2.0 Overall Approach to Ensuring Quality of the 3MRA Modeling System

EPA designed the 3MRA modeling system to be scientifically defensible. To address comments with regard to scientific defensibility, which included recommendations for peer review, the Agency implemented specific steps to build confidence in the system and ensure that the system would produce a reasonable estimate of nationwide risk for a national-level assessment. These activities are described below:

> **Verification and Validation**
>
> **Verification** refers to activities that are designed to confirm that the mathematical framework embodied in the module is correct and the computer code for a module is operating according to its intended design so that the results obtained using the code compare favorably with those obtained using known analytical solutions or numerical solutions from simulators based on similar or identical mathematical frameworks. Or that the data were properly developed based on the methods selected for their generation. For the module code, verification activities would include taking steps to ensure that code was properly maintained, modified to correct errors, and tested across all aspects of the module's functionality. For data generation, example of verification activities include, determining whether data definitions (distributions, ranges) in the database match the data definitions in the 3MRA modeling system technical background documents.
>
> **Validation** is conducted after the verification step. It refers to activities that confirm that the design of a module provides an accurate representation of the physical processes it is intended to simulate, or that the data are accurate and complete. For a module, validation might include comparing simulation results with field data or results from other established models if field data are unavailable. For data generation, validation might include comparing modeling data for a site with site-specific data for that location obtained from a site visit or previously collected data.

1. **Peer Review.** The overall technical approach and each science-based module included in the 3MRA modeling system were peer reviewed. Teams of peer reviewers (at least three per module) provided critical feedback about the science-based modules. More than 45 independent experts reviewed the science modules to ensure that the theoretical concepts describing the processes within the release, fate, transport, uptake, exposure, and risk components were adequate representations of the processes to be evaluated. The peer review process is described in Section 2.2.5.

2. **Verification.** All software components and databases underwent a series of tests to verify that the software and data were performing properly. At the heart of this protocol was the requirement that each component of the modeling system include a designed and peer-reviewed test plan that was executed by both the

module developer and a completely independent modeler (i.e., someone who did not participate in the original module development). These procedures, test plans, test packages, and test results are fully documented and available to the public. The underlying concept of the verification methodology is that if tests are designed to challenge all subroutines, and if decision points in the module and calculations can be duplicated independently of the module, then it can be concluded that the testing is complete and successful. In addition, the methodology was predicated on the premise that the looping functions need not be tested on hundreds of values of the looping parameter. Confirmation of calculations for a small subset of values demonstrates that the looping functions in the module are working as intended. Sections 4, 5, and 6 summarize the verification activities for, respectively, the modules, the site-based data, and the models used to estimate some of the chemical properties.

3. **Validation.** True validation of the 3MRA modeling system for a national application would require validation over the full range of environmental settings that are relevant to the application. However, determining whether the modeling system is valid for the full range of settings is not possible: data sets exist that allow components of the 3MRA modeling system to be validated, but none were found that would allow validation of the complete and integrated multimedia risk assessment. Individual modules and data sets were validated if appropriate data were available. However, instead a comparison study is being conducted using environmental monitoring field data for mercury from an actual industrial site. These data represent the relationship between contaminant source and environmental concentrations; however, the data set is incomplete. This comparison is ongoing; its current status is described in Section 3. The validation efforts for the individual modules, the site-based data, and the chemical properties estimation models are described in Sections 4, 5, and 6, respectively.

4. **Model Comparison Study.** The 3MRA modeling system as a whole is undergoing a comparison analysis with EPA's Total Risk Integrated Methodology (TRIM), which is currently under development. The objective of the model comparison effort is to increase confidence that the 3MRA modeling system produces estimates consistent with other multimedia models. This comparison is ongoing; its current status is described in Section 3.

5. **Representative National Data Set.** A comprehensive data collection approach was developed to parameterize the modeling system for 201 sites in accordance with the site-based approach described in Volume II. The data collection plan described the general collection methodology for the major types of data (for example, facility location, land use, soil characteristics, and receptor locations), including quality assurance and quality control procedures and references for data sources. The resulting data set was used for the modeling system evaluation efforts. The data collection approach for the representative national data set is described in more detail in Volume II.

6. **Sensitivity and Uncertainty Analyses.** As the level of assessment complexity grows, it becomes both more difficult and more important to establish comprehensive and quantitative expressions of uncertainty. Uncertainty analysis is a relatively undeveloped scientific discipline for high order models such as the 3MRA modeling system. Thus, a formal program focusing on sensitivity and uncertainty analysis for high-order modeling systems was initiated by EPA. The initial focus of this program is the investigation of parameter sensitivities and system uncertainties within the 3MRA modeling system. A Supercomputer for Model Uncertainty and Sensitivity Evaluation (SuperMUSE), comprising 160 PCs, was developed to allow exhaustive experimentation with the 3MRA modeling system in Monte Carlo mode. The modeling system is suited to facilitate this new generation of uncertainty analysis and tool development. These efforts are not only laying a sound foundation for this research but also the sensitivity work effort so far has helped in ensuring quality of the modeling system. These analyses are ongoing; its current status is described in more detail in Volume IV.

Figure 2-1 provides an overview of the quality assurance approach for the 3MRA modeling system. The rest of this section provides an overview of verification and validation for the overall system (Section 2.1), the modules (Section 2.2), the site-based data (Section 2.3), and the chemical properties data (Section 2.4).

2.1 Verification and Validation of the 3MRA System

After the development of the components of the 3MRA modeling system, the first step was the verification and validation of each component individually. After components satisfied those tests, they were placed in the complete 3MRA modeling system to confirm their functionality in the context of the whole system. These system integration tests required that components operate correctly while executing within the full system context, that is, running the full set of 3MRA modeling system site/waste management unit combinations for the contaminants of interest and the iterations of the Monte Carlo simulation. The 3MRA representative national data set of 201 sites, executed within a Monte Carlo simulation, tested the robustness of science models in a manner not previously possible. Even legacy codes that had more than a decade of wide use experienced environmental conditions that caused unstable numerical solutions.

The system integration tests were initially conducted on single PCs. Computer time for the 3MRA modeling system was typically on the order of a few minutes per site-based simulation. Thus, a single PC might run continuously for several days before completing a simulation for all combinations of sites and WMUs related to a single contaminant. When runs for multiple contaminants were required, several PCs were used, each running a subset of the full list of required simulations. However, with the ready availability of faster PCs with more and faster memory, the runtimes are expected to be shorter. Recently, the EPA has developed software for distributing the computational load across the Super-computer for Model Uncertainty and Sensitivity Evaluation (SuperMUSE) cluster and retrieving output files. While the SuperMUSE was intended as a research tool for investigating uncertainty and sensitivity related to the 3MRA modeling system, it also serves as a final testing ground for the software

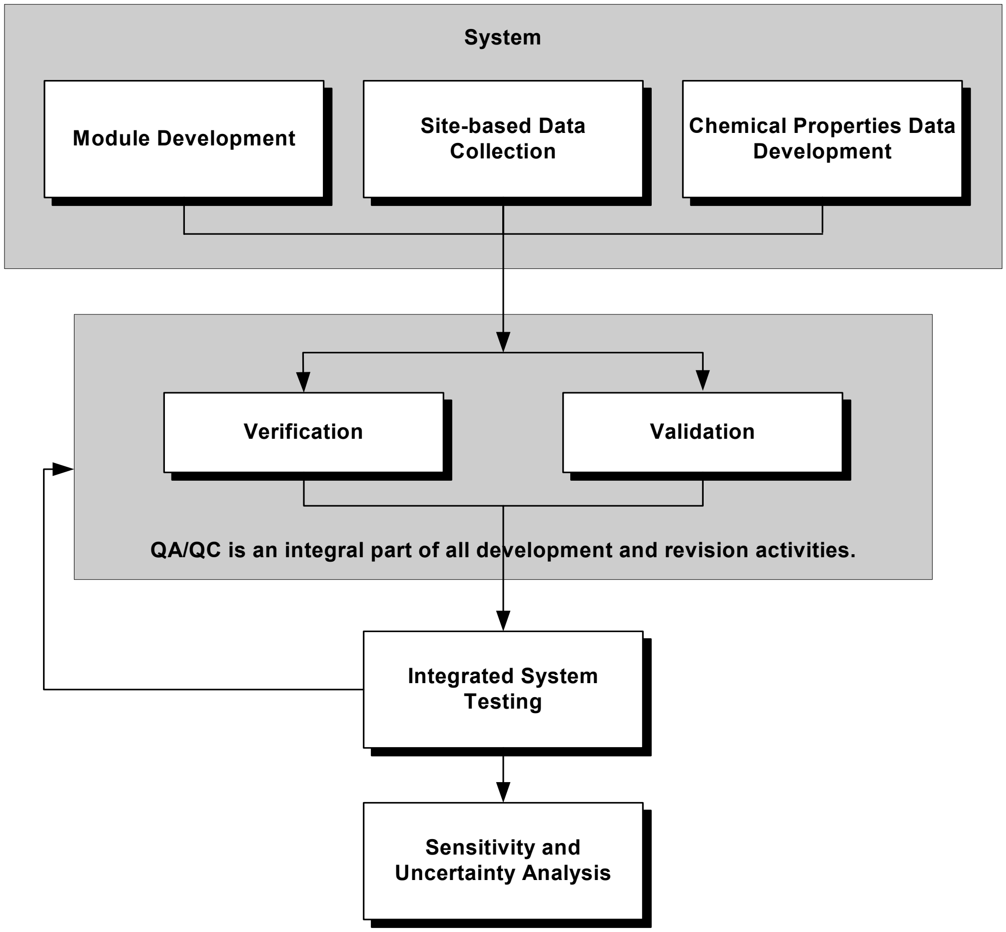

Figure 2-1. Overall approach to ensure the quality of the 3MRA modeling system.

itself. Before Version 1.0 of the 3MRA modeling system was released, the SuperMUSE had successfully executed on the order of one million individual 3MRA modeling system simulations.

2.2 Verification and Validation of the Modules

Some of the 3MRA modules have been adapted from established legacy codes, which have undergone extensive public review, been tested and validated, and been used in rulemakings. They include the Air Module (ISCST3), the Vadose Zone and Aquifer Modules (EPACMTP), and the Surface Water Module (EXAMS). Other modules were developed based on sound science, established methodologies, and accepted QA/QC procedures. Some of those modules also use components of established codes (e.g., the Wastewater Source Modules use CHEMDAT8 and EPACMTP). All modules were subjected to a consistent verification and testing process (see Figure 2-2). The verification steps included

1. **Concept Review and Code Design.** The module conceptual design was discussed among the project team members, developed, and reviewed. The conceptual design included a determination of the module's purpose, essential

functionality, and inputs and outputs. Pseudocode was developed based on the conceptual design and reviewed by senior project team members. Concept review and code design are discussed in more detail in Section 2.2.1.

2. **System-Level Control of Module Input and Output Definitions.** Most module data inputs and outputs are managed by the 3MRA Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES). The system design imposed specific requirements for data definition to ensure that each input and output variable was defined and used consistently with respect to data type, acceptable range, and units. Input and output control is discussed in more detail in Section 2.2.2.

3. **Version Control of Module Code.** The program code for each module went through numerous updates during development and refinement to address errors or add functionality. EPA used version control software to maintain a record of program code updates and to ensure that the latest version of the code was used to generate new executable files. Version control is discussed in more detail in Section 2.2.3.

4. **Preliminary Testing.** Once the code for a module was fully developed, module developers conducted preliminary tests on each module individually to determine whether the code was functioning as expected. In general, these internal tests, which were not documented, were used to identify and resolve errors in the code. Code testing is discussed in more detail in Section 2.2.4.

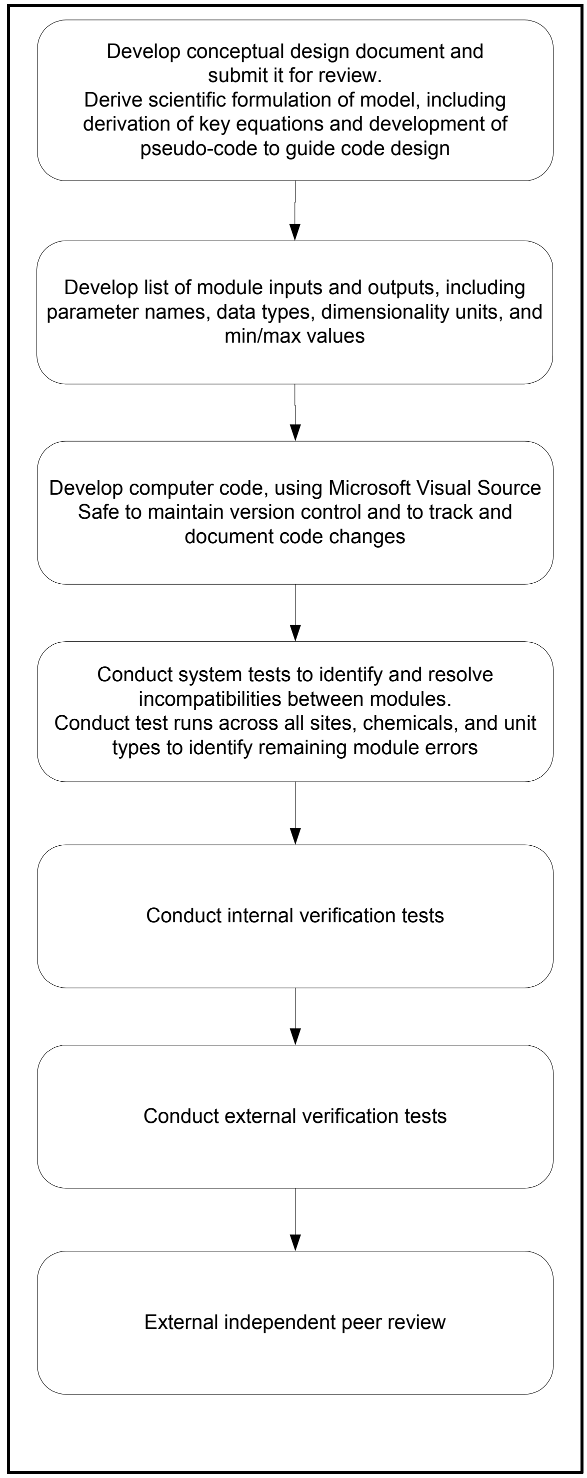

Figure 2-2. Overview of 3MRA module development process.

5. **Preliminary System Tests and Production Runs.** When the code for all modules and the system-level software were complete and data sets were available, EPA ran the complete system, noted module errors, maintained a list of errors generated by this testing, and tracked new versions of modules or data that resolved these errors. Code testing is discussed in more detail in Section 2.2.4.

6. **Internal Verification Testing.** For each module, the module developers developed and implemented a module test plan to rigorously determine whether the program was functioning as designed. External project team members reviewed test plans prior to implementation. This testing usually involved independent verification of calculations. For some modules, internal verification testing included limited sensitivity analysis to determine if the module responded as expected to changes in specific input parameters. The inclusion of such sensitivity analyses varied by module, based on the judgment of the test plan developer. Code testing is discussed in more detail in Section 2.2.4.

7. **External Verification Testing.** For each module, external project team members repeated the internal verification testing to confirm that the modules operated as expected. Code testing is discussed in more detail in Section 2.2.4.

8. **External, Independent Peer Review.** EPA documented the conceptual design and calculations for each module in background documents, which were independently peer reviewed. The module developers reviewed the peer review comments; based on these comments, the module developer, in conjunction with EPA, determined whether a model change was needed to address the comment, and, if so, revised the module. Where necessary, internal verification testing was repeated to verify that the module passed all tests and to ensure that test packages reflected the latest versions of the executable code and of the input and output data files. The peer review process is discussed further in Section 2.2.5.

The steps related to the module design, input/output control, code version control, code testing, and peer review are described in more detail below.

2.2.1 Concept Review and Code Design

Initially, EPA developed and documented the conceptual design and scientific basis for each module for review and discussion by the project team. The documentation generally included a description of the module, background information supporting the module design, key assumptions in the module development, and the mathematical formulation of the module and relevant derivations. The module documentation became the basis for pseudocode that described how the computer program for the module would be designed. The programmers then used the pseudocode to develop the operating code for the module.

2.2.2 System-Level Control of Module Input and Output Definitions

The module background documents included information about the input and output variables for each module. In general, inputs and outputs of each module are managed through the 3MRA modeling system input/output dynamic link library (DLL) routines. The design of these routines includes several inherent quality assurance/quality control (QA/QC) checks. Specifically, the routines require that data be read from or written to ASCII flat data files containing data in a defined format. This file may be either a site specification file (SSF) or a global results file (GRF). SSFs are input files generated by the 3MRA modeling system from the system database as part of the site definition process. GRFs are output files from the 3MRA modeling system modules that are used by either subsequent modules as input files or the system to generate the risk results. Each SSF and GRF has an associated data dictionary (DIC) file. Each DIC file lists each parameter in the associated SSF or GRF and specifies the parameter name, dimensionality, data type (string, floating point, integer, or logical), units, minimum and maximum allowable values, and other parameters on which the parameter is dimensioned. Each parameter entry in the SSF or GRF includes the parameter data type, dimensionality, and units. The 3MRA modeling system reports an error if there is any inconsistency between an SSF or GRF and the associated DIC file, or if a data value is outside of the range determined by the minimum and maximum values specified in the DIC file.

The 3MRA modeling system input/output DLLs include functions for reading data from SSFs and GRFs. The functions are specific to the dimensionality and data type of the parameter, and the function calls include the parameter name and units. The 3MRA modeling system reports an error if there is any inconsistency between the input/output function call and the associated parameter specification in the SSF or GRF and the DIC file.

In a limited number of cases, module data inputs and outputs are not managed through the input/output DLLs. These cases include the reading of meteorological data files, writing files used as inputs for ISCST3, and the reading of ISCST3 output files prior to postprocessing these data to generate the Air Module GRFs. Because these input/output operations do not include the inherent checks of the 3MRA modeling system input/output DLLs, the module developers checked these input/output operations manually in informal tests to ensure they were operating properly.

2.2.3 Version Control of Module Code

EPA wrote the module code in C++ using the Microsoft Visual Studio integrated development environment. Several programmers developed, tested, and corrected the modules over a period of months. To maintain version control and a record of changes made to the modules, EPA maintained code for each module in Microsoft Visual Source Safe (VSS). VSS maintains project code in a central database on a server. Each developer can download a complete set of the current code from VSS. In addition, a developer can "check out" individual project files, make modifications, and check the file back in to VSS. During the time the developer has the file checked out, other developers are prevented from checking out the file or modifying it. When a file is checked back in, the developer can include comments with the new file. VSS maintains a record of the old and new files, and allows the developer to view the history of all changes made to a file and compare different versions of a file to determine the differences in the code between them. If necessary, the current version of a file can be discarded and the project can be "rolled back" to an earlier version of the file. The programmers used VSS to obtain the most current version of a module, ensure that only one developer at a time was implementing changes to a file, and examine the history of code changes to determine whether specific changes had been implemented.

2.2.4 Internal and External Code Testing

The overall purpose of internal and external independent testing was to determine whether the codes for the various modules were operating as designed. This subsection describes the internal testing and verification process.

Errors in codes were identified in several ways. Errors in code syntax were found and corrected as the modules were being compiled. In general, once a module or functional component of a module was developed and successfully compiled, the developer tested the code informally to determine whether the code was operating as designed. This testing involved a number of test cases. When anomalies were found, the developer traced through the code in "debug" mode, tracking the flow of program execution and examining the data values stored in specific registers to determine the potential source of the error. To facilitate module testing, the programmers incorporated output statements into the code to save the values of specific internal program parameters to an output file for review.

The compatibility of the module with the overall 3MRA modeling system was determined through a series of system test runs. This process identified inconsistencies between modules, such as different variable names or passing different variables than those expected by subsequent modules. Once these inconsistencies were resolved, and the entire 3MRA modeling system was operating consistently, the developers conducted thousands of runs across a wide range of contaminants, sites, and unit types. The system developers maintained an error list to track errors uncovered in these test runs. This error list documented the test data that generated the error and the module in which the error occurred. Errors were addressed on a case-by-case basis to identify the cause of the error and implement solutions. In some cases, an error in a module was traced to a problem with the input data from the 3MRA modeling system database or generated by a prior module. Otherwise, the developers traced and corrected the error in the module and reran the case that generated the error to ensure that the error had been satisfactorily resolved. In some cases, the developer conducted a limited number of informal additional runs to confirm that the change had resolved the error. Once the developer was satisfied that the error had been resolved, the developer then submitted the new version of the program to the 3MRA system managers for inclusion in the next version of the system software. The 3MRA system managers maintained a record of module errors and the program version that resolved each error.

Once the 3MRA modeling system was stable and generally operating without errors, each 3MRA modeling system module was tested individually to determine whether it was operating as designed. The testing protocol included internal verification tests conducted by the module developers, followed by independent tests conducted by another organization on the project team. For the internal tests, module developers wrote a test plan for each module; this test plan was reviewed by an external reviewer. The test plan specified the inputs and outputs of the module, the key module operating requirements, and specified tests that would be used to check the compliance of the module with the specified requirements. Several of the tests involved comparing module results with those generated independently from hand calculations or spreadsheet models. Other tests involved comparing module sensitivity to specific input parameters with the behavior expected based on the model design. Internal tests were documented in an internal verification test report, which described the test and results, provided supporting documentation to demonstrate that the program had passed the test, and also provided any supporting comments regarding how the test was conducted.

After a module passed its internal verification test, the developer sent the module and the test plan to another organization on the team (that was not involved in the development of the module) for further review and replication of the verification tests to confirm that the module completed each test successfully. The external verification tests were documented in technical memoranda.

2.2.5 Peer Review

The peer review process followed EPA's protocol for peer reviews (Science Policy Council Peer Review Handbook; U.S. EPA, December 2000) and was used to help ensure scientific defensibility of the 3MRA modeling system and its components. The 3MRA modeling system components were independently peer reviewed by the reviewers shown in Table 2-1. The peer reviewers were independently selected from a national database of experts by an outside firm that was not involved in the development or testing of the 3MRA modeling system in any way. EPA provided a list of areas of expertise needed to review each module, and the consulting firm then selected the reviewers from the database, based on their availability.

Flexibility was built into the 3MRA modeling system design in several ways. First, the modeling system was designed in modular format so any component could be replaced if better science became available. The implementation of the modeling system allowed for varied temporal spatial scales to be user-specified through the data input files. This enhanced the overall efficiency of the development of the system consistent with the best available science methodologies.

Table 2-1. 3MRA Modeling System Peer Reviewers

Component	Year	Reviewer	Affiliation
Science Plan	1998	Dr. Yoram Cohen	University of California, Los Angeles
		Dr. Paul F. Deisler, Jr.	Independent Consultant
		Dr. Mitchell J. Small	Carnegie Mellon University
Surface Impoundment and Aerated Tank Modules	1998	Dr. Patricia Culligan	Massachusetts Institute of Technology
		Dr. Wade Hawthorn	Washington State University
		Dr. Michael Overcash	North Carolina State University
Landfill, Waste Pile, Land Application Unit, and Watershed Modules	1999	Dr. Anita R. Bahe	President, LYNX Group, Ltd.
		Dr. Kirk Brown	Texas A&M University
		Dr. William Inskeep	Montana State University
		Dr. Clyde. Munster	Texas A&M University
		Mr. William Norris	Virginia Dept. Of Environmental Quality
		Mr. Robert Wyatt	President, R. J. Wyatt & Associates

(continued)

Table 2-1. (continued)

Component	Year	Reviewer	Affiliation
Air Module (ISCST3)[a]	1998	Dr. Steven Hanna	George Mason University
		Dr. Fred Mogolesko	President, M & L Environmental Consultants
		Dr. Bruce Turner	Sr. Tech. Associate, Trinity Consultants
Surface Water Module (EXAMS II)[a]	1999	Dr. Mustafa Aral	Georgia Institute of Technology
		Dr. Anthony Donigian	President, AQUA-TERRA Consultants
		Dr. Wilbert Lick	University of California, Santa Barbara
Vadose Zone and Aquifer Modules (EPACMTP)[a]	1999	Dr. Craig Forster	University of Utah
		Dr. M. Akram Hossain	Washington State University
		Dr. Carl Mendoza	University of Alberta
		Dr. Frank Schwartz	Ohio State University
Farm Food Chain Module	2001	Dr. Donald Mackay	Trent University, Ontario
		Dr. Lee Shull	Principal, Montgomery Watson Harza
		Dr. Curtis Travis	Principal, Quest Technologies
Terrestrial Food Web Module	2001	Dr. Anne Fairbrother	Sr. Ecotoxicologist, Parametrix, Inc.
		Dr. Robert Pastorok	Managing Scientist, Exponent
		Dr. Bradley Sample	CH2M Hill
Aquatic Food Web Module	2001	Dr. Lawrence Barnthouse	LWB Environmental Service, Inc.
		Dr. Frank Gobas	Simon Fraser University
		Dr. Paul Jacobson	Langhei Ecology, LLC
Human Exposure and Risk Modules	2000	Dr. James Butler	Argonne National Laboratory
		Dr. William Kastenberg	University of California at Berkeley
		Mr. Stephen Washburn	ENVIRON International Corporation
Ecological Exposure and Risk Modules	2000	Dr. Anne Fairbrother	Sr. Ecotoxicologist, Parametrix, Inc.
		Dr. Lawrence Kaputska	President, Ecological Planning & Toxicology
		Dr. Robin Matthews	Western Washington University
		Dr. Bradley Sample	CH2M Hill, Sacramento, CA
Physical and Chemical Properties (SPARC)[a]	1998	Dr. Richard Lee Dickerson	Texas Tech. University
		Dr. Ryan DuPont	Utah State University
		Dr. Igor Linkov	Menzie-Cura Associates
Aqueous Geochemistry and Sorption (MINTEQA2)[a]	1999	Dr. Lynn Dudley	Utah State University
		Dr. Kathryn Johnson	Johnson Environmental Concepts
		Dr. R. Bruce Robinson	University of Tennessee
Human Health Benchmarks	1999	Dr. Sara Hoover	Golden Associates
		Dr. Daland Juberg	ICTM
		Dr. Gary Pascoe	Independent Consultant
		Dr. Lauren Zeise	California EPA

[a] Denotes legacy code that forms the basis of the module and which has also been peer reviewed independently.

2.3 Verification and Validation of the Site-based Data

2.3.1 Verification of Site-based Data

Data verification includes the activities undertaken prior to and during the data collection effort to ensure that data of the correct type, amount, and quality (i.e., data that meet data quality objectives) are provided in the 3MRA modeling system respresentative national dat set. These activities included

- Developing a data collection plan that specified data sources and how data would be collected from those sources;
- Incorporating a quality assurance/quality control (QA/QC) protocols that were specified as part of the data collection plan, including data entry checks, independent calculations to verify that data were processed correctly in all circumstances, and automated checks of critical parameters, formats, and processes; and
- Conducting independent testing of the major site-based data elements.

EPA updated the data collection plan and it is described Volume II, Data volume. Section 5 describes the verification of the site-based data in more detail.

2.3.2 Validation of Site-based Data

EPA validated the accuracy of the site-based data in the representative national data set by comparing those data with data and model results for two of the sites where more recent data were independently collected during EPA's 1999 Surface Impoundment Study (SIS) Survey (U.S. EPA, 2001). Section 5 describes the validation of the site-based data in more detail.

2.4 Verification and Validation of the Chemical Properties Data

Chemical properties were estimated using the SPARC and MINTEQA2 models. Section 6 describes the verification and validation of the chemical properties models in more detail.

2.4.1 Verification of Chemical Properties Models

For SPARC, EPA has developed quality assurance software that is executed each quarter on the current version of SPARC. This software runs the various property modules for a large number of chemicals and compares the results to historical results obtained over the life span of the SPARC program. For MINTEQA2, EPA tests all code modifications and additions by a combination of compiler tests and model execution tests before final adoption.

2.4.2 Validation of Chemical Properties Models

For SPARC, each calculation used to estimate a chemical or physical property has been validated against numerous measured values for the property of interest. For MINTEQ, validation has been done by conducting tests and studies that show that the geochemical model, implemented by the combination of the user's input parameters, the thermodynamic database, and the computer code, provides an acceptable representation of reality or that it produces an outcome that is an acceptable representation of reality.