wastes are well managed from "cradle to grave", reducing the amount of waste generated, conserving energy and natural resources; and cleaning up environmental problems caused by the mismanagement of wastes.

The RCRA Corrective Action programme, part of Subtitle C, specifies when action is required to clean up contamination at a facility (as opposed to a site, as under CERCLA). Consequently, RCRA corrective actions usually occur at facilities that treat, store or dispose of hazardous waste, and corrective actions can often occur while a facility continues operating.

1.5.2 Risk-based approaches to contaminated site clean-up

Within US EPA's waste and clean-up programmes, and most state programmes, the National Academy of Sciences' Risk Assessment Paradigm provides the framework for informing regulatory and programme decisions to protect human health and the environment. A variety of US EPA reports (US EPA, 1989, 1991a, 1991b, 1996, 1997, 2000c) provide guidance for designing and conducting human health and ecological risk assessments under CERCLA. These documents generally serve as guidance for the RCRA programme as well. Most states also have their own risk assessment guidance.

Risk assessments are generally context- and site-specific. However, all risk assessments share the common element of modelling. Virtually every risk assessment requires underlying fate and transport and food chain modelling to support estimates of risk into the future. These models are used to generate exposure estimates that are used for risk characterisation. The US EPA Center for Exposure Assessment Modeling[10] was established to provide a repository for some of the most commonly used models, but in practice any model (assuming model development was appropriately conducted) can be used to support site-specific decision-making, particularly since all risk assessments and models for the larger sites will undergo peer review. Accordingly, a wide variety of modelling applications are used to support human health and ecological risk assessments in this area.

1.5.3 Hudson River PCB modelling example

The Hudson River flows through New York State for nearly 300 miles (480 km), beginning as a small mountain lake on the side of the State's highest peak, Mt Marcy,

and ending in New York Harbor, one of the world's busiest and most populated metropolitan port areas. Locations along the river are expressed as river miles, representing the number of miles north of New York Harbor. Halfway along the river, approximately 150 miles north of New York Harbor (at river mile 150), the Hudson River flows over the Federal lock and dam at Troy. From this point on the river is an estuary (i.e., a river flowing at sea level, where salt and freshwater mix with tidal flows). The upper freshwater portion of the river consists of a series of locks and dams, whereas the lower river is entirely open. The salt front extends up to river mile 50, and salinity drops off sharply at that point continuing north. In 1973 the Ft Edward dam (at approximately river mile 185) was removed, because of its deteriorating condition, causing a large migration of PCBs into the lower Hudson River. The portion of the river between miles 188 and 195, known as Thompson's Island Pool, represents the most contaminated area, and is considered by US EPA to represent the primary source of PCB contamination to the remainder of the river.

PCB concentrations upstream of Thompson's Island Pool are primarily at non-detect levels, and decline approximately linearly down the river in all media: sediment, water, and biota. PCB levels in the upper river (above the Federal dam) are orders of magnitude higher than for the lower river. Resuspension of highly contaminated sediments from the Thompson's Island Pool area are implicated in the continuing downstream migration of PCBs. In addition, PCB releases from the General Electric (GE) Hudson Falls site due to migration of PCB oil through bedrock have also occurred, although the extent and magnitude of this release are not well known. This leakage was identified after the partial failure of an abandoned mill structure near GE's Hudson Falls plant site in 1991 revealed that PCB-bearing oils and sediments had accumulated within the structure. This failure also served to augment PCB migration from the bedrock beneath the plant to the river.

Over a 30-year period ending in 1977, two GE facilities, one in Fort Edward and the other in Hudson Falls, New York, used PCBs in the manufacture of electrical capacitors. PCBs were considered an ideal insulating fluid because of their nonflammability properties. Various sources have estimated that between 209 000 and 1 300 000 lb (94 800–590 000 kg) of PCBs were discharged between 1957 and 1975 from these two GE facilities (Sofaer, 1976; Limburg, 1984). Discharges resulted from washing PCB-containing capacitors and PCB spills from building and dismantling transformers and capacitors.

PCBs were marketed under the trade name "Aroclor" from 1930 to 1977. Aroclors represent mixtures of individual congeners, but the exact identity and proportion of congeners in any Aroclor mixture is not standard. The most common Aroclors include 1016, 1221, 1242, 1248, 1254 and 1260. The last two digits of any Aroclor number represent the weight percent of chlorine in the mixture (e.g., Aroclor 1254 is 54 percent chlorine by weight). According to scientists at GE, at least 80% of the total PCBs discharged are believed to have been Aroclor 1242, with lesser amounts of Aroclors 1254, 1221 and 1016 (Brown *et al.*, 1985). The exact congener profile of commercial PCBs varied from lot to lot (even in lots from the same manufacturer), creating difficulty in making assumptions about congener profiles in Aroclors unless congener-specific analytical techniques are employed. Specification of the exact

proportion of individual congeners in PCB mixtures requires measurement at a cost of approximately $1000 per sample, versus $300 for the Aroclor standards.

Environmental samples are compared with Aroclor standards, but PCB composition in the environment changes over time through fate processes that include partitioning, chemical transformation, and preferential bioaccumulation into lipid-rich tissues. This results in a congener composition in the environment that differs significantly from the original mixture. Degradation congeners are not accounted for in the Aroclor standards (thus they are not typically detected). US EPA conducted a survey in 1974 showing elevated levels of PCBs in fish. The New York State Department of Environmental Conservation (NYS DEC) subsequently confirmed those findings, and yearly monitoring of fish has been conducted since that time. In February 1976 NYS DEC and the New York State Department of Health (NYS DOH) banned all fishing in the upper Hudson (from the Ft Edward Dam to the Federal dam at Troy), and closed all Hudson River commercial fisheries. In that same year a massive flood (of magnitude such that only one such flood is expected to occur every 100 years) caused a large movement of contaminated sediments from the upper Hudson into the lower river.

In 1984 US EPA issued a Record of Decision identifying GE as the responsible party at the Hudson Site, and called for in-place containment of the remnant deposits along the river bank but no action on sediments at the river bottom. In 1989 NYS DEC petitioned US EPA to reconsider the 1984 Superfund "no action" decision, citing data that suggested continued unsafe levels of PCBs in fish, new information regarding the toxicity of PCBs, and US EPA studies validating the effectiveness of dredging as a clean-up strategy. Consequently, both US EPA and GE developed a series of models to assess site conditions, and to develop risk-based tools and strategies to support clean-up goals for the Hudson River.

The principal questions to be answered by the modelling were:

- When will PCB levels in fish populations recover to levels meeting human health and ecological risk criteria under continued No Action?
- Can remedies other than No Action significantly shorten the time required to achieve acceptable risk levels?
- Are there contaminated sediments now buried that are likely to become "reactivated" following a major flood, possibly resulting in an increase in contamination of the fish population?

The principal fate and transport model developed by US EPA to evaluate these questions is called the Upper Hudson River Toxic Chemical Model (HUDTOX). HUDTOX was developed to simulate PCB transport and fate for 40 miles of the Upper Hudson River from Fort Edward to Troy, New York. The HUDTOX model code was based on an earlier version of the WASP model (WASP4/TOXI4) and updated by US EPA to incorporate a variety of enhancements. HUDTOX simulates PCBs in the water column and sediment bed, and balances inputs, outputs and internal sources and sinks. Mass balances were constructed first for water, then for solids and bottom sediment, and finally for PCBs. External inputs of water, solids loads and PCB loads, plus values for many internal model coefficients, were specified from field observa-

tions. Once inputs were specified, the remaining internal model parameters were calibrated so that concentrations computed by the model would agree with field observations. Model calculations of forecast PCB concentrations in water and sediment from HUDTOX were used as inputs for the forecasts of the bioaccumulation model (FISHRAND).

US EPA also developed the Depth of Scour Model (DOSM). The DOSM was developed principally to provide spatially refined information on sediment erosion depths in response to high-flow events such as a 100-year peak flow. The DOSM is a two-dimensional, sediment erosion model that was applied to the most contaminated portion of the river (and a potential source of PCBs to the remainder of the river, namely the Thompson Island Pool). The Thompson Island Pool is characterised by high levels of PCBs in the cohesive sediments. DOSM was linked with a hydrodynamic model that predicts the velocity and shear stress (force of the water acting on the sediment surface) during high flows. There was also a linkage between the ES-3 US EPA DOSM and HUDTOX. Relationships between river flow and cohesive sediment resuspension were developed using the DOSM for a range of flows below the 100-year peak flow. These relationships were used in the HUDTOX model for representing flow-dependent resuspension.

The bioaccumulation model FISHRAND is based on the food-web bioaccumulation model developed by Gobas (Gobas, 1993; Gobas *et al.*, 1995), and provides a process-based, time-varying representation of PCB accumulation in fish. This is the same form of the model as was used to develop criteria under the Great Lakes Initiative (US EPA, 1995). FISHRAND incorporates distributions instead of point estimates for input parameters, and calculates distributions of fish body burdens from which particular point estimates can be obtained, for example the median, average, or 95th percentile.

Modelling input variables can be described by distributions or point estimates, and users can specify whether parameters should be considered as "variable" (e.g., contributing directly to the population distribution of concentrations) or "uncertain" (e.g., contributing to the uncertainty bounds around the population distribution). There is "true" uncertainty (e.g., lack of knowledge) in the estimated concentrations of sediment and water to which aquatic organisms are exposed, and also variability in parameters contributing to contaminant bioaccumulation. Uncertainty and variability should be viewed separately in risk assessment, because they have different implications for regulators and decision-makers (Morgan and Henrion, 1990; Thompson and Graham, 1996). Variability is a population measure, and provides a context for a deterministic point estimate (e.g., average or reasonable maximum exposure). Variability typically cannot be reduced, only better characterised and understood. In contrast, uncertainty represents unknown but often measurable quantities. Typically, obtaining additional measurements can reduce uncertainty. Quantitatively separating uncertainty and variability allows an analyst to determine the fractile of the population for which a specified risk occurs, and the uncertainty bounds or confidence interval around that predicted risk. If uncertainty is large relative to variability (i.e., it is the primary contributor to the range of risk estimates), and if the differences in cost among management

alternatives are high, collecting and evaluating additional information can be recommended before making management decisions regarding risks from exposures to contaminants. Including variability in risk estimates also allows decision-makers to evaluate quantitatively the likelihood of risks both above and below selected reference values or conditions (for example, average risks as compared with 95th percentile risks).

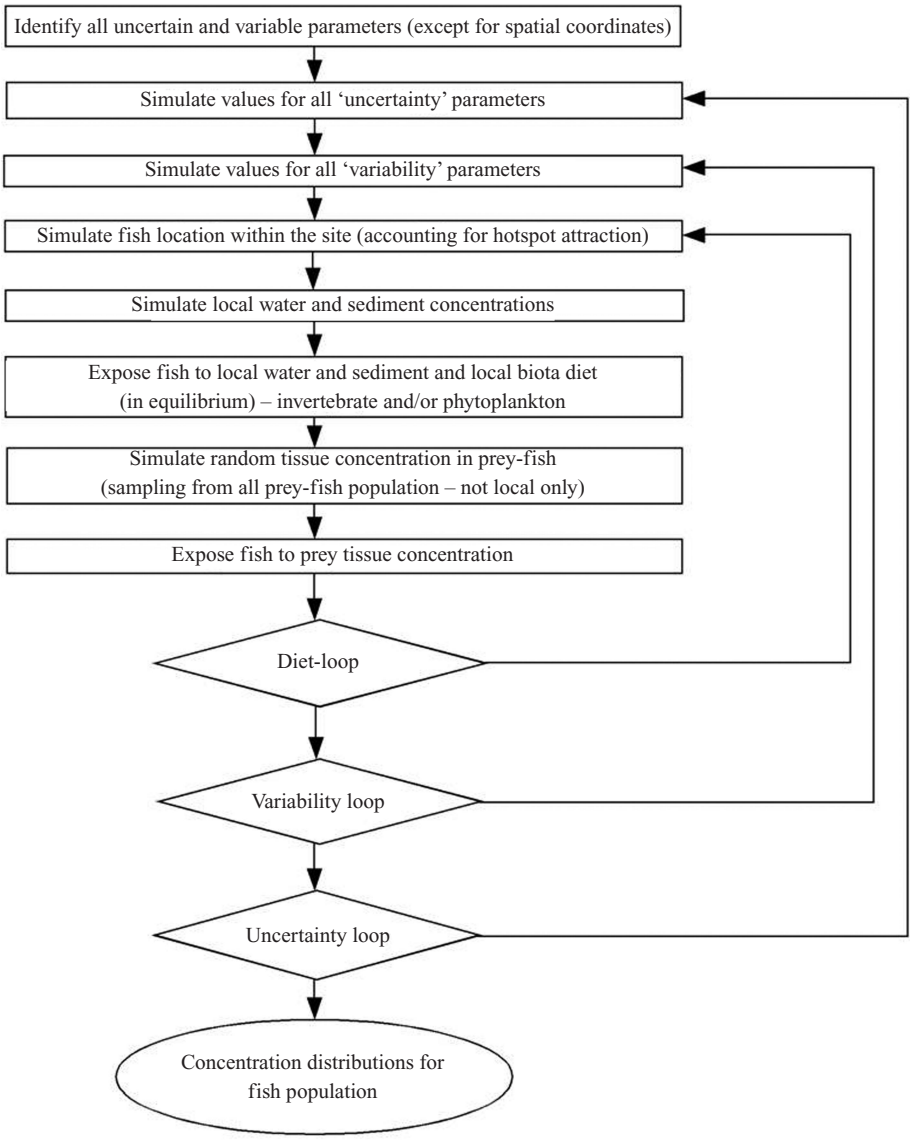
Characterising uncertainty and variability in any model parameter requires informed and experienced judgement. Studies have shown that in some cases, based on management goals and data availability, it is appropriate to "parse" input variables as predominantly uncertain or variable (Cullen, 1995; Kelly and Campbell, 2000; von Stackelberg *et al.*, 2002a, 2002b). Figure 1.5 provides a schematic of the nested modelling framework.

The spatial submodel of FISHRAND is described in detail elsewhere (Linkov *et al.*, 2002; von Stackelberg *et al.*, 2002a). It uses variables that describe fish foraging behaviours to calculate the probability that a fish will be exposed to a chemical concentration in water or sediment. The spatial submodel uses temporally variable sediment and water chemical concentrations, size of the site and hotspots (using GIS-based inputs), attraction factors, migration habits of the fish, fish foraging area sizes and habitat sizes to calculate the probability that a fish will be exposed to chemicals in the site.

The management area or site is divided into background areas and up to 10 hotspots. The model requires that all hotspots be located within the management area, and that they do not overlap. Each area is defined by minimum and maximum x and y coordinates, and the user provides the water and sediment chemical concentrations, organic carbon content of sediments, and water temperature for each area. These inputs can be point estimates or, preferably, distributions. Different areas may have the same sediment and water concentration, organic carbon content, and temperature, or one or all of these values may differ among areas. When a fish is not located within the site, the water and sediment exposures as well as exposure from diet are assumed to be zero.

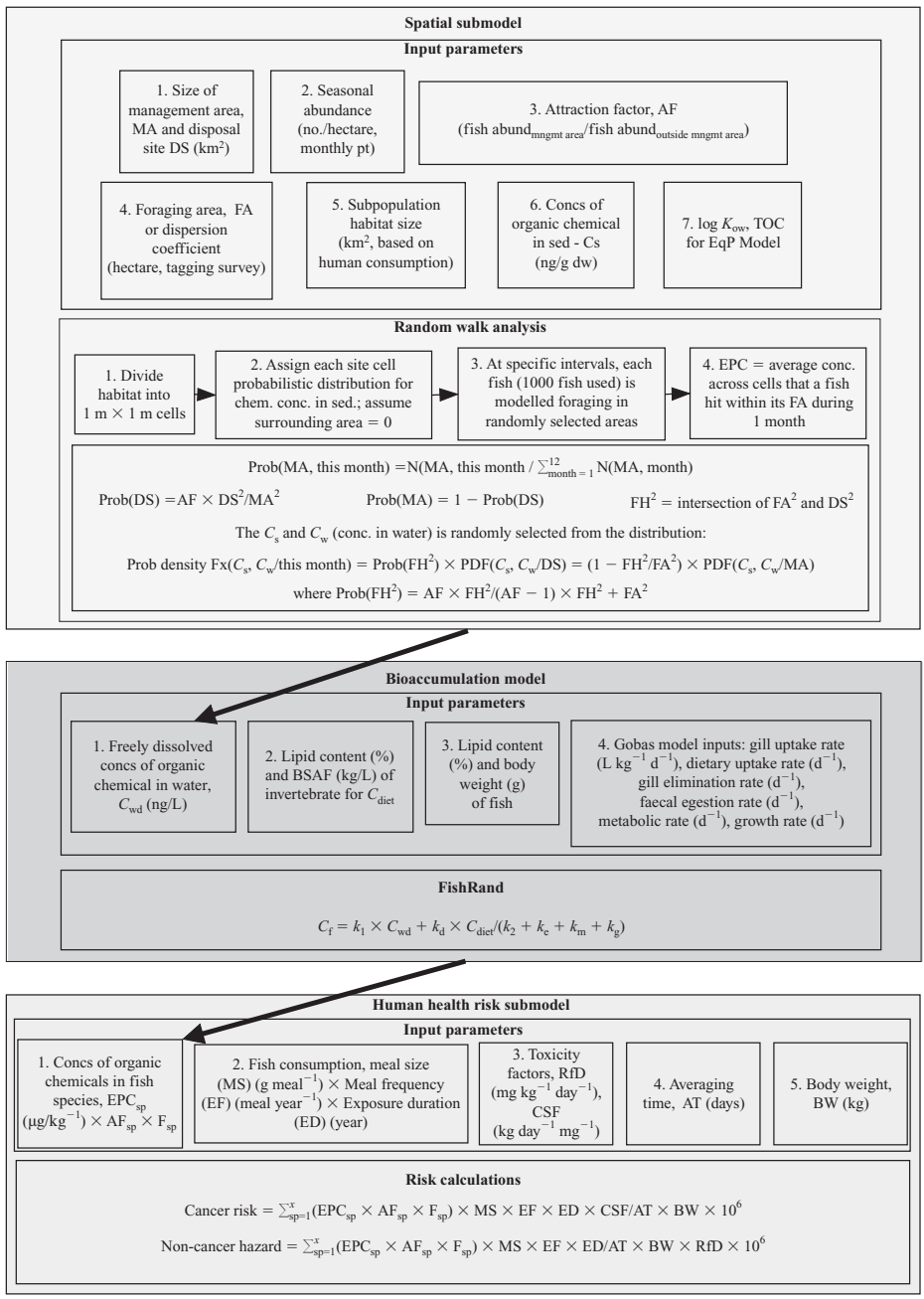
Essentially, FISHRAND starts with a large number of fish (e.g., the number of simulations in the variability loop of the model) and scatters them randomly over the modelling grid. The modelling grid is defined by a GIS-based map of the management area with spatially defined exposure concentrations in sediment and water. These can be defined in as much spatial and temporal detail as is available, including hotspots, background concentrations, and changes in concentrations over different time periods. These fish then move and forage according to their user-specified feeding preferences and foraging areas over the time interval specified in the model (typically one week, although it could be as little as one day or as much as a season). As the fish engage in these individual behaviours, they are exposed to sediment, water and benthic invertebrate concentrations relative to the underlying modelling grid. Figure 1.6 presents a schematic of the modelling equations and the mathematical connections that link model components. In addition to capturing the impact of migratory behaviours on exposure, the spatial submodel also incorporates the impact of heterogeneous chemical distribution across the site.

Figure 1.5: Nested Monte Carlo approach schematic for bioaccumulation modelling.



Model output is presented in various different ways, including tabular and graphical. The basic forms of the model results are individual percentiles of variability (concentrations across the population) and associated uncertainty for each population percentile for each time period and species. The user can select individual percentiles for plotting, or can average the data in different ways (e.g., seasonal or annual average

Figure 1.6: Schematic of FISHRAND modelling equations and the mathematical connections that link model components.



with associated uncertainty). Figure 1.7 presents an example of predicted PCB concentrations for the mean and 95% UCL. These concentrations can then be used to develop exposure point concentrations for human health risk assessment, or be incorporated directly as continuous functions for joint probability estimates of ecological hazard (US EPA, 2000a).

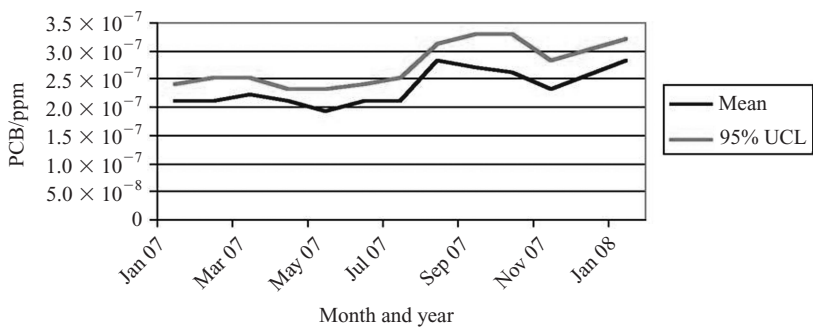
1.6 USE OF EXPERT ELICITATION IN MODELLING ASSESSMENTS

Expert elicitation is an approach for using expert judgements that can supplement other modelling systems. This approach, which uses structured interviews to quantify expert beliefs (typically probabilistic), provides processes that may be useful to address two of the major challenges in environmental modelling: estimating uncertain quantities or events, and characterising uncertainty of quantities or events for quantitative assessments.

Since its origin with the decision-analytic community in the 1950s, expert elicitation has been used for many different types of application, and has seen a recent increase in usage. The foundation of expert elicitation is the idea that individuals' beliefs about the likelihood of something can be expressed meaningfully in terms of probabilities, and can be used by modellers and analysts as part of quantitative analyses. Consequently, in a situation where data to support a model are unavailable (because of cost or time constraints), or where it is impossible to corroborate the output of a model because it is forecasting unique future events, expert elicitation provides a means to obtain quantities that would otherwise be unavailable, or would be impossible to estimate by other methods. In the field of environmental modelling such needs are frequent. Hence recent years have seen an increased interest in the use of expert elicitation as part of environmental modelling systems.

The potential benefits of using expert elicitation have been reflected in recent statements by the National Academy of Sciences (NAS). In its 2002 report *Estimating*

Figure 1.7: Predicted PCB concentrations in the Hudson River using FISHRAND for the mean and 95% uncertainty confidence limit (UCL).



the Public Health Benefits of Proposed Air Pollution Regulation the NAS recommended that US EPA:

> *should begin to move the assessment of uncertainties from its ancillary analyses into its primary analyses by conducting probabilistic, multiple-source uncertainty analyses. This shift will require specifications of probability distributions for major sources of uncertainty. These distributions should be based on available data and expert judgement.*

In addition, the US Office of Management and Budget (OMB) has recognised the utility of expert elicitation methods,and encourages its use in probabilistic uncertainty analyses that support regulatory decisions. In its Circular A-4 (2003), OMB stated:

> *In formal probabilistic assessments, expert solicitation is a useful way to fill key gaps in your ability to assess uncertainty. In general, experts can be used to quantify the probability distributions of key parameters and relationships. These solicitations, combined with other sources of data, can be combined in Monte Carlo simulations to derive a probability distribution of benefits and costs.*

At US EPA, experience with expert elicitation to support the development of air quality standards goes back to the late 1970s (Feagans and Biller, 1981). The Agency anticipates that expert elicitation will continue to be an important approach for characterising uncertainty and filling data gaps. Because it recognises the challenges of applying expert elicitation findings to regulatory and other policy decisions, US EPA has established an Expert Elicitation Task Force. The purpose of this Task Force has been to "initiate a dialogue within the Agency about the conduct and use of expert elicitation and then to facilitate future development and appropriate use of expert elicitation methods". In advancing this objective, the US EPA's Expert Elicitation Task Force has written a *Draft Expert Elicitation Task Force White Paper* that discusses and presents issues that are pertinent to expert elicitation, including a definition of expert elicitation, when to consider it, how it should be conducted, and how the results should be presented and used (US EPA, 2009b).

1.6.1 Example application for environmental fate and transport

Trichloroethene (trichloroethylene, TCE) is a common solvent, a carcinogen, and a frequent groundwater pollutant. The fate and transport of TCE in groundwater is highly dependent on the occurrence of natural biodegradation. When it is active, naturally occurring biodegradation can stop or limit the spread of TCE in groundwater. In the 1990s, phenomena governing this biodegradation were not adequately understood, including the identification of the active bacteria, the optimal environmental conditions for its occurrence, and the presence of degradation by-products.

During this time there were several approaches by the US EPA and other researchers to simulate this biodegradation process, as it was understood. They attempted to estimate when adequate natural biodegradation was occurring, and when it might be enhanced by the addition of nutrients to support bacterial growth (US EPA,

1998). To advance these existing approaches Stiber *et al.* (1999) built a model for this biodegradation process, and used expert elicitation to provide probabilistic relationships for many of its uncertain steps. This research obtained the beliefs of 22 experts through an elicitation protocol that asked the experts to estimate 94 separate probabilities. It showed that these probabilities could be used in a phenomenological model to make predictions about the occurrence of natural biodegradation at real locations of TCE-contaminated groundwater. More generally, the authors (Stiber *et al.*, 1999) concluded that

> *the use of expert knowledge is desirable because: (1) by acquiring expert knowledge, non-experts can make better quality decisions, (2) by breaking up the decision process into discrete components, experts can systematically specify and integrate their knowledge, and (3) by combining the discrete elements of a decision and analysing the outcome, it is possible to identify which components are most critical to the final evaluation, identify significant differences among experts, and determine the value of additional information.*

1.6.2 Example application at US EPA to quantify uncertainty

As part of the development of its NAAQS for fine particles ($PM_{2.5}$) in 2006, the US EPA conducted a regulatory impact analysis (RIA) to inform the public and the states about the potential costs and benefits of implementing these proposed air quality standards. This RIA used expert elicitation of non-EPA experts to better characterise the uncertainty associated with reductions in exposure to $PM_{2.5}$ pollution. In its final report for US EPA, Industrial Economics, Inc. (Industrial Economics, 2006) describes why expert elicitation was used to quantify the health benefits of reductions in $PM_{2.5}$ concentrations:

> *The effect of changes in ambient fine particulate matter ($PM_{2.5}$) levels on mortality constitutes a key component of the EPA's approach for assessing potential health benefits associated with air quality regulations targeting emissions of $PM_{2.5}$ and its precursors … Because it [avoided premature deaths] is such a large component of benefits, obtaining a good characterisation of uncertainties regarding the mortality effects of changes in $PM_{2.5}$ exposure could capture the largest portion of uncertainty characterisation of an entire benefit analysis (aside from unquantified or unmeasurable benefit endpoints).*

Industrial Economics, Inc. used "carefully structured interviews to elicit from each expert his best estimate of the true value for an outcome or variable of interest as well as his uncertainty about the true value". For each of the 12 experts who participated in this study, Industrial Economics, Inc. developed "a subjective probabilistic distribution of values, reflecting each expert's interpretation of theory and empirical evidence from relevant disciplines and ultimately his beliefs about what is known and not known about the subject of the study". These findings were included in US EPA's RIA to better characterise the uncertainty in the estimated health benefits.

1.7 SUMMARY: REGULATORY APPLICATIONS OF FATE AND BIOACCUMULATION MODELS

US EPA's Quality Assurance Plan for modelling applications recommends a tiered approach to model evaluation activities, depending on the importance of modelling results for informing a particular decision and the cost/significance of the environmental decision to be made (US EPA, 2002). For models that are used to inform significant decisions (as defined by the Office of Management and Budget) a variety of practices help ensure the rigour of such applications if subjected to legal challenges. For example, McGarity and Wagner (2003) noted that:

> *an EPA modeling exercise . . . should not suffer reversal . . . if the Agency is careful to describe the model in some detail; identify the assumptions upon which the model relies; explain why those assumptions are valid in the particular context in which it is applying the model and specifically request comments on the validity of the assumptions and their use in the modeling exercise.*

To assist in communication among stakeholders, US EPA guidance (US EPA, 2009a) recommends that model evaluation in the most general sense should answer several straightforward questions (Beck, 2002):

- Is the model based on generally accepted science and computational methods?
- Does it work, that is, does it fulfil its designated task or serve its intended purpose?
- Does its behaviour approximate that observed in the system being modelled?

Developing confidence in environmental modelling applications for policy applications requires effective communication of their underlying science and inherent uncertainties. US EPA uses a wide variety of fate and bioaccumulation models to inform regulatory actions. In order for these models to withstand the judicial review process, both the models themselves and site-specific applications must be transparent, well documented, and peer-reviewed. US EPA has released a "best practices" document for the development, evaluation and application of environmental models (US EPA, 2009a). One of the major recommendations of this guidance document is a philosophical move away from "validating and verifying" models toward a framework for life-cycle model evaluation (i.e., continued updating and testing of a model throughout all applications). Environmental models can never be "verified," meaning be established as true, because they are an imperfect representation of the real world by definition, and thus are untrue (Oreskes *et al.*, 1994). Life cycle model evaluation approaches recognise the pervasive nature of such uncertainties. Thus a key component of the use of fate and bioaccumulation models in regulatory applications is appropriately conveying their uncertainties in a context that is relevant and understandable by decision-makers. Table 1.2 summarises some of the differences in perspectives of environmental managers and modellers (scientific staff) when dealing with environmental information. Recognising these differences is essential for effec-

Table 1.2: Example of differences in perspective between scientists and managers when considering the use of climate information.

Factor	Scientist's perspective	Water manager's perspective
Identifying a critical issue	Based on a broad understanding of the nature of water management	Based on experience of particular system
Time frame	Variable	Immediate (operations) Long-term (infrastructure)
Spatial resolution Goals	Defined by data availability, funding, modelling capabilities Prediction Explanation Understanding of natural system	Defined by institutional boundaries, authorities Optimisation of multiple conditions and minimisation of risk
Basis for decisions	Generalising multiple facts and observations Use of scientific procedures, methods Availability of research funding Disciplinary perspective	Tradition Procedure Professional judgement Training Economics Politics Job risks Formal and informal networks
Expectation	Understanding Prediction Ongoing improvement (project never actually complete) Statistical significance of results Innovations in methods/theory	Accuracy of information Appropriate methodology Precision Save money, time Protect the public Protect their job, agenda or institution
Product characteristics	Complex Scientifically defensible	As simple as possible without losing accuracy
Frame	Physical (atmospheric, hydrologic, economic, etc.) and societal conditions as drivers Dependent on scientific discipline	Safety, well-being Profit Consistency with institutional culture, policy, etc.
Nature of use	Conceptual	Applied

Source: From Jacobs, K. and Pulwarty, R. (2003). Water resource management: science, planning, and decision-making. *In* Lawford, R.G., Fort, D.D., Hartmann, H.C. and Eden, S. (Eds), *Water: Science, Policy, and Management*. American Geophysical Union, Washington, DC, pp. 177–204.

tive communication and therefore the success of modelling applications for informing management decisions and enhancing environmental protection.

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Is this an acceptable place for the notes or would you prefer them to be before the references?

NOTES

1. Criteria air pollutants include: ozone (O_3), fine ($PM_{2.5}$) and coarse (PM_{10}) particulate matter, lead (Pb), sulfur dioxide (SO_2), carbon monoxide (CO), and nitrous oxides (NO_x).
2. For more information see: http: //www.epa.gov/scram001/guidance_permit.htm.
3. All models, a history of their past applications and extensive documentation are available online from US EPA at http: //www.epa.gov/scram001/dispersion_prefrec.htm.
4. http: //www.blueskyrains.org
5. Most of these models are publicly available, and can be downloaded from http: //www.epa.gov/ceampubl/.
6. http: //www.epa.gov/athens/wwqtsc/
7. See: http: //www.epa.gov.athens/wwqtsc.
8. http: //www.epa.gov/region4/mercury/TMDLs.htm
9. Available at: http: //www.rem.sfu.ca/toxicology/models/models.htm
10. http: //www.epa.gov/ceampubl/

1: Because some of you work for the US government, does this mean the chapter is a government work and in the public domain?