4.0 Evaluating Quality of the 3MRA Modeling System Modules

This section describes verification and validation activities for the 3MRA modeling system modules. Figure 4-1 provides an overview of the verification and validation process for the modules. Figure 4-2 shows which subsection describes each module. The five source modules and the watershed module are covered in two sections to avoid duplication, one for Wastewater Source Modules (surface impoundments and aerated tanks) and one for the Land-based Source Modules (landfill, waste pile, and LAU) and the Watershed Module.

4.1 Wastewater Source Modules

This section documents the verification and validation activities for the Aerated Tank and Surface Impoundment Modules. The draft Wastewater Source Module documentation was peer reviewed by the external reviewers shown in the box.

Peer Reviewers for Wastewater Source Modules

- Dr. Patricia Culligan of Massachusetts Institute of Technology
- Dr. Wade Hawthorn of Washington State University
- Dr. Michael Overcash of North Carolina State University

4.1.1 Module Description

The Wastewater Source Modules simulate wastewater management. Two Wastewater Source Modules were developed for the 3MRA modeling system to represent the common management practices for industrial wastewaters for the purposes of flow equalization, storage, treatment (typically biological treatment or neutralization), and solids settling (clarification). These waste management units (WMUs) are

- **Surface Impoundments**, which may be either aerated or quiescent and are used to treat, store, or dispose of many industrial wastewaters; and

- **Aerated Tanks**, which are aerated or mixed tanks used to treat or store many industrial wastewaters.

The two Wastewater Source Modules use a common set of algorithms with similar mass balance and transport equations. Both modules estimate volatile emissions to air. Leaching losses from the bottom of the unit are modeled only for surface impoundments; tanks are assumed to have impervious bottoms. Both modules simulate degradation and solids settling, although solids settling and accumulation are more significant for quiescent units.

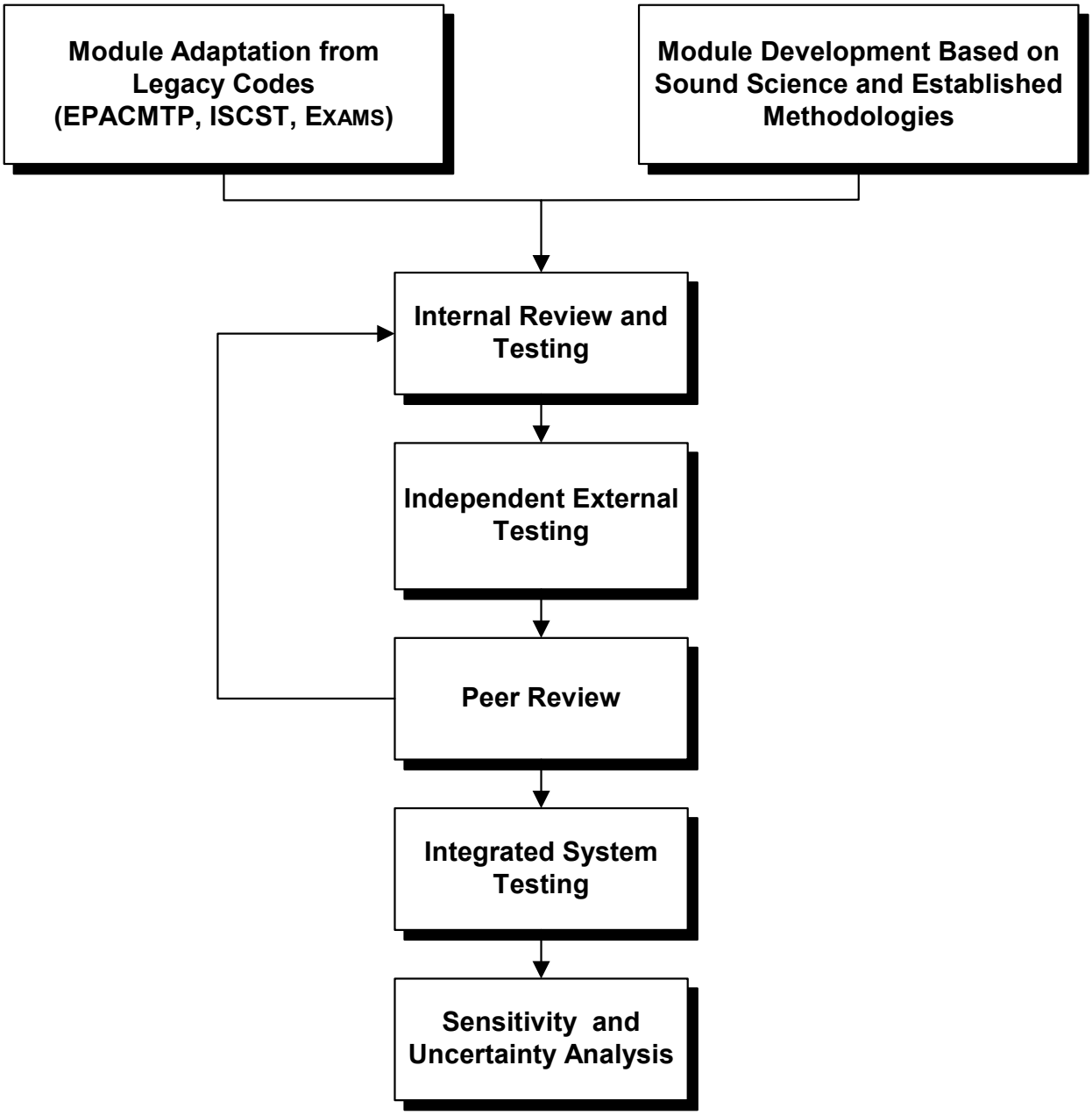

Figure 4-1. Overall approach to ensure the quality of the 3MRA science modules.

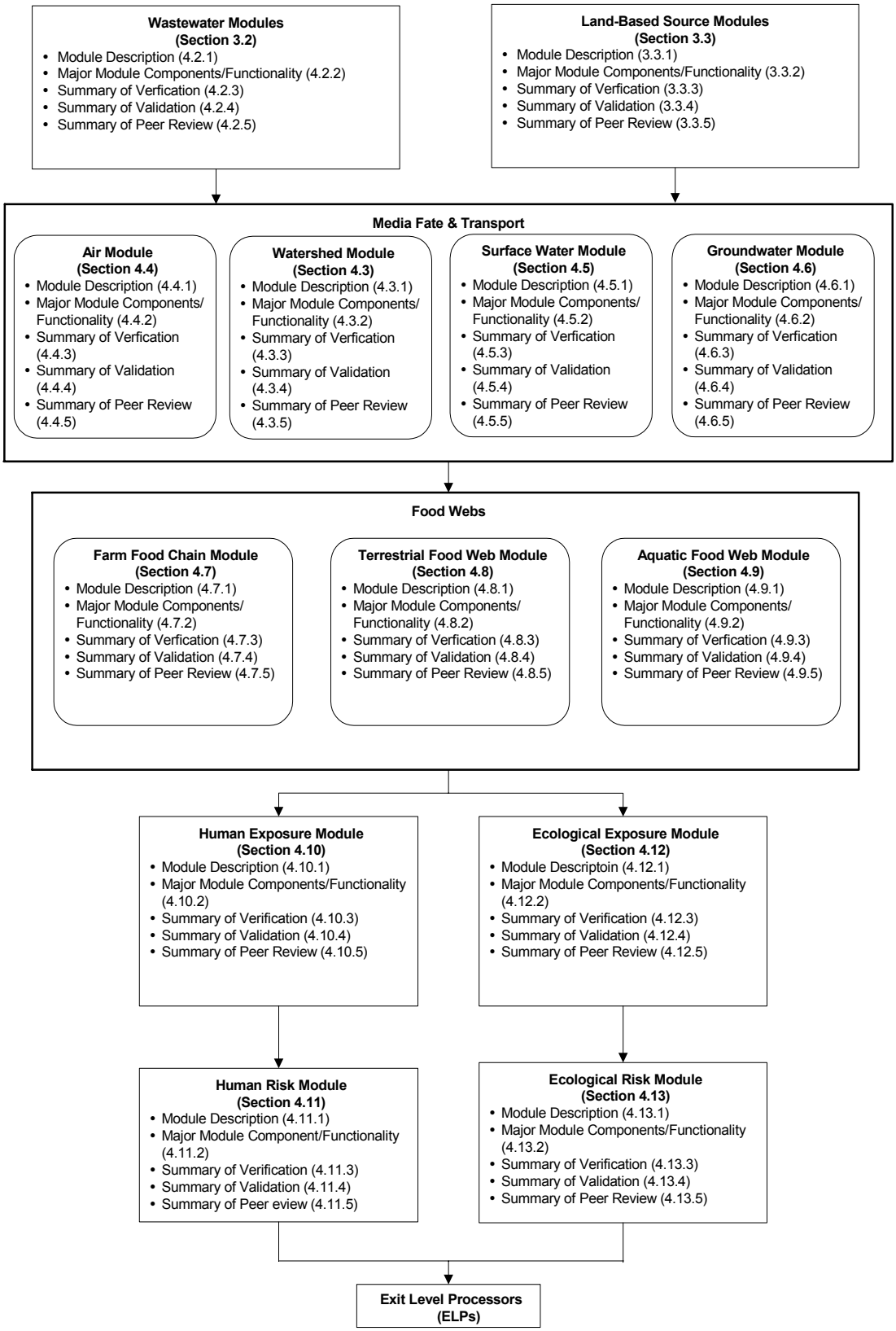

Figure 4-2. Organization of the 3MRA modeling system modules and this section.

The two Wastewater Source Modules were designed to provide estimates of annual average volatilization rates to air, which are used by the Air Module. In addition, the Surface Impoundment Module outputs annual average infiltration rates and leachate contaminant flux rates, which are used by the Vadose Zone and Aquifer Modules, and annual average surface impoundment water concentrations, which are used by the Ecological Exposure Module to estimate exposure to wild animals that may drink or consume organisms from the impoundment. Figure 4-3 shows the information flow for the Wastewater Source Modules to the other modules.

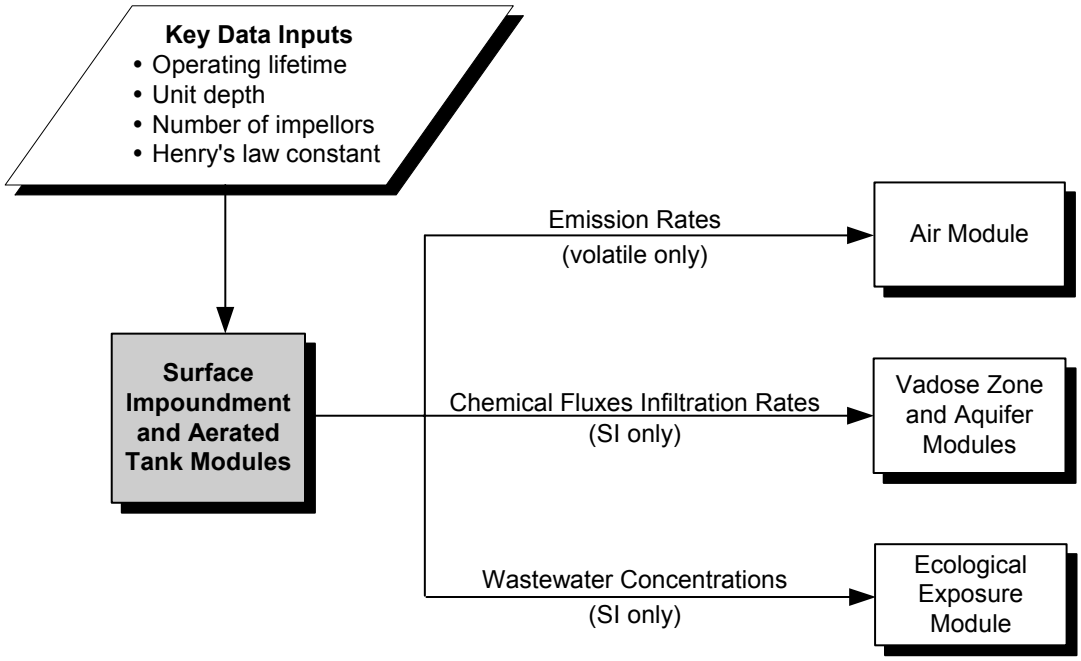

Figure 4-3. Information flow for the Wastewater Source Modules in the 3MRA modeling system.

4.1.2 Major Module Components/Functionality

The Wastewater Source Modules have six major functions, as follows:

1. **Calculate contaminant concentrations within the unit.** The Wastewater Source Modules use a mass-balance, temperature-adjusted approach to estimate contaminant concentrations in the WMU. This approach considers contaminant diffusion between wastewater and sediments, and contaminant removal by volatilization, biodegradation, hydrolysis, partitioning to solids, solids settling, and, for surface impoundments only, infiltration through the bottom of the unit.

2. **Calculate solids concentrations within the unit.** The Wastewater Source Modules use a mass-balance approach to estimate solids concentrations in the WMU.

3. **Calculate volatile emission rates.** The modules calculate volatile emission rates for both aerated and quiescent surfaces.

4. **Estimate resuspension, sedimentation, and burial velocities within the unit.** The modules account for these processes within the tank or surface impoundment.

5. **Estimate contaminant release in leachate.** The Surface Impoundment Module calculates infiltration rates and contaminant leachate flux rates for use in the Vadose Zone and Aquifer Modules. The Aerated Tank Module does not calculate leachate release, as tanks are assumed to have impervious bottoms.

6. **Adjust for temperature effects.** The modules account for the effect of temperature on air viscosity and density, water viscosity, chemical properties, and sediment biodegradation rates.

4.1.3 Summary of Verification

The Wastewater Source Modules were verified through a series of verification tests, which are described in detail in the following documents:

- *3MRA Surface Impoundment Module Test Plan* (RTI, 2002d)
- *3MRA Surface Impoundment Module Test Documentation* (RTI, 2002c).
- *3MRA Aerated Tank Module Test Plan* (RTI, 2002b)
- *3MRA Aerated Tank Module Test Documentation* (RTI, 2002a)

The volatile emissions component of the Wastewater Source Modules is based on CHEMDAT8, which has been verified in previous work. Independent engineering review was conducted on early versions of the CHEMDAT model to ensure that the equations were properly coded. Sample calculations are provided in the CHEMDAT8 model documentation, and those sample calculations verify that the model yields the same results as the sample calculations (U.S. EPA, 1994a). Additionally, the CHEMDAT series of emission models has been publically available for more than 10 years and has been scrutinized by a variety of industries during rule-making efforts. CHEMDAT8 and Water8 represent the culmination of several revisions and modifications made to the emission model over a 5-year period.

EPA developed separate verification test plans for the Surface Impoundment and Aerated Tank Modules. Tables 4-1 and 4-2 summarize the functional requirements and number of test cases executed to verify these two modules. All test cases were completed for both source modules by an independent engineer. Under one of these test cases, the individual and overall volatilization mass transfer coefficients were compared with those calculated using CHEMDAT8. This comparison verified that the mass transfer correlations had been correctly coded in the Wastewater Source Modules. The results of these internal verification efforts are documented in reports for each source module (RTI, 2002a,c).

Table 4-1. General Requirements for Testing the Aerated Tank Module

Step	Description	Number of Test Cases
1	Correct operation of the volatilization mass transfer rate algorithm	13
2	Correct operation of the sediment mass balance	6
3	Correct operation of the annual averaging algorithm	1
4	Correct operation of system requirements	6

Table 4-2. General Requirements for Testing the Surface Impoundment Module

Step	Description	Number of Test Cases
1	Correct operation of the volatilization mass transfer rate algorithm	15
2	Correct operation of the sediment removal algorithm	8
3	Correct operation of the infiltration rate algorithm	6
4	Correct operation of the SI type assignment algorithm	4
5	Correct operation of the annual averaging algorithm	6
6	Correct operation of system requirements	7

4.1.4 Summary of Validation

The volatilization and infiltration rate components of the Wastewater Source Modules are based on well-documented and tested models (CHEMDAT8 and EPACMTP, respectively). The validation of these components is important because the components directly influence the primary outputs that are used in subsequent modules (i.e., the volatile emissions for both the Surface Impoundment and Aerated Tank Modules, and the infiltration and contaminant leaching rate for the Surface Impoundment Module). Therefore, the verification and validation efforts conducted on these module components help support the validity of the overall modules.

The volatilization mass transfer rate equations used in the Wastewater Source Modules are based on generally accepted mass transfer correlations. These correlations have been developed and selected over the past 20 years. Several EPA emission models use these same volatilization mass transfer rate equations (e.g., CHEMDAT8, Water8, Water9 [U.S. EPA, 1994a]), and these equations have been used to support impact estimates for numerous EPA regulations. They have been peer reviewed and publically available for more than 10 years. GCA Corporation performed the initial evaluation and selection of mass transfer rate equations for use in EPA emission models (GCA, 1982). Over time, a few additional mass transfer correlations have been developed (e.g., Springer et al., 1984). Each individual mass transfer correlation was developed from individual studies and data evaluations reported in the literature. The discussion of the validation efforts provided below focuses on the CHEMDAT8 model

because most of the validation efforts performed on the Wastewater Source Modules' volatilization rate equations and emission flux estimates are based on benchmarking with the CHEMDAT8 model. However, the validation of these mass transfer rate equations are not limited to activities performed on CHEMDAT8.

Initial validation of the volatilization mass transfer rate equations and the resulting emission estimates compared measured and predicted fraction emitted from a pilot-scale and several full-scale wastewater treatment units, including both aerated and quiescent units (RTI, 1985; this report also includes sample calculations for the mass transfer correlations and the fraction emitted).

The CHEMDAT8 model was used to develop baseline emissions and emission impact estimates used to support air emission standards developed under RCRA (40 CFR Part 264, Subpart CC). The background information document for the air emissions standard includes summary documentation of the emission model and presents data used to validate the model (U.S. EPA, 1991). The comparisons to measured emissions data for five surface impoundments and both aerated and quiescent tanks indicated that the emission model was relatively unbiased (generating emission estimates higher than some measurements and lower than others). The estimated emission rates agreed with all measured emissions within an order magnitude.

The CHEMDAT8 model equations have been used to develop baseline emissions and emission impact estimates to support several other air emission standards, including the Benzene Waste Operations National Emissions Standard for Hazardous Air Pollutants (NESHAP) (40 CFR Part 61 Subpart FF) and the Hazardous Organic NESHAP (HON) (40 CFR Part 63, Subparts F, G, H, and I). These equations have been publically available, and the emission estimates that result from the application of these equations have been scrutinized. Comments received on the CHEMDAT8 model and the emission estimates are a part of the public record in the dockets of these rule makings. Although no model will perfectly predict the fate of all contaminants from all types of units because of the variability in operating conditions and microbial populations, these equations have consistently provided reasonable estimates of air emissions over a wide range of aerated tank and surface impoundment operating characteristics.

In addition to previous validation of CHEMDAT8, the Wastewater Source Modules were validated by comparing outputs to those calculated by CHEMDAT8. During internal testing of the Wastewater Source Modules, the emissions fluxes calculated by the Surface Impoundment Module were compared with those calculated using CHEMDAT8. Although these models contain the same volatilization mass transfer rate equations, they employ different solids balance algorithms, adsorption correlations, and biodegradation rate models. In addition, CHEMDAT8 does not consider infiltration/leachate flux from the surface impoundment. The Surface Impoundment (and Aerated Tank) Module output agrees well with the CHEMDAT8 module output. This validation effort is documented in RTI (1998).

The infiltration rate equations used in the Surface Impoundment Module are based on EPACMTP (U.S. EPA, 1996b). This model has been peer reviewed (including a Scientific Advisory Board [SAB] review) and publically available for more than 5 years. See Section 4.5.4 for a more detailed discussion of the validation of EPACMTP.

4.2 Land-based Source Modules and Watershed Module

This section documents the verification and validation activities for the Landfill, Waste Pile, Land Application Unit (LAU), and Watershed Modules. The Landfill, Waste Pile, LAU, and Watershed Modules are discussed collectively because of the overall similarity of their functionality and their software components. Indeed, with respect to fundamental theory and underlying calculations, there are relatively few differences among these four modules. The primary differences are in specific parameter values (e.g., anaerobic biodegradation in the landfill and waste pile versus aerobic biodegradation in the LAU), specific particulate emissions processes modeled (e.g., vehicular activity emissions are not relevant to the waste pile), or hydrology-related items (e.g., the landfill is not subject to erosion/runoff), rather than in underlying mathematical models or software.

The Landfill, Waste Pile, LAU, and Watershed Modules and associated data were peer reviewed by the external reviewers shown in the box. The peer-review comments are provided in ERG (1999).

Peer Reviewers for Land-based Source Modules and Watershed Module

- Dr. Anita Bahe of LYNX Group, Ltd.
- Dr. Kirk Brown of Texas A&M University
- Dr. William Inskeep of Montana State University
- Dr. Clyde Munster of Texas A&M University
- Mr. William Norris of VA Department of Environmental Quality
- Mr. Robert Wyatt of R.J. Wyatt and Associates

4.2.1 Module Description

The Land-based Source Modules simulate partitioning and emission of contaminants from land-based waste management units (WMUs). Three Land-based Source Modules were developed for the 3MRA modeling system to represent the major management practices where wastes are put into or on the land for recycling, recovery, reuse, treatment, or disposal. These modules simulate waste management practices in the following types of WMUs:

- **Landfills,** which are a common disposal unit for many nonliquid industrial wastes;
- **Waste piles,** which are temporary storage areas on the ground for nonliquid industrial waste, such as ash or slag; and
- **Land application units (LAUs),** which are used to reuse, treat, or dispose of industrial waste in liquid, semiliquid, or solid form. Some wastes are used as a soil amendment, which is a reuse practice; some wastes are applied to land for treatment through biological degradation; and some wastes are applied to land as a disposal method.

Each of the three Land-based Source Modules provides some similar and some different features in terms of the ways contaminants of concern can be released to the environment. All three modules have the potential to release contaminants to the air by volatilization or particle entrainment, and to the vadose zone and ground water by leaching. Waste piles, because they are elevated and have more surface area exposed, are assumed to have a greater potential for air emissions than the other two source types. Waste piles and LAUs have the additional release

mechanism of erosion and runoff to the surrounding watershed and the nearest stream or other waterbody. Landfills are assumed to be below grade and thus do not release contaminants through erosion or runoff.

The three Land-based Source Modules were designed to provide estimates of annual average contaminant concentrations in surface soil and contaminant mass emission rates to air, surface water, and ground water, and to maintain mass balance between the source and all release routes. The emission rate estimates are then used in the 3MRA modeling system, which links source modules with environmental fate and transport modules. Figure 4-4 shows the information flow for the Land-based Source Modules.

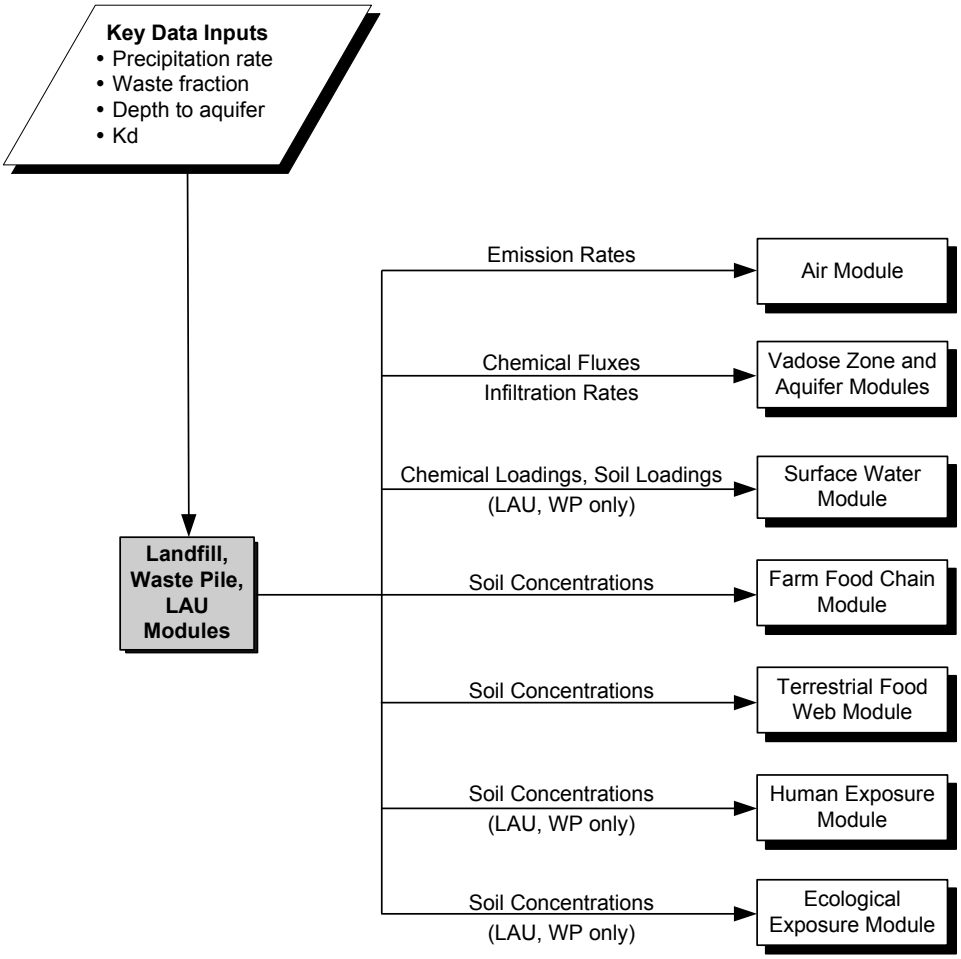

Figure 4-4. Information flow for the Land-based Source Modules in the 3MRA modeling system.

The Watershed Module estimates contaminant concentrations in soil resulting from aerial deposition of contaminants throughout the area of interest (AOI) around each modeled site and the resulting contaminant loadings to surface waterbodies from runoff and erosion. It also estimates some hydrological inputs for the Surface Water Module (flows, eroded soil loads) and the Vadose Zone and Aquifer Modules (infiltration rates). Figure 4-5 shows how the Watershed Module fits into the 3MRA system.

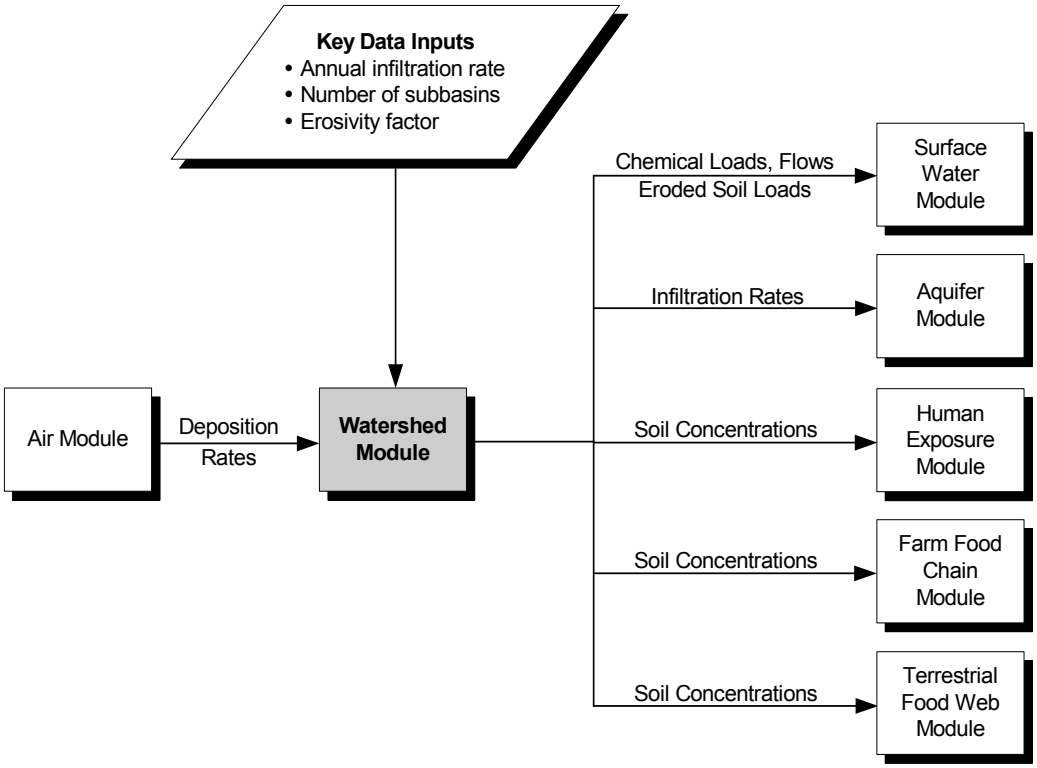

Figure 4-5. Information flow for the Watershed Module in the 3MRA modeling system.

4.2.2 Major Module Components/Functionality

The Land-based Source Modules contain the following four models:

1. **The Generic Soil Column Model (GSCM)** was developed to describe the contaminant fate and transport in a porous medium, such as soil or waste. It provides the vertical concentration profile in the soil/waste column at various times.

2. **The Local Watershed Model** (for waste piles and LAUs) is based on mass balances of solids and contaminants in the runoff and the top layer of the soil column modeled by the GSCM. The "local watershed" comprises the land area between the waterbody and the top of the hillside containing the WMU and may include an upslope area, the WMU, and a downslope or buffer area between the WMU and the waterbody.

3. **The Particulate Emissions Model** was designed to provide estimates of the annual average emission rate of contaminant mass adsorbed to particulate matter less than 30 μm in diameter. The release mechanisms considered differ for each WMU, but may include wind erosion, vehicular activity, unloading operations, tilling, and spreading/compacting operations.

4. **The Hydrology Model** is a water balance algorithm that performs a daily water balance for the surface soil layer. Moisture inputs are daily precipitation and beginning soil moisture; outputs are daily runoff, evapotranspiration, percolation to deeper layers, and changes in soil moisture. Runoff estimates are based on the U.S. Department of Agriculture's (USDA's) Soil Conservation Service Curve Number method (USDA, 1986). Evapotranspiration is based on the Hargreaves equation (Hargreaves, 1975)—to estimate potential evapotranspiration—and a function of the soil's current moisture, wilting point, and field capacity to estimate actual evapotranspiration. Remaining soil moisture in excess of the field capacity is released as percolation.

The Watershed Module includes one additional component:

5. **The Regional Baseflow Model** estimates waterbody baseflow (dry weather flow, i.e., flow not derived from direct surface runoff) based on regional regression models. Baseflow was assumed to be represented by the 30Q2 flow—the minimum 30-day average flow with a return period of 2 years—which was estimated for each of 18 Hydrologic Unit Code (HUC) areas in the conterminous United States from STOrage and RETrevial Database (STORET) flow data. The regional baseflow regression models were then developed by regressing the estimated 30Q2 flow onto the drainage area (watershed area) tributary to the flow gages for all flow gages within the HUC. The Watershed Module then estimates baseflow on a watershed-specific basis by selecting the regression model for the HUC region corresponding to the site being simulated and estimating baseflow as a function of watershed surface area for each watershed at the site.

4.2.3 Summary of Verification

Internal verification activities and tests were performed for each of the four modules and are documented in the following verification testing reports:

- *Landfill Module Verification Testing* (RTI, 2000d)
- *Wastepile Module Verification Testing* (RTI, 2000f)
- *Land Application Unit Module Verification Testing* (RTI, 2000b)
- *Land Application Unit Module Verification Testing: ERRATA* (RTI, 2000c)
- *Watershed Module Internal Verification Testing* (RTI, 2000g).

Following internal verification, independent external peer review and verification were also performed on each module. The external verification is documented in the following reports:

- *Independent Tests for Landfill Module* (Tetra Tech, 2000d)
- *Independent Tests for Waste Pile Module* (Tetra Tech, 2000f)
- *Implementation of the Test Plan for the HWIR99 Land Application Unit Module* (HGL, 2000)
- *Independent Tests for the Watershed Module* (PNNL, 2000).

Finally, responses by the module developers to questions or issues raised by the independent testers are documented in the following memoranda. All verification tests were considered to be completed successfully.

- *Response to Independent Reviewer Comments on Landfill Module Verification Testing* (Little and Baskir, 2000b)
- *Response to Independent Reviewer Comments on Waste Pile Module Verification Testing* (Little and Baskir, 2000c)
- *Response to Independent Reviewer Comments on LAU Module Verification Testing* (Little and Baskir, 2000a)
- *Response to Independent Reviewer Comments on Regional Watershed Module Verification Testing* (Little and Baskir, 2000d).

The design of the verification tests followed an initial assessment of each module's software "requirements," or desired functionality. Requirements included correctly performing individual calculations in specific code sections, such as simulating contaminant fate and transport in a soil column (the GSCM); overall module mass balance conservation; and system-level requirements such as correctly writing warning and error messages and proper communication with other modules. For each identified requirement, one or more test cases were then proposed that specifically verify that requirement. Some test cases served to verify more than one requirement.

Testing to verify internal calculations (as opposed to, for example, testing to verify that the program is correctly reading or writing inputs and outputs) was the most demanding aspect of the verification activities because of the quantitative standard set by the 3MRA modeling system team. In addition to "verifying" an internal calculation (or set of calculations) by qualitative, sensitivity-type tests, testing ensured that each calculation was "hand-reproducible," either by a hand calculation or replication of the calculation in another program, such as a spreadsheet or independent program. For purposes of verifying the Land-based Source Modules and Watershed Module, the definition of "calculation" was interpreted as including any line of code that involved two or more variables and also performed any type of mathematical operation. Most of the "hand" calculations were performed using a spreadsheet. One part of the modules, the GSCM, was too complex to allow either a true hand verification or replication in a spreadsheet. Therefore, a separate computer program was written in BASIC to independently solve the GSCM governing equations. The BASIC programmer took the underlying GSCM equations and independently developed a program to solve those equations, without considering how they had been implemented in the 3MRA modeling system. Once that independent program was completed, the outputs from the two codes were compared to verify the GSCM.

As previously explained, much of the functionality of the Land-based Source Modules and the Watershed Module is common to all four modules, with code that is also common and called by each module. It was only necessary to verify the common functionality and code for one of these modules. EPA used the LAU Module to verify the common functionality, as well as any functionality unique to the LAU Module. Once the LAU Module verification was completed, verification of the remaining three modules was limited to functionality specific to those modules. Tables 4-3 through 4-6 present a summary of the functional requirements and

number of test cases executed to verify these four modules. Detailed descriptions of the requirements and test cases are provided in the verification testing reports (RTI, 2000b,c,d,f,g).

Table 4-3. General Requirements for Testing the Land Application Unit Module

Step	Description	Number of Test Cases
1	Correctly read input data	1
2	Correct presimulation calculations	1
3	Correct operation of the GSCM	9
4	Correct year-end, post-processing calculations	1
5	Correct simulation-end, leachate flux postprocessing calculations	1
6	Correct operation of the subarea coupling processes	3
7	Correct operation of the water balance algorithm	4
8	Correct operation of the soil erosion algorithm	1
9	Correct operation of the particulate emissions algorithm	1
10	Correct writing of outputs	27
11	Correct operation of system requirements	7
12	Robustness	1

Table 4-4. General Requirements for Testing the Landfill Module

Step	Description	Number of Test Cases
1	Correctly read input data	1
2	Correct presimulation calculations	1
3	Correct operation of the GSCM	8
4	Correct intrayear changes in modeled spatial domain for cell 1	1
5	Correct cell 1, year-end, postprocessing calculations	1
6	Correct cell 1, simulation-end, leachate flux postprocessing calculations	1
7	Correct end-of-simulation, LF cell aggregation calculations	1
8	Correct operation of the water balance algorithm	4
9	Correct operation of the particulate emissions algorithm	2
10	Correct writing of outputs	17
11	Correct operation of system requirements	6
12	Robustness	1

Table 4-5. General Requirements for Testing the Waste Pile Module

Step	Description	Number of Test Cases
1	Correctly read input data	1
2	Correct presimulation calculations	1
3	Correct operation of the GSCM	10
4	Correct year-end, postprocessing calculations	1
5	Correct simulation-end, leachate flux postprocessing calculations	1
6	Correct operation of the subarea coupling processes	3
7	Correct operation of the water balance algorithm	4
8	Correct operation of the soil erosion algorithm	1
9	Correct operation of the particulate emissions algorithm	1
10	Correct writing of outputs	7
11	Correct operation of system requirements	7
12	Robustness	1

Table 4-6. General Requirements for Testing the Watershed Module

Step	Description	Number of Test Cases
1	Correctly read input data	1
2	Correct presimulation calculations	1
3	Correct operation of the GSCM	4
4	Correct year-end, postprocessing calculations	1
5	Correct operation of the water balance algorithm	3
6	Correct operation of the soil erosion algorithm	1
7	Correct writing of outputs	12
8	Correct operation of system requirements	5
9	Robustness	1

4.2.4 Summary of Validation

Validation activities for the Land-based Source Modules and Watershed Module include both implicit and explicit validation. Several of the modules' software components are based on empirical data. Because these components are based on observed data rather than theoretical models, they can be considered to be implicitly validated by definition if the code is verified as operating correctly. Empirical components include aspects of the hydrology model (runoff calculations based on the curve number methodology and the Hargreaves evapotranspiration equation), the soil erosion calculations (based on the Universal Soil Loss Equation [USLE]), and the particulate emissions calculations.

Explicit validation involves comparing predicted results to monitored data or the results of other models that are regarded as credible. Monitored data are preferred. EPA validated the hydrology model component by comparison with EPA's Hydrologic Evaluation of Landfill Performance (HELP) model and the LAU Module by comparison of simulated half-lives of dioxin in soil with monitored half-life data. In addition, EPA validated the LAU Module using data from a large soil-column study. These three validation activities are described below.

HELP Model Comparison. The HELP model benchmarking tests are fully described in Test Case 7.3 of the LAU Module verification testing report (RTI, 2000b). The benchmarking tests compared predicted runoff and infiltration for six sites throughout the country (San Diego, CA; Miami, FL; Madison, WI; Denver, CO; Dallas, TX; and Seattle, WA) using 5 years of data per site. The hydrology model in the Land-based Source and Watershed Modules is not completely functionally equivalent to the HELP model, so close agreement between the two was not necessarily expected. Rather, EPA expected long-term average results to be in reasonable agreement. The comparative results were mixed. At some sites, the two models' predictions were quite similar. At other sites, the predictions showed relatively large differences. With regard to differences in infiltration, no consistent bias in the 3MRA modeling system hydrology model predictions versus the HELP model predictions was apparent. With regard to differences in runoff, the 3MRA modeling system hydrology model predicted more runoff than the HELP model for all tested sites. To determine whether this apparent bias in runoff prediction was of concern, EPA compared runoff estimates from both models at the six sites to long-term average observed runoff as reported in the *Water Atlas* (Geraghty et al., 1973). The 3MRA modeling system hydrology model's predictions were in closer agreement with observed runoff than were the HELP model's predictions; however, this conclusion should be regarded as tentative because of the relatively limited number of sites compared and uncertainty about the relevance of the specific comparisons made. In summary, the benchmarking analysis suggested that the 3MRA modeling system hydrology model's results were adequate for the 3MRA modeling system's national screening-level purposes.

LAU Dioxin Half-life Comparisons. The LAU dioxin half-life comparisons were performed as part of an application of the LAU Module to simulate the persistence of dioxin compounds in sewage sludge applied to agricultural lands. That work, including the half-life validation comparisons, is fully described in *Exposure Analysis for Dioxins, Dibenzofurans, and Co-Planar Polychlorinated Biphenyls in Sewage Sludge* (RTI, 2001). The LAU Module was used in that project to provide LAU concentrations of dioxins in agricultural soils, and those concentrations were then used in a probabilistic (Monte Carlo) human health risk assessment. For the half-life comparison, the output LAU soil concentrations associated with specific percentiles (10th, 20th, 50th, 75th, 90th, 95th, and 99th) of the final risk distribution (based on 3,000 Monte Carlo simulations) were used to calculate the half-life for each percentile. Each risk distribution percentile represents a somewhat different physical environment, which gives rise to different half-lives. Half-lives were estimated from the module's outputs by finding the peak concentration in soil—corresponding to the end of the sludge application period—and then counting the years until the peak concentration had been reduced by one-half. The resulting range of simulated half-lives was compared to measured half-lives as reported in the technical literature. The range of half-lives over the selected percentiles was 20 to 48 years, which is in reasonable agreement with observed half-lives at several monitored sites. Thus, EPA concluded

that the monitored data corroborated the modeled results for highly persistent contaminants, at least in a broad sense.

Soil-Column Study Data. The LAU Module has been validated using data from a large soil-column study conducted to investigate the behavior of organic chemicals (including halogenated aliphatic hydrocarbons, substituted benzenes, and phenols) during infiltration of municipal wastewater into soil by the Ground Water and Ecosystem Restoration Division (GWERD) of EPA's National Risk Management Research Laboratory (NRMRL). The experiment design and conditions were very close to the assumptions and application conditions of the LAU Module, making these data suitable for use in evaluating the LAU Module.

The evaluation on LAU source module included:

- Whether volatilization of organic chemicals could be correctly accounted for;
- Whether the conceptualizations on different attributes of the module (such as boundary conditions and the assumption of first order decay for contaminant transformation) are adequate;
- Whether the quasi-analytical approach employed for solving the mathematical model to describe the flow, fate and transport is appropriate; and
- Whether the LAU thickness and temperature parameters have significant effects on the amount of volatilization of organics.

A stand-alone LAU program was obtained by modifying the LAU Module from the 3MRA modeling system to achieve the small intervals of time and space needed to compare the results to the experimental lab data. This modified LAU program was compared to the LAU Module and verified to be consistent with the original module. The necessary input parameters to the LAU program were obtained from the lab experiment design and literature review. The simulated and the observed volatilization rates were compared to validate the LAU Module. Sensitivity analyses were implemented to examine the effect of thickness and temperature parameters of the LAU Module on the evaluation. Furthermore, the evaluation was performed based on the chemical categories and the volatility of organic compounds.

Overall, the volatilization rate modeled by the LAU program is in the right order of magnitude for all categories of compounds involved in the experiment, although the simulated volatilization is consistently lower than the observed volatilization for highly volatile organic compounds. Moreover, sensitivity analyses indicated that the model outputs of LAU program are not sensitive to the thickness parameter for volatilization of organic chemicals, but show certain sensitivity to changes in temperature.

4.3 Air Module

This section documents the verification and validation activities for the Air Module. The Air Module was reviewed by the external reviewers listed in the box.

Peer Reviewers for Air Module

- Dr. Steven Hanna of George Mason University
- Dr. Fred Mogolesko of M&L Environmental Consultants
- Dr. Bruce Turner of Trinity Consultants

4.3.1 Module Description

The Air Module estimates the annual average air concentration of dispersed contaminants and the annual deposition rates of vapors and particles at various receptor points in the area of interest (AOI). This module simulates the transport and diffusion of contaminants in the form of volatilized gases or fugitive dust emitted from area sources into the air. The predicted air concentrations are used to estimate bio-uptake into plants, and human exposures due to direct inhalation. The predicted deposition rates are used to determine contaminant loadings to farm crops and soils, watershed soils, and surface waterbodies. Figure 4-6 shows the information flow for the Air Module.

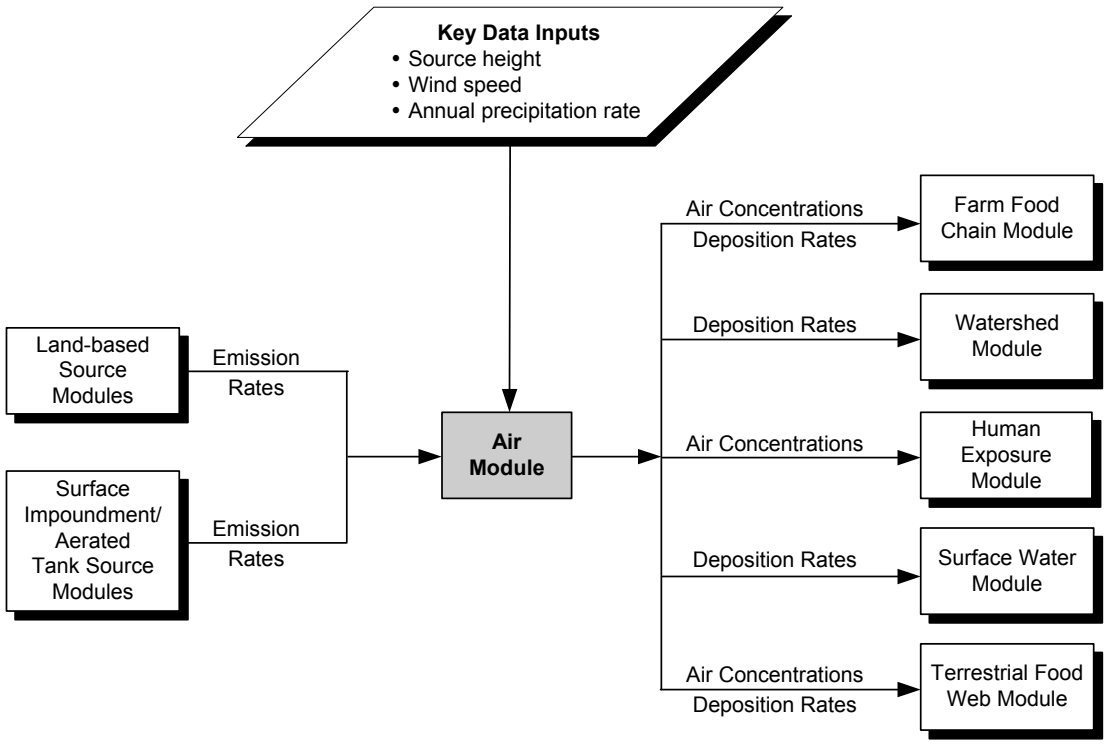

Figure 4-6. Information flow for the Air Module in the 3MRA modeling system.

4.3.2 Major Module Components/Functionality

The Air Module performs four major functions, as follows:

1. **Characterize source-specific parameters.** For each AOI, the Air Module characterizes emission sources based on waste management unit (WMU) dimensions, wastes being managed, and the site-layout. As an option, the module can calculate the source-specific long-term average particulate mass fraction distribution from the outputs of the Land-based Source Modules (Landfill, Waste Pile, or Land Application Unit [LAU] Module). All sources are assumed to be at ground level except for waste piles and aerated tanks. The height of these units are imputed from the WMU area and waste loading data.

2. **Calculate receptor locations (polar grid or site specific).** The Air Module provides the option to model directly to all site-specific output coordinates needed by the 3MRA modeling system or to model to a fixed set of polar coordinates and then use a two-dimensional (2-D) cubic spine method to interpolate from the polar set to the larger set of interest. The spline interpolation is used to reduce the ISCST3 run time.

3. **Calculate receptor-specific concentration and deposition estimates.** The Air Module calculates annual average air concentration and deposition rates for each receptor location specified. Concentrations and deposition rates calculated include

   – Air concentration of vapors,
   – Air concentration of particles,
   – Wet deposition rate for vapors and particles, and
   – Dry deposition rate for particles.

4. **Calculate contaminant-specific annual average concentrations and deposition rates.** The Air Module converts the receptor-specific concentrations and deposition rates based on unit emission rates (e.g., 1 g/m^2-s) to contaminant-specific estimates by multiplying the values by the contaminant-specific emission rate for each year.

ISCST3 may be run by the 3MRA modeling system during a run, or it may be run outside of the 3MRA modeling system and the results of those runs used when the Air Module runs.

4.3.3 Summary of Verification

EPA has used the ISCST model to simulate sources of nonreactive pollutants since 1979 (Bowers and Anderson, 1981). Over the years, EPA has updated ISCST as needed to address particular applications. A history of the development of ISCST may be found in Irwin (2002). Throughout ISCST's development, EPA has undertaken numerous verification efforts to show that the FORTRAN program accurately solves the intended equations. These efforts are described in more detail in Appendix A, and include the following:

- **Creation of ISCST2.** EPA performed a significant overhaul of the program in 1992 to produce ISCST2. During this effort, EPA did a substantial amount of recoding to make the code more modular. EPA developed and followed a detailed test plan to ensure that the re-coded model produced results equivalent to the original model (U.S. EPA, 1992a).

- **Area source algorithm.** A comparison of area source algorithms used by various dispersion models (U.S. EPA, 1989) showed that the finite line source approach used in ISCST to model area sources predicted unrealistic concentrations for receptors located in or near the area source. In 1992, EPA implemented and tested a new area source algorithm that uses an integrated line source algorithm (U.S. EPA, 1992b; U.S. EPA 1992c). EPA released this new area source algorithm to the public in draft form as AREA-ST.

- **Dry deposition velocity of particles.** The need for better estimates of the intermedia transfer of pollutants from the atmosphere to land, water, and vegetation to support multimedia environmental analyses prompted a comparison of existing algorithms for calculating the dry deposition velocity of particles (U.S. EPA, 1994b). This study also compared plume depletion algorithms. In addition, the deposition algorithm in the original ISCST2 model was not designed for small particles. As a result, EPA implemented new deposition velocity and plume depletion algorithms and released them to the public in draft form as DEP-ST.

- **Wet and dry deposition and terrain.** In 1993, the EPA Administrator announced that risk assessments including indirect exposure would be required for permitting hazardous waste incinerators and industrial furnaces. No regulatory models capable of quantifying wet and dry deposition in all terrains existed, so EPA Region 5 sponsored further development of the ISCST2 model to address this need. In this effort, EPA made several revisions to ISCST. First, EPA combined the AREA-ST and DEP-ST versions of ISCST2 into a single version referred to as ISC-COMPDEP. EPA performed testing to demonstrate that ISC-COMPDEP produced equivalent results to AREA-ST and DEP-ST. Second, EPA added the methodology used in the COMPLEX I model for modeling point sources in complex terrain to ISC-COMPDEP and performed tests to ensure that the results were equivalent to those of the original COMPLEX I model. Third, EPA selected and implemented wet deposition and depletion algorithms in ISC-COMPDEP. The development and testing of the ISC-COMPDEP model, including tests to establish equivalent results with the component models, is documented in Strimaitis et al (1993).

ISC-COMPDEP was renamed ISCSTDFT, and proposed as part of Supplement C to the Guideline on Air Quality Modeling. As part of the rulemaking process, the model and associated documentation was subject to public review and comment. Supplement C was promulgated on August 9, 1995 (60 FR 40465). At that time, the model was renamed ISCST3 and released to the public for use in regulatory applications.

ISCST3 was further modified to meet some of the needs and constraints of the proposed 3MRA application. A major area of concern for application in the 3MRA modeling system was ISCST3's runtime. EPA made two modifications to ISCST3 to address the runtime issue.

- **Sampled Chronological Input Methodology.** EPA added an option called the Sampled Chronological Input Methodology (SCIM) to sample from the meteorological data at regular intervals rather than run each consecutive hour. This option is used to calculate annual values for concentration and deposition. EPA tested the use of this option over a range of sources, climate regimes, and sampling rates (U.S. EPA, 1998d). Based on the results of that testing, EPA recommended a sampling interval for the 3MRA modeling system. The 3MRA modeling system does not require the use of the SCIM option, nor does it require the use of the recommended sampling interval if the SCIM option is used.

- **Plume depletion algorithm.** The plume depletion algorithm for area sources is numerically intensive, contributing to the long runtime for area sources. EPA conducted a comparison of available depletion schemes and implemented and tested a new algorithm (Venkatram, 1998) to replace the existing scheme (Horst, 1983).

In addition to the testing of the individual model components as described above, the ISCST model, preprocessors, and postprocessors that comprise the Air Module have undergone internal and independent testing as part of the software development process supporting the 3MRA application. Table 4-7 summarizes the functional requirements and the number of test cases executed to verify the Air Module.

Table 4-7. General Requirements for Testing the Air Module

Step	Description	Number of Test Cases
1	Correctly manage files generated by the pre- and postprocessor	14
2	Correctly detect when the core model does not need to run	1
3	Read normalized concentration and deposition values from the air database correctly and output annualized values correctly	13
4	Correctly implement the spline option and produce a reasonable spline surface	3
5	Correctly implement the massfrax option	3
6	Correctly estimate plume depletion due to dry and wet deposition.	3
7	Ensure that the use of the SCIM option provides estimates close to those of running the full meteorological record	2

4.3.4 Summary of Validation

ISCST3 provides point estimates of concentration, dry deposition, and wet deposition. Although numerous studies have compared concentrations predicted by ISCST3 (or its

predecessors) with observed data, the deposition estimates are harder to validate because field studies of dry and/or wet deposition flux from point or area sources are seldom found in the literature. The subsections that follow discuss validation studies that have been performed on the various components of the ISCST3 model with the intent to show that the modeling approach adequately represents the physical processes in the atmosphere. Appendix A describes the validation of the Air Module; a summary is provided here.

4.3.4.1 Concentration estimates. The ISCST model (Bowers and Anderson, 1981) evolved from earlier plume models such as CRSTER (U.S. EPA, 1977), inheriting the same dispersion algorithms and adding building downwash algorithms. Therefore, evaluation studies done for CRSTER (and its derivatives) are also applicable to ISCST and subsequent revisions to it. Concentration estimates from CRSTER were extensively evaluated for a number of point sources using databases for coal-fired power plants. These studies are listed in Table 4-8.

Table 4-8. Coal-Fired Power Plants used for ISCST3 Evaluation

Database	Location	Stack height(s)	Terrain type	Reference
Clifty Creek	Indiana	3 stacks; all 208 m	low ridges and rolling hills	Londergan et al (1982)
Muskingum	Ohio	2 stacks; all 252 m	low ridges and rolling hills	Cox and Moss (1985)
Paradise	Kentucky	3 stacks; 183 m, 183 m, 244 m	flat terrain surrounded by rolling hills	Cox et al (1987)
Kincaid	Illinois	1 stack; 187 m	flat terrain	Cox et al (1986)

Separate studies were performed to evaluate the concentrations predicted for area sources. Field studies of area sources, particularly ones measuring impacts near and within the source, are scarce. Therefore, EPA used alternative methods for evaluating the algorithm before recommending it for regulatory modeling applications. As described above, EPA conducted a comparison of area source algorithms used by various dispersion models (U.S. EPA, 1989) to select an algorithm for inclusion in ISCST2. In this study, EPA developed a set of prediction scenarios for testing and comparing the algorithms. A follow-on study examined the sensitivity of the selected area source algorithm across a range of source characteristics and compared the results to those from the original ISCST model algorithm. Finally, EPA compared results from the selected algorithm to data from a wind tunnel study (U.S. EPA, 1992d).

4.3.4.2 Dry deposition estimates. ISCST3 calculates particle dry deposition flux by multiplying the air concentration by the deposition velocity. Studies of particle deposition flux attributable to individual sources are difficult to find. In the absence of flux studies to be used for validation, EPA has focused on validating the algorithm to estimate particle deposition velocity and relied on the previously noted validations of the concentration algorithms. To select the dry deposition algorithm to be added to ISCST3, EPA evaluated and compared a number of deposition velocity algorithms and implemented the "most appropriate approach" (U.S. EPA, 1994b). EPA evaluated the algorithms on their ability to parameterize important physical processes while requiring only readily available meteorological, chemical, and physical input data. In addition, Schwede and Paumier (1997) did sensitivity tests that exercised the algorithms and demonstrated the ability of the model to produce estimates within expected ranges.

Another aspect of the deposition calculation is accounting for the material lost from the plume as a result of deposition. This is referred to as depletion. For use in 3MRA, EPA changed the depletion algorithm in ISCST3 to one that was shown to be faster and more robust (Venkatram, 1998). That algorithm was validated against a full numerical solution to the eddy diffusivity equation (Venkatram, personal communication).

4.3.4.3 Wet deposition estimates. ISCST3 is used in 3MRA to calculate the wet deposition of both particles and gases. Wet deposition is dependent on the air concentration, the scavenging coefficient, and the precipitation rate. For wet deposition of particles, the scavenging coefficient is specified for ISCST3 by particle size category. For wet deposition of vapors, the scavenging coefficient is contaminant-specific. To reduce the number of model runs required for a 3MRA application, EPA configured the Air Module to use a single vapor-phase scavenging coefficient value for all contaminants that causes them to be scavenged as if they were small particles. The general approach for calculating the wet deposition flux and resulting depletion was proposed by Maul (1980) based on an analysis of ambient data.

4.4 Surface Water Module

The Surface Water Module is based on EPA's legacy model Exposure Analysis Modeling System (EXAMS II), which has been thoroughly verified and validated in numerous applications. EXAMS II was extended for use in the Surface Water Module primarily through development of the pre- and postprocessor, EXAMS IO. EXAMS IO is the interface between EXAMS II and the rest of the 3MRA modeling system. It reads data from other modules and 3MRA modeling system databases, builds the EXAMS input files describing the waterbody environment and chemical properties, builds a command file that specifies the contaminant loading history, and controls the EXAMS simulation. EXAMS IO passes control to EXAMS II, which conducts the simulation and produces intermediate results files. EXAMS IO then processes the intermediate files and passes the output data back to the proper 3MRA modeling system database. While the EXAMS component of the Surface Water Module is a fully functional model independent of the 3MRA modeling system, it is driven and constrained in various ways by EXAMS IO and the 3MRA modeling system databases.

The external peer reviewers for the Surface Water Module are listed in the box.

Peer Reviewers for Surface Water Module

- Dr. Mustafa Aral of Georgia Institute of Technology
- Dr. Anthony Donigian of AQUA-TERRA Consultants
- Dr. Wilbert Lick of University of California, Santa Barbara

4.4.1 Module Description

The Surface Water Module simulates contaminant concentrations in surface waterbodies throughout the AOI around each site modeled. Inputs to the Surface Water Module include contaminant loadings from direct air deposition onto surface waters, contaminant loadings from runoff and soil erosion from land areas associated with sources (LAU and waste pile only), contaminant loadings from contaminated ground water plumes that are intercepted by surface waters, contaminant loadings from runoff and soil erosion from watersheds in the AOI, and hydrological inputs (flows, soil loads) from watersheds. Surface Water Module outputs include water column and sediment concentrations, which are then used

by the Aquatic Food Chain Module, Farm Food Chain Module, and Ecological Exposure Module. All inputs and outputs are annual average time series. Figure 4-7 shows the information flow for the Surface Water Module.

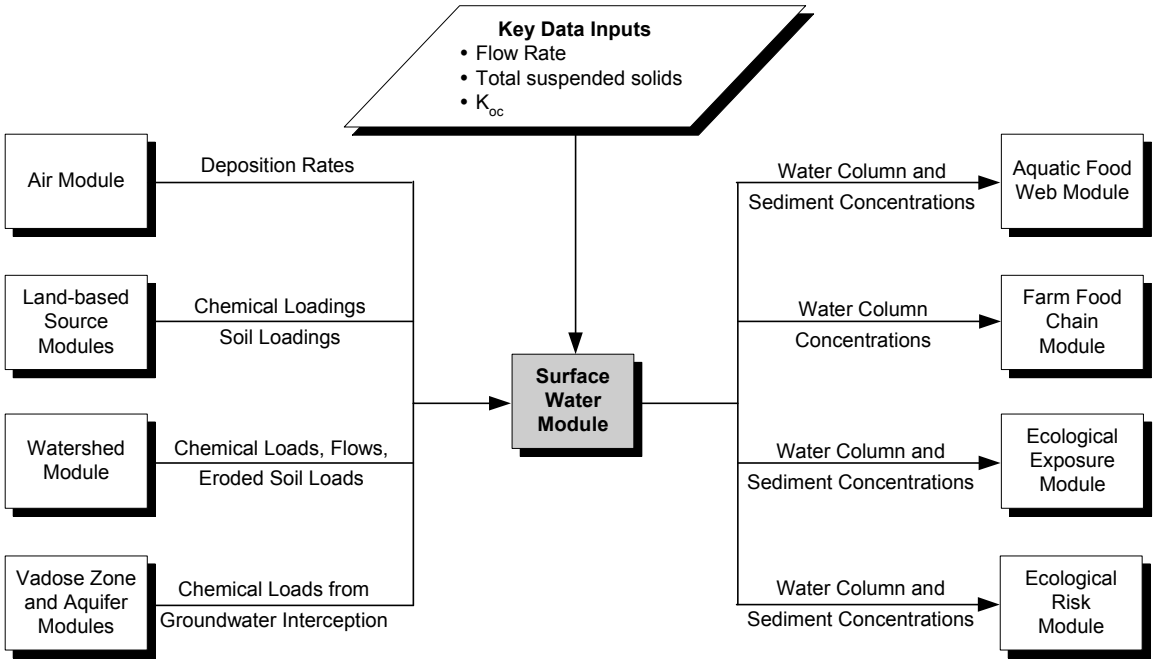

Figure 4-7. Information flow for the Surface Water Module in the 3MRA modeling system.

4.4.2 Major Module Components/Functionality

The major tasks performed by the Surface Water Module to simulate contaminant concentrations throughout the surface waterbody network in the AOI are as follows:

1. **Construct waterbody network.** For each AOI, the Surface Water Module identifies the streams, wetlands, ponds, lakes, and bay reaches to be modeled and assigns lengths, areas, depths, and volumes to them.

2. **Route hydraulic flow and solids through the waterbody network.** The Surface Water Module conducts water and solids balances for each waterbody in each year of the simulation.

3. **Construct and solve the mass balance equations describing contaminant fate and transport throughout the waterbody network.** The Surface Water Module calculates the contaminant concentration in each waterbody for each year. Outputs include total water column concentration and dissolved concentration.

4.4.3 Summary of Verification

The Surface Water Module was subjected to a series of tests to verify that it accurately performs its prescribed computations. These tests were intended to verify that the Surface Water Module correctly implements EXAMS within the 3MRA modeling system. In addition, some verification testing was performed to ensure that the Surface Water Module accurately reproduces available analytical solutions for a set of simplified test cases. The verification testing is described in detail in the EPA document, *Quality Assurance Verification and Validation Tests for the Exposure Analysis Modeling System—EXAMS* (U.S. EPA, 2002a). A summary of that testing is presented here; the complete document is included as Appendix B.

The Surface Water Module must automatically construct and execute a simulation for each waterbody system at a site using the databases that are created by each Monte Carlo iteration in a 3MRA modeling system implementation. As mentioned previously, the general steps in a simulation are to construct a proper waterbody network, conduct water and solids balances, and calculate contaminant transport and fate. These general steps also formed the structure of the module testing program. The general requirements of the Surface Water Module are presented in Table 4-9 along with the number of verification test cases examined for each requirement.

Table 4-9. General Requirements for Testing the Surface Water Module

Step	Description	Number of Test Cases
1	Construct the water body network	3
2	Construct dispersive exchanges	3
3	Conduct the water balance	3
4	Calculate solids transport	3
5	Calculate conservative contaminant transport	3
6	Calculate ionic speciation for ionizing organic chemicals	2
7	Calculate partitioning to solids and DOC	2
8	Calculate volatilization loss	13
9	Calculate contaminant transformation	5
10	Test for robustness	16

All tests in Steps 1 through 9 were performed using one of three simplified waterbody networks at a hypothetical site (Figure 4-8). The first two networks are simple one-reach water bodies. Network 1 is a pond with outflow, and network 2 is a lake with no surface outflow. Network 3 is composed of four reaches: two headwaters reaches (1 and 2, a pond and a wetland), which are connected to reach 3 (a stream), which is connected to exiting reach 4 (a lake).

Within each reach, the surface-water modeling system disaggregates the waterbody into a set of "compartments." The Surface Water Module constructs a differential equation for each compartment, and then solves the resulting system of equations representing interactions among

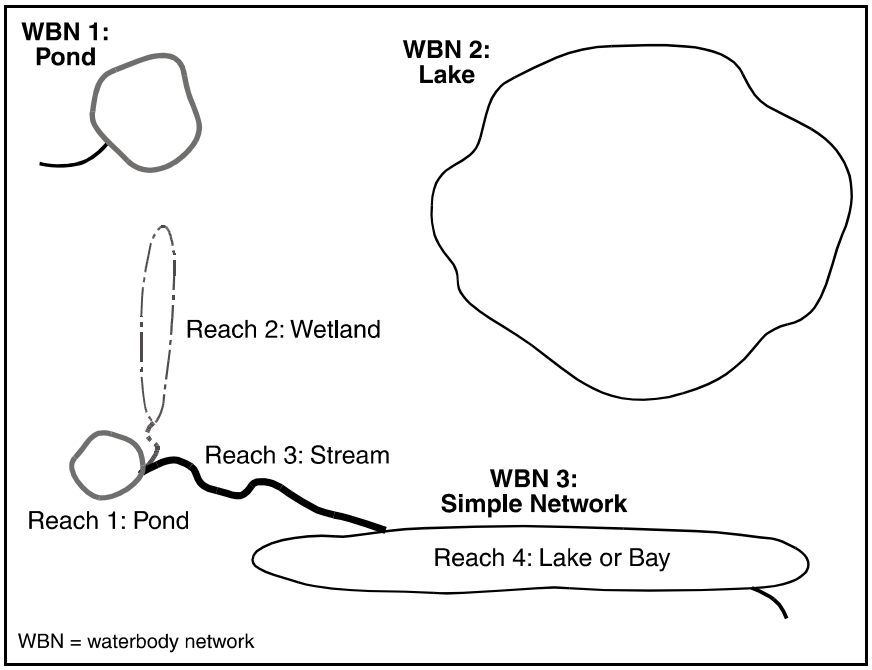

Figure 4-8. Surface Water Module test waterbody networks.

all modeled compartments. For example, for the pond reach-type, the Surface Water Module simulates three compartments: the littoral zone, the surficial benthic layer, and the underlying benthic layer. For the lake reach-type, it simulates four compartments: the epilimnion (water column above the thermocline), the hypolimnion (water column below the thermocline), the surficial bethnic layer, and the underlying benthic layer.

All test cases were verified and the module requirements in Table 4-9 were considered to be met.

4.4.4 Summary of Validation

Since EXAMS was first released in 1983, it has been applied many times to waterbodies throughout the world. This section summarizes studies that report model performance against measured data in either a calibration or validation mode. These studies cover a wide range of waterbodies, chemicals, and fate processes, including

- Environments—small streams, rivers, ponds, rice paddies, and bays;
- Chemicals—dyes, herbicides, insecticides, phenols, and other organic chemicals with a variety of chemical properties; and
- Fate processes—advection, sorption, sediment-water exchange, volatilization, hydrolysis, photolysis, water column and benthic biodegradation, and oxidation.

Chemical coefficients were supplied from the open technical literature and, in some cases, from site-specific experiments. Table 4-10 lists the calibration/validation case studies

Table 4-10. EXAMS Calibration/Validation Case Studies

Reference	Description
Games (1982)	EXAMS was applied to model the fate of linear alkylbenzene sulfonate (LAS) discharged in treated sewage effluent in Rapid Creek, SD. The important chemical fate reactions for LAS are partitioning to solids and biodegradation, both of which vary with the isomer chain length. The most sensitive model parameters were found to be the sediment-water dispersion coefficient and the sediment biodegradation rate constant. Because these are two of the least-understood parameters, the authors suggest that "wide error limits would need to be placed on predicted LAS concentrations... using EXAMS, and probably any evaluative model in a safety assessment." Nevertheless, the authors concluded that "given the proper assumptions, EXAMS can successfully predict the concentration of LAS resulting from its steady-state input to a flowing stream."
Pollard and Hern (1985)	EXAMS was tested against phenol data in an 18-mile reach below a steel plant discharge to the Monongahela River, PA. After calibration, the authors observed a "nearly perfect fit of observed and predicted concentrations by station."
Schramm et al. (1988)	EXAMS was tested by simulating Disperse Yellow Dye 42 introduced to an experimental outdoor pond. The model network included a water column segment and two benthic layers. Although some departures between predicted and observed concentrations were observed during the course of the study, the authors characterized the overall model performance as good.
Kolset and Heiberg (1988)	EXAMS was calibrated and tested with three contaminants from a kraft mill effluent to a heavily polluted bay on the east coast of Sweden. Four compounds identified in the effluent were used to test EXAMS – 2,4,6-trichlorophenol (2,4,6-TrCP), 3,4,5-trichloroquaiacol (3,4,5-TrCG), tetrachloroguaiacol (TeCG), and tetrachlorocatechol (TeCC). Calculated and measured concentrations agree well for 2,4,6-TrCP, 3,4,5-TrCG, and TeCG, but not for TeCC. The authors conclude that EXAMS is capable of predicting the concentrations of some selected chlorophenolics in the Norrsundet area with reasonable accuracy. EXAMS describes all important transformation and loss processes except for sedimentation reasonably well.
Woodrow et al. (1990)	Volatilization flux was measured for three rice herbicides—MCPA, molinate, and thiobencarb—and one insecticide—methyl parathion—from a laboratory chamber and two flooded rice fields. The flux measurements were compared to predicted fluxes using EXAMS with chemical properties and chamber or field conditions as input. The normalized volatilization flux values predicted by EXAMS compared well overall with the observed values, within 10%–20% for molinate, a factor of 2 for MCPA acid, and a factor of 3 for methyl parathion. The calculated flux rate for thiobencarb, however, was low by a factor of 5. The authors attribute this discrepancy to possibly incorrect vapor pressure and/or solubility data. The authors conclude that EXAMS "appeared to be promising as a predictive tool for estimating volatilization, when the appropriate chemical properties and environmental conditions were used as input data."
Tynan et al. (1991)	EXAMS was tested against data for a variety of contaminants in a 7 km reach below a sewage treatment works (STW) effluent to a small, unnamed lowland river in England. In general, EXAMS predictions are described as being reasonably close to measured values, with "fairly close predictions" for styrene, m-dichlorobenzene, and p-dichlorebenzene. The authors conclude that EXAMS produces quantitative predictions that compare well with observations for those contaminants for which reliable rate data exist.

(continued)

Table 4-10. (continued)

Reference	Description
Cousins et al. (1995)	EXAMS was tested against aniline and lindane data in a 7 km reach below an STW effluent to the large lowland River Calder in West Yorkshire, England. EXAMS predicted very slight losses for both contaminants, a result consistent with two surveys. Fairly good correlations were achieved between measured and predicted dissolved water column concentrations, with predictions falling within a factor of 2 of station means. Measured suspended particulate concentrations in the river were significantly higher than predicted, probably because of limitations in the equilibrium partitioning assumption. The measured high particulate concentrations from the STW appeared to be either irreversibly or strongly bound with a slow desorption rate. By contrast, predicted bed sediment concentrations were "a little lower than measured," all falling within an order of magnitude of observations. From this study, the authors conclude that EXAMS is useful for predicting the fate of non-ionic organic chemicals in rivers, provided that adequate physicochemical and environmental data are available.
Armbrust et al. (1999)	EXAMS was calibrated to bensulfuron methyl (BSM) and azimsulfuron (AZM) data taken in experimental lysimeters that contained 5 cm of water overlying 50 cm of paddy soil. EXAMS successfully predicted the partitioning and degradation reactions that led to observed contaminant half-lives in paddy water. Predicted water column concentration responses generally matched the observed data. EXAMS overestimated soil concentrations by factors of 2 to 4. The authors conclude that a "definitive characterization of the rate of degradation and mobility of the two contaminants at a specific site would require additional information on environmental parameters and site-specific soil-chemical interactions."

performed to date in chronological order. These case studies are described in more detail in U.S. EPA (2002a). EXAMS requires a combination of environmental, chemical, and loading data in order to properly specify the model parameters. Erroneous, uncertain, or missing data can result in improper model parameterization, which leads to errors in model predictions. Overly simple process equations can also lead to errors in model predictions. The case studies referenced here highlight both parameter uncertainty and model uncertainty. However, despite these sources of uncertainty, it appears that EXAMS, and thus the Surface Water Module, is able to predict the concentrations of most organic chemicals within a factor of 2 or better in the water column, and within an order of magnitude in the sediment.

4.5 Vadose Zone and Aquifer Modules

The Vadose Zone and Aquifer Modules simulate the migration of chemical constituents in the subsurface and were extracted from EPA's Composite Model for Leachate Migration with Transformation Products (EPACMTP) (U.S. EPA, 1996a,b,c; 1997a). This model is used in EPA regulatory efforts by OSW and has been subject to extensive peer review and public comment. EPACMTP is the best currently available tool to predict potential ground water pathway exposure at a downstream receptor well for regulatory development purposes.

Peer Reviewers for Subsurface Module

- Dr. Craig Forster of University of Utah
- Dr. M. Akram Hossain of Washington State University
- Dr. Carl Mendoza of University of Alberta
- Dr. Frank Schwartz of Ohio State University

The Vadose Zone and Aquifer Modules were reviewed by the external reviewers listed in the box.

4.5.1 Module Description

The Vadose Zone and Aquifer Modules simulate the subsurface movement of chemical constituents contaminants in leachate from surface impoundments, landfills, waste piles, and land application units (LAUs) to downgradient drinking water wells and waterbodies. The modules are not used for aerated tanks, because tanks are assumed not to leak. Figure 4-9 shows the information flow for the Vadose Zone and Aquifer Modules.

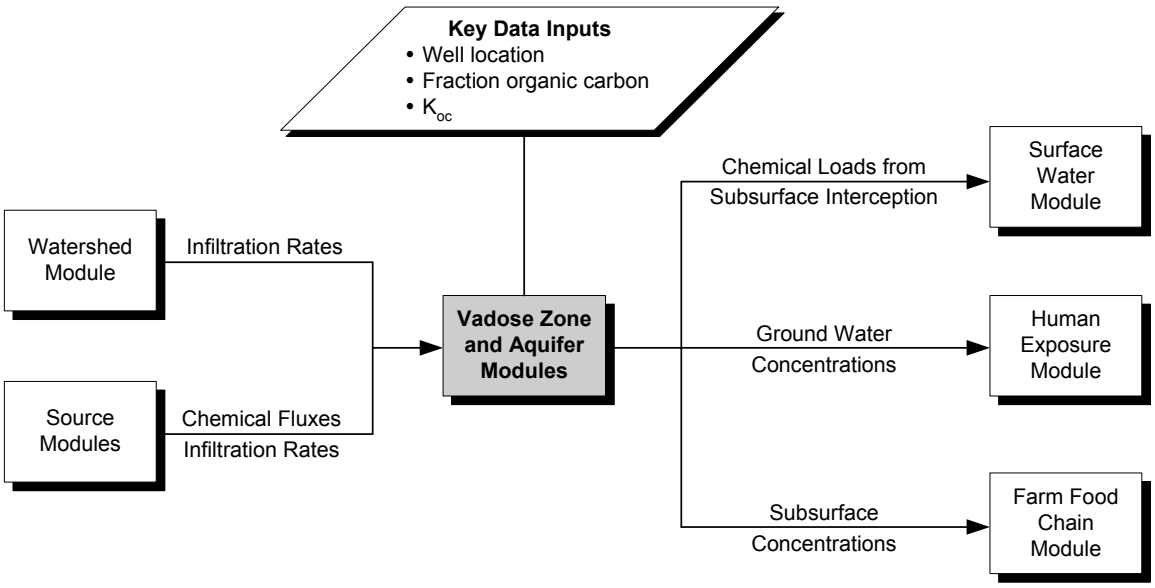

Figure 4-9. Information flow for the Vadoze Zone and Aquifer Modules in the 3MRA modeling system.

The Vadose Zone and Aquifer Modules simulate the fate and transport of dissolved contaminants from a point of release at the base of a WMU, through the underlying soil (the vadose zone), and through a surficial aquifer (or ground water source). Module outputs include ground water contaminant concentrations in wells, which are used by the Human Exposure Module to estimate exposures through drinking water and showering and by the Farm Food Chain Module to estimate contaminant concentrations in beef and milk from farm well use; and contaminant fluxes into waterbodies, which are used by the Surface Water Module, along with contaminant fluxes from atmospheric deposition and overland flow, to estimate contaminant concentrations in streams, lakes, and wetlands.

The Vadose Zone and Aquifer Modules are used by the 3MRA modeling system only if there are wells or downgradient streams, lakes, or wetlands at a site. Waterbodies are downgradient if they are in the direction of ground water flow away from the WMU.

4.5.2 Major Module Components/Functionality

The Vadose Zone and Aquifer Modules perform the following functions:

1. **Model vadose zone flow and transport.** The one-dimensional (1-D) Vadose Zone Module simulates infiltration and dissolved contaminant transport, by advection and dispersion, from the WMU through the soil above the water table (i.e., the vadose zone) to estimate the contaminant and water flux to the underlying ground water.

2. **Model ground water flow and transport.** The quasi-3-D Aquifer Module simulates ground water flow and contaminant transport, by advection and dispersion, from the base of the vadose zone to estimate contaminant concentrations in drinking water wells and contaminant discharge fluxes to waterbodies.

3. **Model subsurface chemical reactions.** Both the Vadose Zone and Aquifer Modules simulate sorption to soil or aquifer materials and biological and chemical degradation, which can reduce contaminant concentrations as contaminants move through soil and ground water. In cases where degradation of a contaminant yields other contaminants that are of concern, the Vadose Zone and Aquifer Modules can account for the formation and transport of up to six different daughter and granddaughter degradation products. The modules use sorption isotherms for metal contaminants, which allow adjustment of sorption behavior to account for varying metal concentrations and geochemical conditions.

4.5.3 Summary of Verification

Verification of EPACMTP began in 1991. These activities compared numerical and analytical results from EPACMTP to analytical and numerical solutions from other verified sources. Initially, the flow and transport mechanisms in the vadose zone and saturated zone (aquifer) models were verified. Testing continued in 1999 on the portions of EPACMTP extracted for use in the Vadose Zone and Aquifer Modules. In 2000, EPA conducted comprehensive verification efforts on all components of the Vadose Zone and Aquifer Modules.

These verification efforts are summarized in "*Verification and Validation of the EPA's Composite Model for Transportation Products (EPACMTP) and its Derivatives*." (HGL, 2003) That summary is included here as Appendix C. A synopsis of this summary is provided here and in Table 4-11. For additional information, please refer to the original source documents.

EPA's ORD conducted its first verification of EPACMTP in 1992. EPA tested 14 components of the model, including aquifer flow, vadose-zone transport, multiple species transport with decay, and full-3D aquifer flow and transport. The tests were conducted to confirm the developer's verification results using the same data sets and to provide an independent verification of the model using alternate test criteria. Analysts used EPA's verification activities to identify some technical limitations of EPACMTP. As a result, the model's code was modified to expand its capabilities.

Table 4-11. Summary of Verification Activities for the 3MRA Vadose Zone and Aquifer Modules[1]

Name of Verification Activity (Year) (Original Source Document)	Component Tested	Verification Tools	Number of Test Cases	Results
U.S. EPA Office of Research and Development (1992-1993) (U.S. EPA, 1992e; HGL, 1993)	Composite model—flow and transport	Reverification of original test problems and data files; independent verification using alternative test criteria	21	Some technical limitations identified; modifications were conducted
Module-Level Verification (1993-1994) U.S. EPA, 1996d, U.S. EPA, 1996e)	Vadose Zone Module—Infiltration and transport	Compared to analytical and numerical solutions from VADOFT, FECTUZ, HYDRUS, MOB1, Ogata and Banks (1961), van Genuchten and Alves (1982), Shamir and Harleman (1967), Hadermann (1980), and Hodgkinson and Maul (1985)	10	verified
	Vadose Zone Module—metals transport with nonlinear sorption	Compared to total mass input or analytical and numerical solutions from HYDRUS and Ogata (1970)	4	verified
	Saturated Zone—flow and transport	Compared to analytical and numerical solutions from MNDXYZ, EPACMTP, MOB1, FECTUZ, DSTRAM, VAM2D, VAM3D, and Sudicky et al. (1991)	7	verified
Module- and Model-Level Verification as EPACMTP (1997) (U.S. EPA, 1997b)	Vadose Zone—flow, infiltration, and transport	Compared to analytical and numerical solutions from STAFF3D, EPACMTP, and VAM2D	4	verified
	Saturated Zone—flow and transport	Compared to analytical and numerical solutions from MNDXYZ, EPACMTP, VAM3DF, and STAFF3D	3	verified
	Composite Model—flow and transport	Compared to analytical and numerical solutions from VAM3DF	2	verified

(continued)

Table 4-11. (continued)

Name of Verification Activity (Year) (Original Source Document)	Component Tested	Verification Tools	Number of Test Cases	Results
3MRA's Ground water Pathway Module Verification (1999) (U.S. EPA, 1999b; U.S. EPA, 1999c; U.S. EPA, 1999d)	Vadose and Saturated Zones—extracted flow and transport mechanisms	Compared to results from EPACMTP	12	verified
	Vadose Zone—1-D flow and transport	Compared to results from MODFLOW-SURFACT	2	verified
	Saturated Zone—pseudo 3-D flow and transport	Compared to Darcy's Law, Ogata (1970), and 3MRA	3	verified
Final Verification of 3MRA Ground water Pathway Module (2000) (U.S. EPA, 2000c; U.S. EPA, 2000d)	Vadose Zone—all components	NA[2]	40	verified
	Saturated Zone—all components	NA	69	verified

[1]Adapted from HGL (2003)
[2]Not available

Further testing was conducted in 1993 and 1994 to verify the model's flow and transport components in the vadose and saturated zones. Researchers compared the results of these tests to analytical and numerical solutions from several simulators with comparable frameworks. Ten cases verified the model's ability to calculate infiltration and transport mechanisms in the vadose zone. Another four test cases were conducted to examine metals transport mechanisms with non-linear sorption in the vadose zone. The cases verified the model's ability to calculate these mechanisms. The flow, transport, and sorption of contaminants in the saturated zone were verified in seven test cases.

Verification activities for EPACMTP continued in 1997. These activities focused on single problem geometry and were developed in accordance with the ASTM "*Standard Guide for Developing and Evaluating Ground-Water Modeling Codes*" (ASTM, 1996). The first four test cases verified the flow, infiltration, and contaminant transport mechanisms in the model's vadose zone module. The 3-D flow and transport components of the saturated zone module were verified in the next three test cases. Finally, two test cases were used to examine the composite module. These cases verified the model's ability to calculate composite flow and transport mechanisms in the subsurface.

In 1999, the flow and transport mechanisms in EPACMTP were extracted from the vadose zone and saturated zone modules for use as the Vadose Zone and Aquifer Modules in the 3MRA modeling system. EPA conducted 12 case studies to ensure that the extracted components functioned correctly in the new module. Two cases verified 1-D contaminant flow and transport mechanisms in the vadose zone using the 3-D MODFLOW-SURFACT model. The flow and transport mechanisms in the 3MRA modeling system's pseudo-3-D model for the saturated zone were also verified in three test cases.

EPA conducted final verification of the vadose zone model and pseudo-3-D saturated zone model contained in the Vadose Zone and Aquifer Modules in 2000. Tables 4-12 and 4-13 summarize the functional requirements and number of test cases executed to verify the Vadose Zone and Aquifer Modules, respectively.

Table 4-12. General Requirements for Testing the Vadose Zone Module

Step	Description	Number of Test Cases
1	Correctly read and screen source and site-specific input data	5
2	Correctly perform any required presimulation processing of input data	3
3	Correct operation of flow component	2
4	Correct operation of the nonmetals transport component	8
5	Correct operation of the metals transport component	10
6	Correct operation of postsimulation output	2
7	Robustness	24

Table 4-13. General Requirements for Testing the Aquifer Module

Step	Description	Number of Test Cases
1	Correctly read and screen source and site-specific input data	10
2	Correctly perform any required presimulation processing of input data	69
3	Correctly calculate the appropriate hydraulic conductivity multiplier for sites with fracture media	9
4	Correctly calculate the appropriate concentration multipliers to account for effects due to heterogeneous saturated media	2
5	Correctly read and screen contaminant-specific, biodegradation, and metal-specific data	20
6	Correctly generate numerical grid for simulation	10
7	Correctly simulate ground water flow subject to various conditions	4
8	Correctly simulate contaminant fate and transport subject to various conditions	21
9	Robustness	29

4.5.4 Summary of Validation

Simulations using EPACMTP and its predecessors have been validated using four sites in North America (see Table 4-14). Site-specific data were modeled and compared to observed field data at the sites. These validation activities are summarized in "*Verification and Validation of the EPA's Composite Model for Transformation Products (EPACMTP) and its Derivatives*" (HGL, 2003). That document is included here as Appendix C. A synopsis of the information from this report is provided here.

Table 4-14. Summary of EPACMTP Validation Activities

Site Description and Location	Validation Mechanism	Results
Borden Landfill, Borden, Ontario, Canada	Compared to observed values and simulation values from Frind and Hakkanen (1987)	Accurately predicted plume size and shape
Agricultural Site, Long Island, New York	Compared to observed values at the site	Demonstrated reasonable agreement; relative error decreased as distance from source increased
Triasulfuron and bromide spill, Dodge City, Kansas	Compared to observed values	Demonstrated reasonable agreement; conservative predictions slightly underestimated; non-conservative concentrations overestimated
Manufactured Gas Plant, New York	Compared to observed naphthalene near to source of contamination	Demonstrated qualitatively similar results

A predecessor to EPACMTP was compared to field and calculated data from the Borden Landfill in 1990. A site contained a chloride plume in a glaciofluvial aquifer beneath the landfill. Contaminants at the site are not transported through the vadose zone because the base of the landfill is located just above the water table. The results of the simulation were compared

to observed field data and calculated data derived from the procedure described in Frind and Hokkanen (1987). The model accurately predicted the size and shape of the chloride plume.

In 1990, pesticide concentrations in ground water were modeled using the saturated zone and vadose zone models from the predecessor to EPACMTP. The results of the simulation were compared to field data from a pesticide-contaminated potato field on Long Island, New York. Site-specific data were combined with calculations from EPA's Pesticide Root Zone Model (PRZM) to provide input for the simulation. Researchers found reasonable agreement between the simulated and observed ground water concentrations. The relative error decreased as the distance from the site increased.

EPACMTP was used in 1993 to model a controlled release of triasulfuron pesticide and bromide. The triasulfuron simulation was conducted using a non-conservative flow and transport model. Bromide was modeled conservatively. These models were compared to an actual controlled release of these contaminants at a site in Dodge City, Kansas. Compared to observed data, the simulated, non-conservative triasulfuron concentrations tended to be overestimated. The model tended to underestimated the conservative bromide concentrations. Overall the simulated data demonstrated reasonably good agreement with the observed data.

In 1995, EPACMTP was validated against observed field results from a coal tar manufactured gas plant in New York. Coal tar had been disposed at the surface and migrated into the aquifer beneath the site. Naphthalene was the contaminant of concern at the site. The results from the model were qualitatively similar to the observed ground water concentrations near the source.

The Vadose Zone Module has also been validated using data from a large soil-column study conducted to investigate the behavior of organic chemicals (including halogenated aliphatic hydrocarbons, substituted benzenes, and phenols) during infiltration of municipal wastewater into soil columns by the Ground Water and Ecosystem Restoration Division (GWERD) of EPA's National Risk Management Research Laboratory (NRMRL). The experiment design and conditions were very close to the assumptions and application conditions of the Vadose Zone Module, making these data suitable for use in evaluating the Vadose Zone Module.

The evaluation of the Vadose Zone Module included:

- Whether modeling without accounting for gas phase could acceptably describe the contaminant fate and transport processes in vadose zone;
- Whether the assumption of first order decay of contaminant transformation is valid;
- Whether the conceptualizations on different attributes of the model (such as boundary conditions and the mathematical model to describe the flow, fate, and transport, as well as its solutions) are adequate; and

- Whether suggestions on how to appropriately apply the Vadose Zone Module could be made through the evaluation.

An individual standalone Vadose Zone program was obtained by modifying the Vadose Zone Module from the 3MRA modeling system to achieve the small intervals of time and space as well as outputs for any depths along the soil column needed to compare the results to the experimental lab data. This modified Vadose Zone program was compared to the Vadose Zone Module and verified to be consistent with the original module. The necessary input parameters to the Vadose Zone program were obtained from the lab experiment design, literature review, and parameter calibrations. Concentrations of organic compounds of interest at selected sampling ports were compared with the model simulation results. The Vadose Zone Module was examined directly using the parameters from the lab experiment design and literature review. It was further evaluated by taking the calibrated first-order transformation rates obtained based on the concentrations from part of sampling ports. Then model verifications were carried out using the concentration data from the other sampling ports.

Comparisons were also performed between the simulation results from the Vadose Zone Module and the other tested and accepted models with similar or enhanced functions (such as CHEMFLO) in order to investigate the compatibility of the Vadose Zone Module with those models. In addition, the simulation outputs of leachate concentrations from the LAU program described in section 4.2.4 were used as input to the Vadose Zone Module, the results of which were used in comparison with the lab experiment data to assess the overall errors from applications of both LAU and Vadose Zone Modules. Moreover, the evaluation was performed based on the chemical categories and the volatility of organic compounds.

Generally, the Vadose Zone Module functioned quite well in simulating the fate and transport of organic chemicals in vadose zones, although noticeable differences between the simulated and observed results could be observed for highly volatile organics. The Vadose Zone Module and the CHEMFLO model generate comparable results. In addition, the overall final outputs from both the LAU and Vadose Zone Modules gave a good estimate of the leachate concentration for organics undergoing both volatilization and transformation, but slightly overestimated for organics with high volatility and low transformation rates.

4.6 Farm Food Chain Module

This section describes the verification and validation activities for the Farm Food Chain Module. The external reviewers listed in the box reviewed the Farm Food Chain Module.

Peer Reviewers for Farm Food Chain Module

- Dr. Donald Mackay of Trent University, Ontario
- Dr. Lee Shull of Montgomery Watson Harza
- Dr. Curtis Travis of Quest Technologies

4.6.1 Module Description

The Farm Food Chain Module predicts the accumulation of contaminants in the edible parts of plants through the uptake of contaminants from soil and the deposition of vapor-phase and particle-bound contaminants from the air. Concentrations are predicted for fruits and vegetables that are grown above ground, as well as for root vegetables. In addition, the module predicts the annual average contaminant concentration in beef and milk products from cattle

raised on farms. The concentrations in produce, beef, and milk are used as inputs to the Human Exposure Module to calculate the applied daily dose to human receptors that consume fruits and vegetables from home gardens or consume produce, beef, or milk from on a farm. Figure 4-10 shows the information flow for the Farm Food Chain Module.

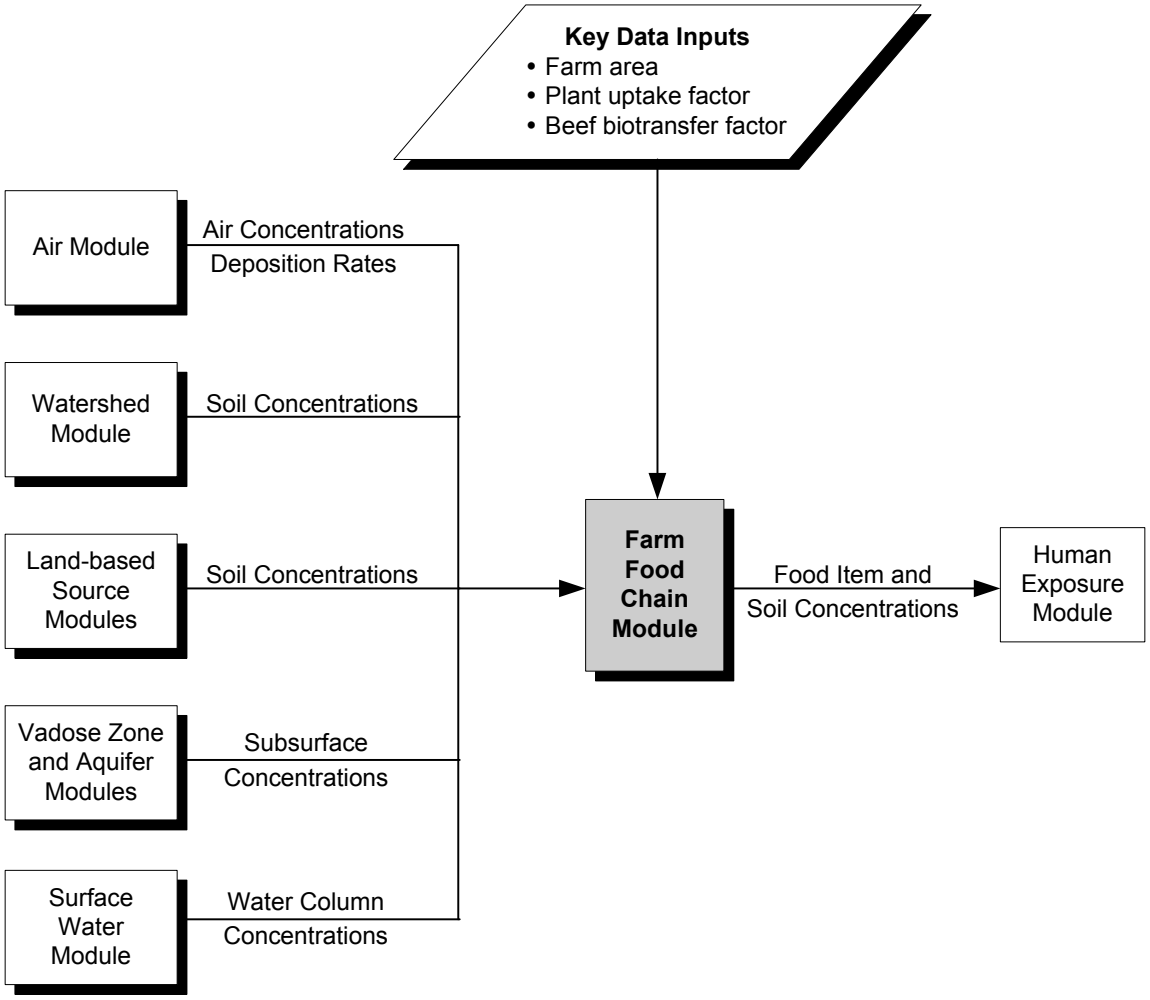

Figure 4-10. Information flow for the Farm Chain Module in the 3MRA modeling system.

The modeling construct for the Farm Food Chain Module is based on recent and ongoing research conducted by EPA ORD and presented in *Methodology for Assessing Health Risks Associated with Multiple Pathways of Exposure to Combustor Emissions* (U.S. EPA, 1998b).

4.6.2 Major Module Components/Functionality

The Farm Food Chain Module performs the following four functions:

1. **Calculate contaminant concentrations in plants due to contaminants in air.** The Farm Food Chain Module calculates the contaminant concentration in plants due to the deposition of particle-bound and vapor-phase contaminant contaminants onto fruits, vegetables, and feed crops that grow above the ground.

2. **Calculate contaminant concentrations in plants due to contaminants in soil.** The Farm Food Chain Module calculates the contaminant concentration in plants due to uptake and translocation of contaminants from the soil into the edible parts of fruits, vegetables, and feed crops that grow above the ground.

3. **Calculate total contaminant concentrations in plants.** The Farm Food Chain Module sums plant concentrations across relevant mechanisms, including direct deposition of particle-bound contaminants, vapor-phase uptake, and translocation of contaminants from soil into the edible parts of plants.

4. **Calculate contaminant concentrations in beef and milk.** The Farm Food Chain Module calculates exposures to beef and dairy cattle through ingestion of contaminated forage, feed crops, soil, and drinking water, and the resulting beef and milk concentrations.

For each year in the simulation, the module predicts point estimates and spatially averaged concentrations within the AOI. Point estimate concentrations are used to evaluate exposures to residential home gardeners that grow and eat fruits and/or vegetables within the AOI. The point estimates reflect the locations of residential receptors that are used to represent the populations in various Census tracts throughout the AOI. The spatially averaged concentrations are used to evaluate exposures to farmers that raise and eat their own produce, beef, or milk products. The spatial averages reflect the farm boundaries that are delineated in the site layout that defines all of the characteristics of the AOI.

4.6.3 Summary of Verification

The Farm Food Chain Module was verified through a series of tests, which are described in detail in the following documents:

- *Farm Food Chain (FFC) Module—Test Plan* (RTI, 2002k)
- *Farm Food Chain Module Internal Verification Testing* (RTI, 2002m)
- *HWIR Farm Food Chain—Review of Compiled Code Executables and Review of the Implementation of the Test Plan* (Snyder, 2000).

EPA originally completed internal verification testing in 2000, followed by external verification testing. Since then, EPA has made a few minor changes to the module. Therefore, EPA repeated internal verification testing on the updated version of the module in 2002 to ensure that the updated version passed all tests and that the test files reflected the outputs from the updated version. EPA also updated internal verification test plans and testing documentation to reflect this second round of testing.

To verify that the module was working properly, EPA designed an Excel spreadsheet using the equations from the module documentation. The testing included a comparison of the output concentrations (and intermediate concentrations) calculated by the Farm Food Chain Module to those calculated using the Excel spreadsheet. The comparison verified that the

concentrations in air, soil, fruits, vegetables, feed, beef, and milk calculated by the module were correct. Table 4-15 summarizes the functional requirements and number of test cases executed to verify the Farm Food Chain Module.

Table 4-15. General Requirements for Testing the Farm Food Chain Module

Step	Description	Number of Test Cases
1	Correctly read results files from the Air, Watershed, Surface Water, and Source modules	3
2	Correctly identify the constituent type as dioxin-like, organic, metal, mercury, or special	3
3	Correctly read site layout file	3
4	Correctly calculate the area-averaged soil concentrations at root zone depth and in the surficial soil for the farm	3
5	Correctly calculate the contaminant concentrations in produce for each constituent type	1
6	Correctly calculate the contaminant concentrations in beef and milk for each constituent type	1
7	Correctly calculate intermediate concentrations, including area-averaged air concentrations and deposition rates onto plants, and concentrations in feed crops for cattle	3
8	Correctly calculate output concentrations when input data include multiple time series that do not start or end in the same year or are discontinuous	1

All total produce, beef, and milk concentrations and area-averaged soil concentrations matched for years 1, 5, 10, 15, and 20, demonstrating that the module handles discontinuous time series correctly. All area-averaged soil concentrations; concentrations in produce, beef, and milk; and intermediate concentrations calculated by the Farm Food Chain Module were verified by the spreadsheet calculations.

The independent testing of the Farm Food Chain Module confirmed the internal testing results: all tests were successfully completed with the executable provided by the development team. All tests were also successfully completed with an independently generated executable.

4.6.4 Summary of Validation

The Farm Food Chain methodology is based primarily on EPA's MPE methodology (U.S. EPA, 1998b). The MPE methodology represents the state of the science with respect to providing reliable guidance in the proper conduct of assessments of risks that may result from multimedia and multipathway exposure. The National Center for Environmental Assessment (NCEA) prepared the MPE methodology as an update to EPA's 1990 indirect exposure document (U.S. EPA, 1990), which is generally known as the Indirect Exposure Methodology, or IEM. Most of the revisions in the MPE methodology are based on SAB and public comments

on IEM. Earlier versions of this document have undergone internal Agency and external peer review. However, this methodology has not been formally validated using field data.

4.7 Terrestrial Food Web Module

This section documents the verification and validation activities that were performed for the Terrestrial Food Web Module. The reviewers listed in the box reviewed the Terrestrial Food Web Module.

Peer Reviewers for Terrestrial Food Web Module

- Dr. Anne Fairbrother of Parametrix, Inc.
- Dr. Robert Pastorok of Exponent
- Dr. Bradley Sample of CH2M Hill

4.7.1 Module Description

The Terrestrial Food Web Module calculates the annual average contaminant concentrations in terrestrial plants and prey (such as earthworms or small mammals) that are eaten by wildlife. In addition, the module calculates spatially averaged soil concentrations in two soil horizons—surficial soil and root zone soil—for the receptor home ranges placed within each of the habitats delineated within the AOI. These concentrations are used as input to the Ecological Exposure Module in calculating the applied does to receptors of interest, and the root zone soil concentration is used by the Ecological Risk Module to predict risks to terrestrial plants and soil communities. Figure 4-11 shows the information flow for the Terrestrial Food Web Module.

For each home range delineated within the AOI, the Terrestrial Food Web Module predicts a time series of annual average concentrations of contaminants in soil, along with concentrations in specific plant and prey categories. The Terrestrial Food Web Module uses the same algorithms and contaminant-specific data as the Farm Food Chain Module to calculate concentrations in plants.

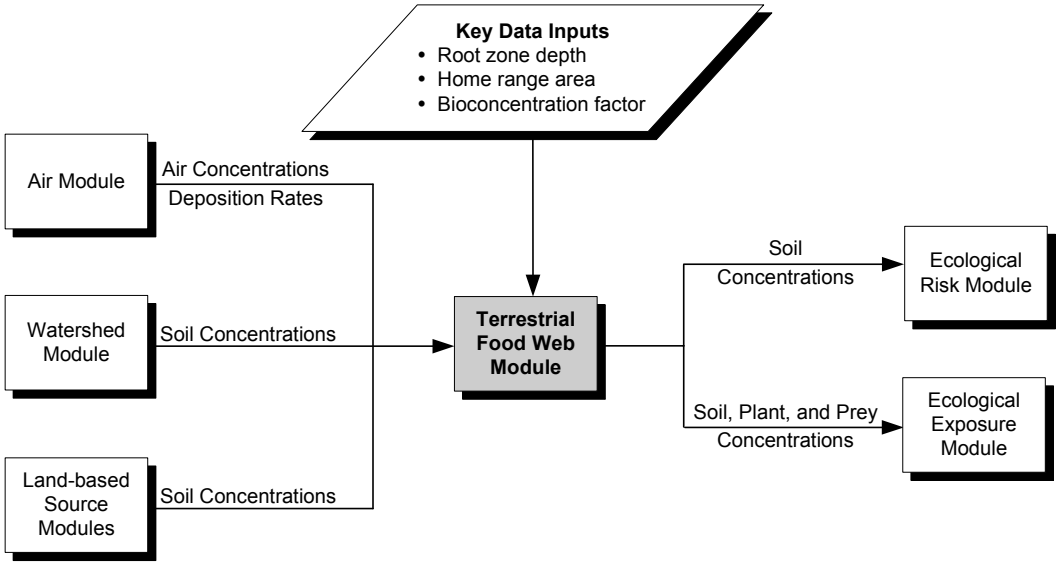

Figure 4-11. Information flow for the Terrestrial Food Web Module in the 3MRA modeling system.

4.7.2 Major Module Components/Functionality

The Terrestrial Food Web Module uses both predictive models and empirical data to calculate contaminant concentration in terrestrial food items. Specifically, the Terrestrial Food Web Module performs the following four functions:

1. **Calculate contaminant concentrations in soil.** The module calculates spatially averaged soil concentrations for each home range in each habitat. The soil concentrations reported by the Land-based Source Modules and the Watershed Module are defined by the WMU, and the watershed subbasins, respectively, at each site. The Terrestrial Food Web Module determines the spatial average based on the proportion of subbasins and/or WMU that overlaps the home range of wildlife species assigned to a given habitat.

2. **Calculate total contaminant concentrations in plants.** The Terrestrial Food Web Module sums plant concentrations across relevant mechanisms, including direct deposition of particle-bound contaminants, vapor-phase uptake, and translocation of contaminants from soil into the edible parts of plants. The module uses the same approach as described for the Farm Food Chain Module to calculate total contaminant concentrations in plants. The only significant difference in the respective modules is that the Terrestrial Food Web Modules defines plant categories for consumption by wildlife rather than humans.

3. **Calculate contaminant concentrations in soil invertebrates.** Earthworms and other soil invertebrates constitute a significant dietary component for many wildlife species. Contaminant-specific soil-to-biota bioconcentration factors are used to calculate the contaminant concentrations in soil invertebrates based on the spatially averaged, root zone soil concentration for each wildlife species' home range.

4. **Calculate contaminant concentrations in vertebrate prey categories.** Small to medium sized terrestrial vertebrates are eaten by larger predators (e.g., fox, black bear, and red tailed hawk). Contaminant-specific soil-to-vertebrate bioconcentration factors are used to estimate the tissue concentrations of contaminants in vertebrate prey categories based on the spatially averaged, root zone soil concentration for each wildlife species' home range.[1] The module reports the minimum and maximum tissue concentrations in each vertebrate prey category; these outputs allow the Ecological Exposure Module to sample from the spatial variability of possible prey species.

The Terrestrial Food Web Module is applied to the margin habitats in freshwater systems and wetlands and to terrestrial habitats, such as the representative forest or grassland. Simple terrestrial food webs were constructed for each terrestrial habitat to depict the major functional

[1] The root zone, rather than surficial, soil concentrations were used to be more representative of the types of exposures likely to be reflected in soil-to-organism bioaccumulation factors (e.g., direct ingestion of soil invertebrates from deeper soil horizons; ingestion of prey that feed primarily on plant matter).

and structural components of healthy terrestrial ecosystems. The components represent major dietary categories for terrestrial wildlife, and represent a broad range of sizes, feeding guilds, and taxa typical of terrestrial food webs. In addition, the terrestrial prey categories reflect available methods and data required to estimate prey concentrations. For example, the category of "small mammals" was developed specifically to take advantage of recent research (Sample et al., 1998) on estimating tissue concentrations of contaminants in small mammals as a function of the soil concentration. This research provides a significant improvement over previous approaches that aggregated a variety of prey items into a single category of "terrestrial invertebrates."

4.7.3 Summary of Verification

The Terrestrial Food Web Module was verified through a series of verification tests, which are described in detail in the following documents:

- *Terrestrial Food Web (TFW) Module—Test Plan* (RTI, 2002p)
- *Terrestrial Food Web Internal Verification Testing* (RTI, 2002n)
- *Independent Tests for Terrestrial Food Web Module* (Tetra Tech, 2000e).

EPA originally completed internal verification testing in 2000, followed by external verification testing. Since then, EPA has made a few minor changes to the module. Therefore, EPA repeated internal verification testing on the updated version of the module in 2002 to ensure that the updated version passed all tests and that the test files reflected the outputs from the updated version. EPA also updated the internal verification test plans and testing documentation to reflect this second round of testing.

Table 4-16 summarizes the functional requirements and number of test cases executed to verify the Terrestrial Food Web Module.

Table 4-16. General Requirements for Testing the Terrestrial Food Web Module

Step	Description	Number of Test Cases
1	Correctly read output files from the Air, Watershed, and Source modules	3
2	Correctly identify the constituent type as dioxin-like, organic, metal, mercury, or special	3
3	Correctly read site layout file	3
4	Correctly calculate depth averaged and surficial soil concentrations for each home range in both aquatic (e.g., stream margin) and terrestrial habitats	3
5	Correctly calculate the contaminant concentrations in plants for each constituent type	1
6	Correctly report the minimum and maximum tissue concentrations for each prey category	3
7	Correctly loop over home ranges (by receptor)	3
8	Correctly loop over habitats	3
9	Correctly loop over years and ensure correct time series management	2

The testing confirmed that the module correctly calculates concentrations in terrestrial biota for all years with nonzero concentrations during the simulation period. Biota concentrations were calculated in a module verification spreadsheet and compared with those

from module runs to confirm that the equations are coded properly and that the module is fully functional.

4.7.4 Summary of Validation

Although the Terrestrial Food Web Module has not been directly validated, it is based on accepted science. The Terrestrial Food Web methodology is based primarily on EPA's MPE methodology (U.S. EPA, 1998b). The MPE methodology represents the state of the science with respect to providing reliable guidance in the proper conduct of assessments of risks that may result from multimedia and multipathway exposure. The NCEA prepared the MPE methodology as an update to EPA's 1990 Indirect Exposure document (U.S. EPA, 1990), which is generally known as the Indirect Exposure Methodology, or IEM. Most of the revisions in the MPE methodology are based on SAB and public comments on IEM. Earlier versions of this document have undergone internal Agency and external peer review.

For contaminant uptake in soil invertebrates, the Terrestrial Food Web Module uses uptake factors developed by the Oak Ridge National Lab (ORNL) (Sample et al., 1998). ORNL validated these uptake factors to evaluate their predictive utility. Validation consisted of separating the available data into two groups, a "model" data set and a "validation" data set. ORNL applied the uptake factors developed from the model data set to the soil concentration data in the validation data set, and compared the resulting estimated concentrations in earthworms with the measured earthworm concentrations in the validation data set. The difference between the estimated values and the measured values was expressed as a proportion deviation as follows:

$$\text{proportion deviation} = (\text{measured} - \text{estimated})/\text{measured}$$

The proportion deviations for the median uptake factors used in the Terrestrial Food Web Module ranged from -6.35 for mercury to 0.76 for chromium. A negative proportion deviation indicates an overestimation; a positive one indicates an underestimation.

4.8 Aquatic Food Web Module

This section describes verification and validation activities for the Aquatic Food Web Module. The external reviewers listed in the box reviewed the Aquatic Food Web Module.

Peer Reviewers for Aquatic Food Web Module

- Dr. Lawrence Barnthouse of LWB Environmental Service, Inc.
- Dr. Frank Gobas of Simon Fraser University
- Dr. Paul Jacobson of Langhei Ecology, LLC

4.8.1 Module Description

The Aquatic Food Web Module calculates steady-state contaminant concentrations in aquatic organisms (e.g., fish, benthic invertebrates, aquatic plants) that are consumed by human and ecological receptors. These concentrations are used as input to the Human Exposure and Ecological Exposure Modules in calculating the applied dose to receptors of interest. Figure 4-12 shows the information flow for the Aquatic Food Web Module.

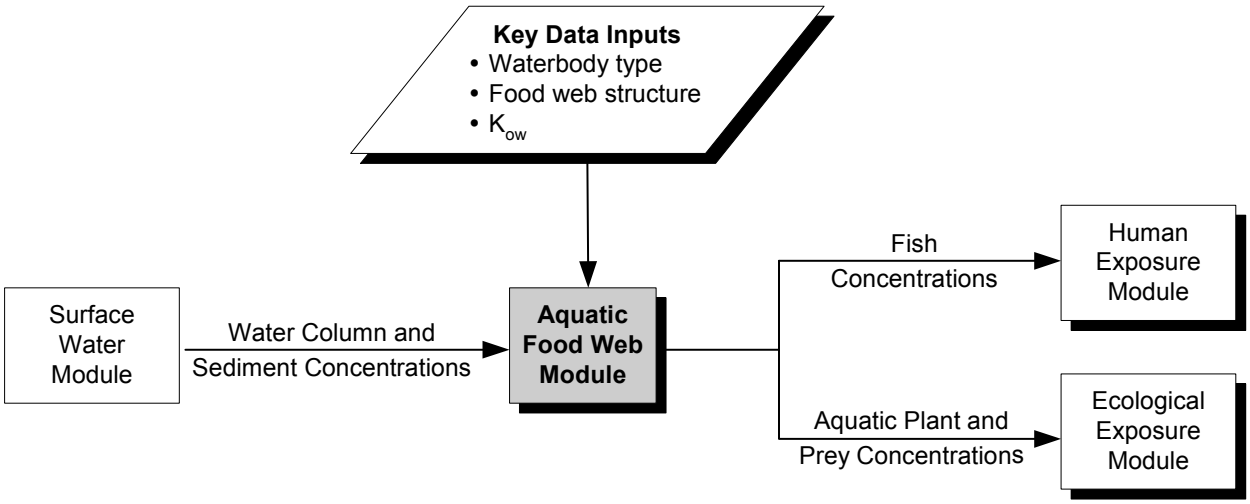

Figure 4-12. Information flow for the Aquatic Food Web Module in the 3MRA modeling system.

For each year in the simulation, the Aquatic Food Web Module predicts contaminant concentrations in aquatic biota for freshwater waterbodies in the AOI considered capable of supporting fish (referred to as "fishable" waterbodies). The model is flexible enough to be applied to different types of waterbodies, including stream reaches, rivers, lakes, ponds, and permanently flooded wetlands. Simple freshwater food webs were constructed for each type of waterbody to depict the major functional and structural components of "healthy" freshwater ecosystems. The components of each food web represent major categories of aquatic biota in freshwater systems: aquatic macrophytes, phytoplankton, periphyton, zooplankton, benthic detritivores, benthic filter feeders, and various feeding guilds of fish. Some of these concentrations are used internally to calculate concentrations in fish, while other concentrations are reported as a time series for use in calculating exposures to wildlife and humans, as well as to calculate ecological hazard (e.g., hazard to sediment dwellers). Thus, the Aquatic Food Web Module determines which data are appropriate for use in a given waterbody and calculates concentrations in the aquatic biota assigned to that waterbody.

4.8.2 Major Module Components/Functionality

The Aquatic Food Web Module performs the following functions:

1. **Select food web appropriate for each waterbody.** The Aquatic Food Web Module matches an appropriate food web with each waterbody identified as fishable within the AOI. Eight freshwater food webs were developed to capture the variability in freshwater systems. They represent warmwater streams/rivers, wetlands, ponds, and lakes; and coldwater streams/rivers, wetlands, ponds, and lakes.

2. **Construct dietary matrix for food web.** The Aquatic Food Web Module uses a constrained, random prey preference sampling approach that selects preference

fractions at random between the minimum and maximum, assuming a uniform distribution. This approach allows for the dietary composition to reflect the full range of variability inherent in the diets of freshwater fish.

3. **Calculate contaminant concentrations in food web.** The Aquatic Food Web Module calculates concentrations for the biota assigned to each freshwater food web. The model will only calculate concentrations for biota that are assigned to a particular food web and waterbody. The calculations involve mechanistic models or the use of empirical data on bioaccumulation.

4. **Report contaminant concentrations for fish consumed by wildlife and humans.** Food webs for freshwater aquatic systems typically have a single apex predator species (trophic level 4 [TL4]) and a number of other fish species that occupy different feeding guilds, such as benthic feeders (e.g., catfish). These other species are, for the purposes of exposure assessment, often grouped into the category of trophic level 3 (TL3), indicating that they are both predator and prey in the food web. To predict exposures for wildlife and humans that eat TL3 fish, the model calculates an average concentration—both wholebody and filet—for fish that fall into the category of TL3. In addition, the Aquatic Food Web Module predicts the tissue concentration for the apex predator fish in each waterbody. The wholebody fish concentrations are used by the Ecological Exposure Module, and the filet concentrations are used by the Human Exposure Module.

4.8.3 Summary of Verification

The Aquatic Food Web Module was verified through a series of verification tests that are described in detail in the following documents:

- *Aquatic Food Web (AFW) Module—Test Plan* (RTI, 2002e)
- *Aquatic Food Web Internal Verification Testing* (RTI, 2002f)
- *Independent Tests for Aquatic Food Web Module* (Tetra Tech, 2000a).

EPA originally completed internal verification testing in 2000, followed by external verification testing. Since then, EPA has made a few minor changes to the module. Therefore, EPA repeated the internal verification testing on the updated version of the module in 2002 to ensure that the updated version passed all tests and that the test files reflected the outputs from the updated version. EPA also updated internal verification test plans and testing documentation to reflect this second round of testing.

Table 4-17 summarizes the functional requirements and number of test cases executed to verify the Aquatic Food Web Module.

Table 4-17. General Requirements for Testing the Aquatic Food Web Module

Step	Description	Number of Test Cases
1	Correctly read output files from the Surface Water Model	4
2	Correctly identify the constituent type as dioxin-like, organic, metal, mercury, or special	4
3	Correctly read site layout file	1
4	Correctly assign the food web (i.e., biota) types for each waterbody	1
5	Correctly assign prey preferences to all elements in the aquatic food web	1
6	Correctly calculate the contaminant concentrations in each element in the food web for each constituent type	4
7	Correctly average concentrations in T3 fish	4
8	Correctly loop over aquatic habitats	2
9	Correctly loop over all fishable reaches within each aquatic habitat	2
10	Correctly loop over years and ensure correct time series management	3
11	Correctly read the chemical properties and surface water data associated with methylmercury when multiple chemical species of mercury are present	1

The testing confirmed that the module correctly calculates concentrations in aquatic biota for all years with nonzero concentrations during the simulation period. A comparison of the output biota concentrations in the spreadsheet and those from the module runs ensured that the equations were coded properly and that the module was fully functional.

4.8.4 Summary of Validation

The Aquatic Food Web Module methodology for calculating tissue concentrations for organic chemicals for fish and other aquatic biota is based on methods identified in refereed journals. In addition, the Gobas model (Gobas, 1993) and other major elements of the calculation framework are currently used by EPA in various guidance documents and rule makings. The methodology for hydrophobic organics (based on the work by Gobas [1993]) has been validated for coldwater lakes and has been validated for other aquatic systems as well. Nevertheless, validation exercises comparing output from the Aquatic Food Web Module with measured concentrations from field studies have not been performed.

4.9 Human Exposure Module

This section describes the verification and validation activities for the Human Exposure Module. The Human Exposure Module and associated data (e.g., spatial layout, human exposure factors) were reviewed by the external reviewers shown in the box. The peer-review charge, a summary of the reviewer comments, and original comments submitted by each individual

reviewer were included in the peer review of the Background Document for the Human Exposure and Human Risk Modules for the 3MRA Model (U.S. EPA, 2000e).

Peer Reviewers for Human Exposure Module

- Dr. James Butler of Argonne National Laboratory
- Dr. William Kastenberg of the University of California at Berkeley
- Mr. Stephen Washburn of ENVIRON International Corporation

4.9.1 Module Description

The Human Exposure Module calculates the applied dose to human receptors from ingestion and inhalation of contaminated media and food. Figure 4-13 shows the information flow for the Human Exposure Module. The Human Exposure Module uses media and food concentrations calculated in the media and food web modules to calculate applied doses. These doses are used by the Human Risk Module to calculate risk measures.

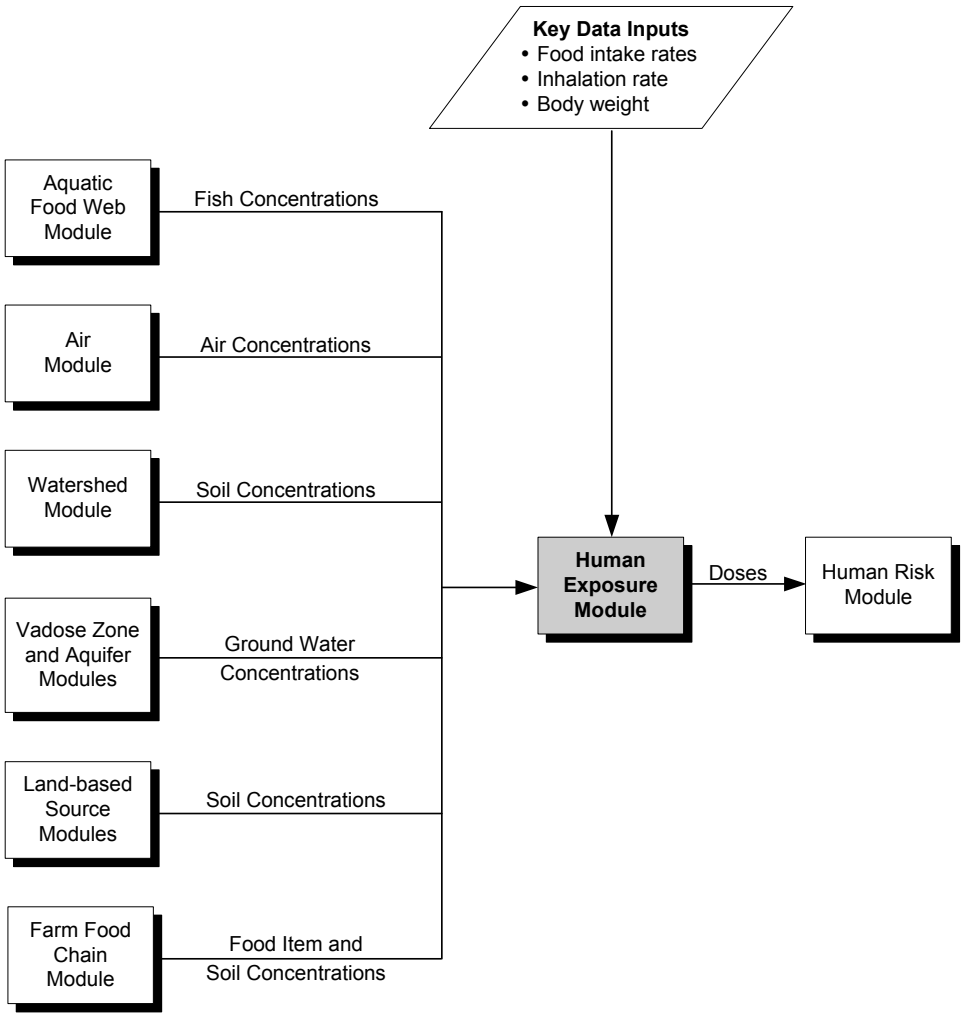

Figure 4-13. Information flow for the Human Exposure Module in the 3MRA modeling system.

4.9.2 Major Module Components/Functionality

The purpose of the Human Exposure Module is to calculate the inputs needed by the Human Risk Module to calculate risk and hazard. For carcinogens, risk is calculated from applied dose (in mg/kg-d). For noncarcinogens, hazard via the ingestion pathway is also based on dose, whereas hazard via the inhalation pathway is based on the air concentration to which a receptor is exposed. Thus, the Human Exposure Module has the following functions:

1. **Calculate ambient air concentrations.** The Human Exposure Module calculates areal average ambient air concentrations for farms. Ambient (outdoor) air concentrations for residents are calculated by the Air Module and used by the Human Exposure Module.

2. **Calculate shower air concentration.** The Human Exposure Module calculates shower air concentration from ground water concentration. Ambient air concentrations are calculated by the Air Module.

3. **Calculate dose from inhalation of carcinogens.** The Human Exposure Module calculates dose from inhalation of ambient (outdoor) air and shower air for carcinogens. Noncarcinogenic risk for inhalation exposures is based directly on air concentration, not dose; thus, the Human Exposure Module does not calculate inhalation dose for noncarcinogens.

4. **Calculate dose from ingestion of contaminants in media or food.** The Human Exposure Module calculates dose for carcinogens and noncarcinogens from ingestion of soil, ground water, produce (fruits and vegetables), beef, milk, and fish.

5. **Calculate dose from ingestion of contaminants in breast milk.** The Human Exposure Module calculates dose to infants from ingestion of contaminated breast milk. This route of exposure is assessed only for dioxin-like chemicals and only for infants.

Doses and air concentrations are calculated for each contaminant and site, as well as for each

- **Receptor type.** The module calculates exposures for two types of human receptors: residents and farmers. These are distinguished by how they are located—residents at a single exposure point and farmers on an area representing a farm. Residents are further defined by various kinds of behavior that lead to different profiles of exposure, such as home gardening and recreational fishing. Farmers may also be defined by behavior such as recreational fishing. Human receptor types considered in the 3MRA modeling system are a function of the goals of a particular analysis and are defined by the receptor data used for the analysis.

- **Age cohort.** The human receptors are divided into five age cohorts (infants under 1 year, children aged 1 to 5 years, children aged 6 to 11 years, children aged 12 to 19 years, and adults) that are used to determine the most appropriate exposure factor data for various pathways, such as body weights, inhalation rates, and consumption rates for various food products.

- **Exposure pathway.** The Human Exposure Module considers nine exposure pathways. Depending on the exposure inputs entered into the model, all pathways could be considered for all receptor types. Table 4-18 shows the pathways modeled and indicates which receptor types are modeled for each pathway by default. All pathways are modeled by default for all age cohorts with two exceptions: the breast milk pathway is modeled only for infants (and no other pathways are modeled for infants), and shower inhalation is modeled only for children aged 12 to 19 years and adults.

Table 4-18. Default Pathways Considered by Receptor Type

	Receptor Type							
Pathway	**Resident**	**Resident Fisher**	**Home Gardener**	**Home Gardener Fisher**	**Beef Farmer**	**Beef Farmer Fisher**	**Dairy Farmer**	**Dairy Farmer Fisher**
Air inhalation	✓	✓	✓	✓	✓	✓	✓	✓
Shower inhalation	✓[a]	✓[a]	✓[a]	✓[a]	✓	✓	✓	✓
Ground water ingestion	✓[a]	✓[a]	✓[a]	✓[a]	✓	✓	✓	✓
Soil ingestion	✓	✓	✓	✓	✓	✓	✓	✓
Produce ingestion			✓	✓	✓	✓	✓	✓
Beef ingestion					✓	✓		
Milk ingestion							✓	✓
Fish ingestion		✓		✓		✓		✓
Breast milk ingestion	✓	✓	✓	✓	✓	✓	✓	✓

[a] Ground water and shower pathways are considered for residents and home gardeners only if Census data indicate the presence of private wells in the Census block group. All farms are assumed to have a private well.

- **Location.** The Human Exposure Module calculates exposures for residents for a single point, placed in the current data set at the centroid of each Census block in the area of interest (AOI). The module calculates exposure for farmers at a single farm in each census block group in the AOI that has Census data for farmers and agricultural land areas.

- **Year.** The module calculates exposures for each year of the simulation. The exposures predicted by the Human Exposure Module are reported as a time series of annual average applied doses or air concentrations. Thus, the equations presented in this section are applied to input data for each year. All temporal averaging for exposure durations exceeding 1 year is done by the Human Risk Module.

4.9.3 Summary of Verification

The Human Exposure Module was verified through a series of verification steps that are described in detail in the following documents:

- *Test Plan for the HWIR Human Exposure Module* (RTI, 2000e).
- *HWIR Human Exposure Module Internal Verification Testing* (U.S. EPA, 2000a).

The scope of the testing was to verify all major requirements of the Human Exposure Module. The internal verification included hand-calculation verification of internal calculations, as well as visual examination of the GRF to verify that certain switches work as designed. Table 4-19 summarizes the functional requirements and number of test cases executed to verify the Human Exposure Module.

Table 4-19. General Requirements for Testing the Human Exposure Module

Step	Description	Number of Test Cases
1	Correctly recognize the presence of farms and residential receptor areas and correctly calculate inhalation (non-shower) and ingestion (food, soil, water) doses	5
2	Correctly recognize and differentiate contaminants that are only carcinogenic, contaminants that are only noncarcinogenic, and contaminants that are both carcinogenic and noncarcinogenic, output the appropriate variables, and correctly calculate inhalation (nonshower) and ingestion (food, soil, water) doses	3
3	Correctly calculate and assign exposures per receptor, cohort, and exposure area	5
4	Correctly process continuous and discontinuous time series of varying length per pathway	1
5	Correctly calculate shower concentrations and inhalation doses by means of a dynamic solution to a system of differential equations	1
6	Correctly assign shower concentrations and inhalation doses only to adults and child 4 cohorts	1
7	Correctly assign and compute breastmilk ingestion doses only to Child 1 (infant) cohorts	1
8	Correctly perform random selection of 3 fishable waterbody reaches for farmer fishers and resident fishers and calculate doses from fish ingestion	2
9	Correctly recognize and respond to error/warning traps	3

A series of test cases was developed to test these requirements. The Human Exposure Module was tested using a variety of contaminants and site layouts (e.g., sites with and without fishable reaches, sites without any farms, sites without residential receptors). A variety of contaminants (e.g., pentachlorophenol, acetonitrile, toluene, 2,3,7,8-TCDD, mercury, chloroform, carbon disulfide, and benzene) were tested, because the decision to perform certain calculations depends on whether the contaminant is a carcinogen or a noncarcinogen or has an

inhalation and/or oral health benchmark available; breastmilk ingestion doses are calculated for infants only for 2,3,7,8-TCDD.

The verification testing of the Human Exposure Module was based on the doses and concentrations reported to the output file. All food (total vegetable and fruit, beef, milk, fish), breastmilk, ground water, and soil ingestion doses and ambient air (non-shower) and shower inhalation concentrations and doses calculated for each appropriate receptor/cohort by the Human Exposure Module matched the independently calculated values in Excel spreadsheets. Existing error traps operated as expected.

All decision points, functions, and contaminant-specific switches required of the Human Exposure Module were adequately tested to confer a high degree of confidence in the module's ability to correctly calculate ingestion and inhalation doses. The combination of basic mathematics and the selection of a diverse group of contaminants and site layouts provides a sufficient basis to conclude that the verification was successful.

4.9.4 Summary of Validation

The Human Exposure Module has not been validated because no data set exists to do so. However, the module is based on widely accepted state-of-the-science formulations.

4.10 Human Risk Module

This section describes the verification and validation activities for the Human Risk Module. The Human Risk Module was reviewed by the external reviewers shown in the box.

Peer Reviewers for Human Risk Module

- Dr. James Butler of Argonne National Laboratory
- Dr. William Kastenberg of the University of California at Berkeley
- Mr. Stephen Washburn of ENVIRON International Corporation

4.10.1 Module Description

The Human Risk Module calculates risk measures for a given contaminant, waste concentration, and site. Figure 4-14 shows the information flow for the Human Risk Module.

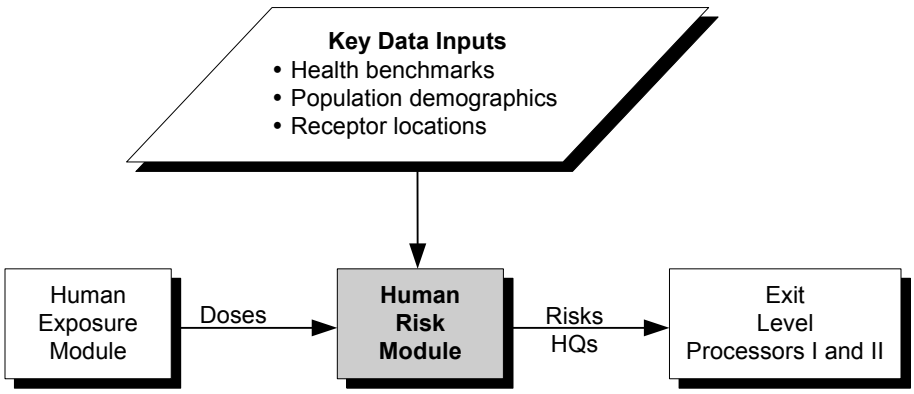

Figure 4-14. Information flow for the Human Risk Module in the 3MRA modeling system.

The Human Risk Module uses the annual average daily doses calculated in the Human Exposure Module to calculate risk statistics. These risk statistics are used by the Exit Level Processors to determine national-level risk distributions.

4.10.2 Major Module Components/Functionality

For each contaminant, waste concentration, and site, the Human Risk Module generates risk estimates for each receptor location in the AOI and then calculates the number of receptors that fall within a specified risk or hazard range to describe the distribution of risks for the population at each site. The module also determines the timing of maximum risks. The Human Risk Module has the following functions:

1. **Calculate risk measures.** The Human Risk Module calculates cancer risk, noncancer hazard quotient (HQ), and noncancer margin of exposure (MOE) (for breastfeeding infants only). Depending on the contaminant, the Human Risk Module may calculate risk, HQ, or both. MOE is only calculated for breastfeeding infants for dioxin-like chemicals. These risk measures are specific to a receptor type, an age cohort, an exposure pathway, a receptor location, and a specific exposure period (identified by starting year). The Human Risk Module also aggregates risks and HQs from individual exposure pathways (e.g., ground water ingestion) to determine risk for groups of pathways (e.g., all ingestion pathways).

2. **Process results for decision making.** The Human Risk Module puts exposed and unexposed population into risk bins to estimate the number of receptors that experience risk within a specified range. Each risk bin is a range of risks or HQs. For any given pathway and exposure period, the Human Risk Module uses Census data on population for each receptor location to determine the number of people of each receptor type and age cohort that experience risk from the specified pathway in the specified exposure period at risk levels within that bin. Population is summed across receptor locations that have risks within the same bin. For each pathway or pathway group, the Human Risk Module estimates total risk by multiplying the population at a location by the risk for that location and uses this to determine the exposure period for which the total risk or HQ across all receptor types and age cohorts is the greatest. This estimate of total risk is not intended as a final risk measure but is used to identify the timing of maximum risk. The exposure period is identified by the year in which the risk averaged over a specified exposure period starts.

4.10.3 Summary of Verification

The Human Risk Module was verified through a series of verification steps that are described in detail in the following document:

- *Draft Test Plan for the HWIR Human Risk Module* (U.S. EPA, 2000e)

The scope of the testing was to verify all major requirements of the Human Risk Module. Table 4-20 summarizes the functional requirements and number of test cases executed to verify the Human Risk Module.

Table 4-20. General Requirements for Testing the Human Risk Module

Step	Description	Number of Test Cases
1	Correctly calculate risk, hazard quotient (HQ,) and MOE for appropriate receptor, cohort, pathway, and distance ring	1
2	Correctly calculate total population for any receptor, cohort, distance, pathway combination	1
3	Correctly find critical year for risk/HQ/MOE for any receptor, cohort, distance, pathway combination	1
4	Correctly detect whether the contaminant is carcinogenic, noncarcinogenic, or both; whether the carcinogenic and noncarcinogenic effects are additive; and whether a human risk assessment is to be done	1
5	Correctly develop risk/HQ/MOE histograms for aggregate pathways	1
6	Correctly respond to NumFarm or NumHumRcp	1
7	Correctly respond to ChemBreastMilkExp switch (MOE)	1
8	Correctly respond to ExDur	1
9	Correctly respond to RegPercentile criterion	1
10	Correctly age child cohorts during exposure periods so that cohort-specific, varying exposures are considered	1
11	Report an error message if a farm index or a human receptor index is not used in any ring or if a farm index or human receptor index refers to an undefined farm or human receptor	1
12	Report an error message if an the human receptor point is not defined	1
13	Report an error message if too many or too few arguments are set in the Arguments environment variable or if the Arguments variable has files out of order	1
14	Report an error message for a number of consistency checks of the site layout information	1

The Human Risk Module was tested using a variety of contaminants and a simple site layout that included two distance rings and all receptor types. A variety of contaminants were tested, because the decision to perform certain calculations depends on whether the contaminant is a carcinogen or a noncarcinogen or has an inhalation and/or oral health benchmark available; breastmilk MOEs are calculated for infants only for 2,3,7,8-TCDD.

The internal verification included hand-calculation verification of calculations. For some requirements, EPA created an Excel spreadsheet to reproduce the intended functionality. The results calculated by hand and by the spreadsheet were compared with those from the module runs to ensure that all equations were coded properly and that the module was fully functional. All cumulative frequency distributions calculated by the Human Risk Module matched the values calculated by hand or using the spreadsheet. Consequently, it was concluded that the module correctly manages all requirements listed above.

4.10.4 Summary of Validation

The Human Risk Module can not be validated because no data set on human risk values exists.

4.11 Ecological Exposure Module

This section provides a summary of verification and validation efforts relating to the Ecological Exposure Module. The Ecological Exposure Module was reviewed by the external reviewers shown in the box.

Peer Reviewers for Ecological Exposure Module

- Dr. Anne Fairbrother of Parametrix, Inc.
- Dr. Lawrence Kapustka of Ecological Planning and Toxicology, Inc.
- Dr. Robin Matthews of Western Washington University
- Dr. Bradley Sample of CH2M Hill

4.11.1 Module Description

The Ecological Exposure Module calculates the applied dose (in mg/kg-d) to ecological receptors that may be exposed to contaminants via ingestion of contaminated plants, prey, and media (i.e., soil, sediment, and surface water). The Ecological Exposure Module uses input concentrations from the Surface Impoundment, Surface Water, Terrestrial Food Web, and Aquatic Food Web Modules. Figure 4-15 shows the information flow for the Ecological Exposure Module.

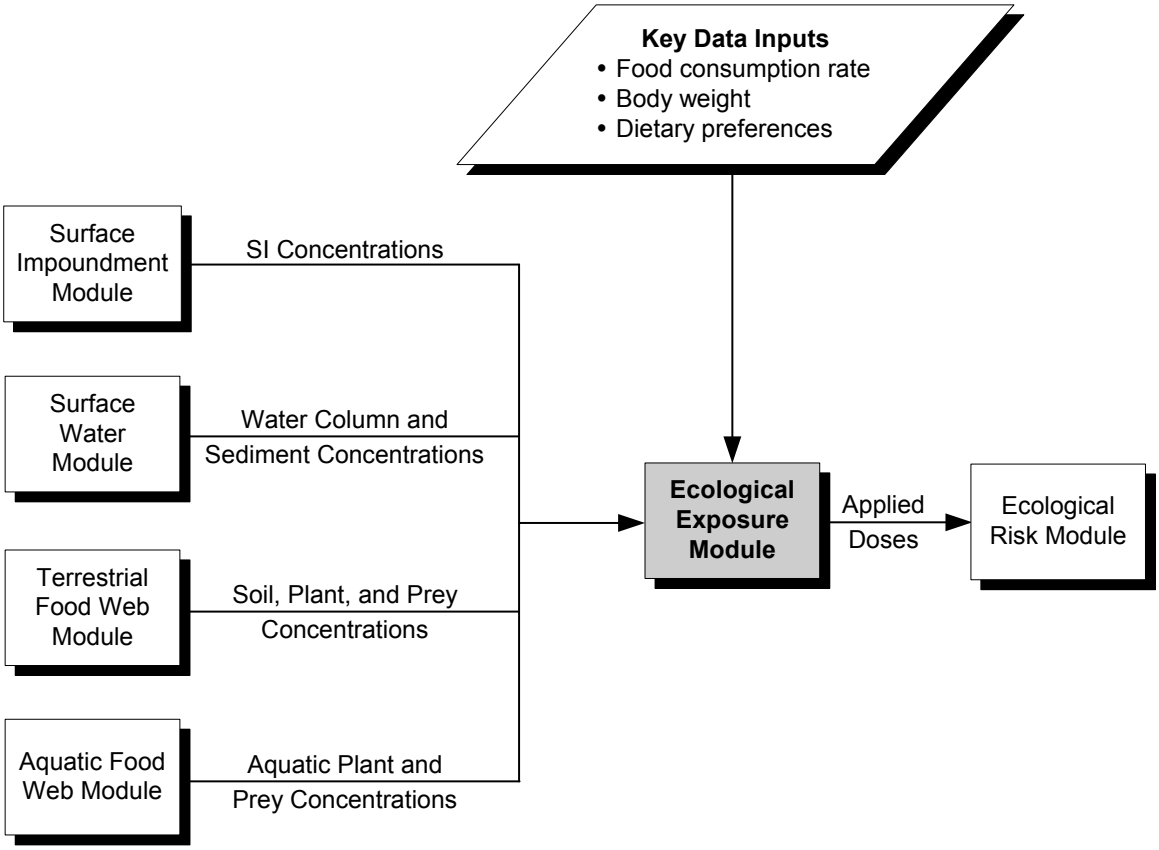

Figure 4-15. Information flow for the Ecological Exposure Module in the 3MRA modeling system.

The methodology and equations used to calculate the applied dose to mammals and birds assigned to habitats within the AOI are consistent with the principles and guidelines described in the *Guidelines for Ecological Risk Assessment* (U.S. EPA, 1998a). The basic forms of these equations have been used by OSW and other EPA programs to predict applied doses in a variety of ecological risk analyses, and they are similar to the exposure equations recommended by other non-EPA risk assessors (see, for example, the *Methods and Tools for Estimation of the Exposure of Terrestrial Wildlife to Contaminants*, Sample et al., 1997).

4.11.2 Major Module Components/Functionality

The Ecological Exposure Module performs the following three functions:

1. **Construct a dietary matrix for each receptor for each habitat in the AOI.** The Ecological Exposure Module creates a diet for each ecological receptor based on dietary preferences.

2. **Calculate applied doses for animals in terrestrial habitats.** Using the dietary matrix and the media,[2] plant, and prey concentrations calculated by the Terrestrial Food Web Module, the Ecological Exposure Module calculates applied doses for each avian and mammalian receptor species assigned to terrestrial habitats in the AOI.

3. **Calculate applied doses for animals in margin habitats (wetland or waterbody).** Using the dietary matrix and the media,[1] plant, and prey concentrations calculated by the Aquatic Food Web and Terrestrial Food Web Modules, the Ecological Exposure Module calculates applied doses for each avian and mammalian receptor species assigned to margin habitats in the AOI.

4.11.3 Summary of Verification

The Ecological Exposure Module was verified through a series of verification tests that are described in detail in the following documents:

- *Ecological Exposure (EcoEx) Module—Test Plan* (RTI, 2002g)
- *Ecological Exposure Module Internal Verification Testing* (RTI, 2002h).
- *Independent Tests for Ecological Exposure Module* (Tetra Tech, 2000b).

EPA originally completed internal verification testing in 2000, followed by external verification testing. Since then, EPA has made a few minor changes to the module. Therefore, EPA repeated internal verification testing on the updated version of the module in 2002 to ensure that the updated version passed all tests and that the test files reflected the outputs from the updated version of the module. EPA also updated internal verification test plans and testing documentation to reflect this second round of testing.

[2] Contaminant concentrations in surface impoundments may also be used to calculate exposure if the receptor's home range overlaps the impoundment.

In order to verify that the module processed the data correctly, EPA created an Excel spreadsheet using the equations from the module documentation. The testing included confirmation that the module correctly calculates the applied doses to mammals, birds, and herpetofauna for all relevant years (i.e., years with nonzero concentrations and media, plants, or prey) during the simulation period. The applied doses calculated with the spreadsheet were compared to those from the module runs to verify that the equations were coded properly and that the module was fully functional.

Table 4-21 summarizes the functional requirements and number of test cases executed to verify the Ecological Exposure Module.

Table 4-21. General Requirements for Testing the Ecological Exposure Module

Step	Description	Number of Test Cases
1	Correctly read output files from the Terrestrial Food Web, Aquatic Food Web, Surface Water, and Source modules	3
2	Correctly read site layout file	3
3	Correctly calculate the applied dose to mammals, birds, and herpetofauna in both aquatic (e.g., stream margin) and terrestrial habitats	3
4	Correctly assign prey preferences to all elements in the food web	3
5	Correctly loop over receptors	3
6	Correctly loop over habitats	2
7	Correctly loop over years and ensure correct time series management	1
8	Correctly select prey concentrations for each receptor	1
9	Correctly read the chemical properties and surface water data associated with methyl mercury when multiple chemical species of mercury are present	1

4.11.4 Summary of Validation

The Ecological Exposure Module has not been validated because no adequate data set exists to do so. However, the module is based on generally accepted science-based formulations.

4.12 Ecological Risk Module

This section provides a summary of verification and validation efforts for the Ecological Risk Module. The Ecological Risk Module was reviewed by the reviewers shown in the box.

Peer Reviewers for Ecological Risk Module

- Dr. Anne Fairbrother of Parametrix, Inc.
- Dr. Lawrence Kapustka of Ecological Planning and Toxicology, Inc.
- Dr. Robin Matthews of Western Washington University
- Dr. Bradley Sample of CH2M Hill

4.12.1 Module Description

The Ecological Risk Module calculates the HQ for species of mammals, birds, and herpetofauna and, through inference, for communities of organisms that live in close contact with soil (including plants and soil invertebrates), sediment (benthic invertebrates), and surface water (e.g., fish, aquatic invertebrates, algae, and aquatic plants). The HQ is the ratio of the annual average environmental exposure (in units of concentration or dose) to a benchmark for ecological effects (in units of concentration or dose) and quantifies the potential for contaminants to elicit an adverse ecological response once released into the environment. To calculate the HQs, the Ecological Risk Module uses input concentrations from the Surface Water and Terrestrial Food Web Modules, as well as applied doses calculated by the Ecological Exposure Module, and compares those values to ecotoxicological benchmarks (EBs, in units of dose) and chemical stressor concentration limits (CSCLs, in units of concentration), as appropriate. The module calculates an HQ for every ecological receptor assigned to habitats within the AOI for a given site. Figure 4-16 shows the information flow for the Ecological Risk Module.

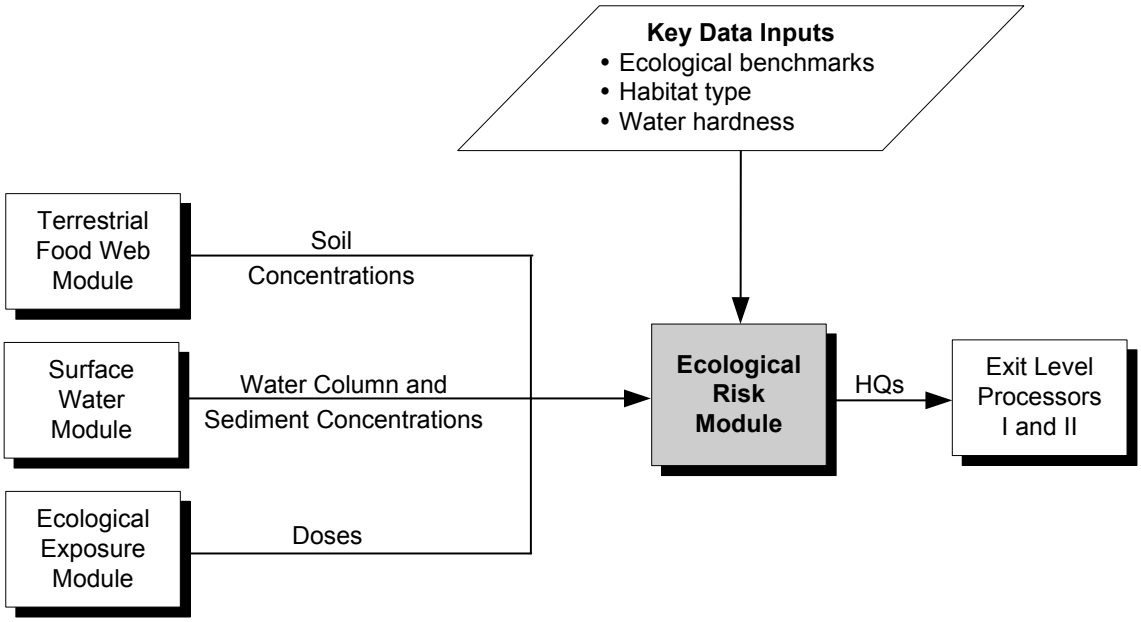

Figure 4-16. Information flow for the Ecological Risk Module in the 3MRA modeling system.

The conceptual approach to characterizing the potential for adverse ecological effects depends on the assessment endpoints used. Assessment endpoints are explicit expressions of the actual environmental values that are to be protected (U.S. EPA, 1998a). Candidates for assessment endpoints often include threatened or endangered species, functional attributes that support food sources or flood control, or aesthetic values such as the existence of charismatic species (e.g., eagles) that have special value to society (U.S. EPA, 1998a). The assessment endpoints must be defined with respect to the valued ecological entity (e.g., a particular species), and an attribute of that entity that is to be protected (e.g., reproductive fitness). For the 3MRA modeling system, the assessment endpoints were selected to represent multiple levels of biological organization (e.g., populations, communities), key functional elements of natural

communities (e.g., primary producers), and biota throughout the trophic continuum. Although the 3MRA modeling system does not restrict the selection of assessment endpoints for future applications, the Ecological Risk Module and supporting databases were developed to evaluate three primary assessment endpoints:

- Survival of species that comprise key structural and functional elements of soil, freshwater, and benthic (sediment) communities;
- Reproductive fitness and survival of mammalian, avian, and herpetofaunal wildlife populations; and
- Growth and survival of primary producers (e.g., plants) in terrestrial and freshwater systems.

These endpoints are ecologically relevant to the habitat types used to represent ecological variability in the 3MRA modeling system and are sensitive to a broad range of chemical stressors.

4.12.2 Major Module Components/Functionality

The Ecological Risk Module performs two major functions:

1. **Calculate Hazard Quotients (HQs).** The Ecological Risk Module calculates HQs for each receptor at each site according to spatial, temporal, and environmental characteristics of the site.
2. **Process the HQ Results for Decision Making.** The Ecological Risk Module tracks various attributes such as taxa and habitat type to process the HQ results for decision making. This processing includes placing results in bins and determining the timing of maximum risks.

4.12.3 Summary of Verification

The Ecological Risk Module was verified through a series of verification tests, which are described in detail in the following documents:

- *Ecological Risk Module—Test Plan* (RTI, 2002j)
- *Ecological Risk Module Internal Verification Testing* (RTI, 2002i)
- *Independent Tests for Ecological Risk Module* (Tetra Tech, 2000c).

EPA originally completed internal verification testing in 2000, followed by external verification testing. Since then, EPA has made a few minor changes to the module. Therefore, EPA repeated internal verification testing on the updated version of the module in 2002 to ensure that the updated version passed all tests and that the test files reflected the outputs from the updated version. EPA also updated internal verification test plans and testing documentation to reflect this second round of testing.

To verify that the module processes the data correctly, EPA created an Excel spreadsheet and an Access database using the equations from the module documentation. The testing included confirmation that the module (1) correctly calculates HQs for ecological receptors for all relevant years (i.e., years with nonzero concentrations) during the simulation period, and (2) correctly creates cumulative frequency distributions for each of the ecological risk attributes considered by the module (e.g., receptor group, habitat type, distance). The HQs calculated by the spreadsheet and database were compared with those from the module runs to ensure that the equations were coded properly and that the module was fully functional.

Table 4-22 summarizes the functional requirements and test cases executed to verify the Ecological Risk Module.

Table 4-22. General Requirements for Testing the Ecological Risk Module

Step	Description	Number of Test Cases
1	Correctly read output files from the Surface Water, Terrestrial Food Web, and Ecological Exposure modules	2
2	Correctly identify the constituent type as dioxin-like, organic, metal, mercury, or special	2
3	Correctly read site layout file	2
4	Correctly calculate average sediment and surface water concentrations for each aquatic habitat delineated at the site	2
5	Correctly adjust ecological benchmarks according to site-based conditions (e.g., water hardness) and constituent type	2
6	Correctly calculate the hazard quotients for each ecological receptor and identify the max HQ and associated risk attributes (e.g., receptor group) for each site	2
7	Place the HQ values in the correct bins by risk attribute and build cumulative frequency distribution	2
8	Correctly loop over receptors	2
9	Correctly loop over habitats	2
10	Correctly loop over years to ensure correct time series management	1
11	For mercury, correctly select the chemical species based on the receptor, and read the chemical properties and surface water data associated with that species	2

All cumulative frequency distributions calculated by the Ecological Risk Module matched the values calculated using the spreadsheet and database. Consequently, it was concluded that the module correctly manages all requirements listed above.

4.12.4 Summary of Validation

Modules like the Ecological Risk Module are very difficult to validate because of lack of useful data for validation purposes. We have not found any data set suitable for the validation of this module.