3.0 Ensuring Quality of the 3MRA Modeling System

This section addresses the ensurance of the quality of the 3MRA Modeling System at the system level. Figure 3-1 provides a broad overview of the system verification and validation.

3.1 Verification of the Modeling System

Verification of the 3MRA modeling system requires that the software components of the system function according to their individual and collective design. Verification of the 3MRA modeling system implies that the science-based modules and data processors are codified in software form correctly. This section describes the key aspects of the software development and verification protocols followed for the 3MRA modeling system.

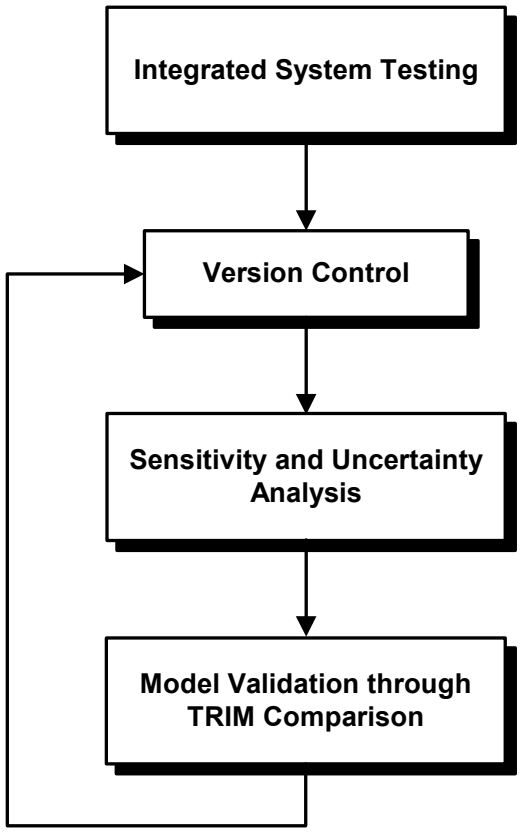

Figure 3-1. Overall approach to ensure the quality of the 3MRA modeling system technology.

The 3MRA modeling system represents the integration of more than twenty-five independent software components developed by five different software development groups located across the country and possessing different levels of expertise with respect to system software development. Because of this technically diverse and geographically dispersed development team, there was a need to formulate a comprehensive and rigorous approach for executing and managing software development and quality assurance. Four key elements contributed to the successful development, testing, and delivery of the 3MRA modeling system: (1) open and regular team communications, (2) a documented top-down approach to software design, (3) a rigorous implementation of software quality assurance and testing, and (4) a sound strategy for archiving the software. The following sections describe the manner in which each of these elements was implemented for the 3MRA modeling system.

3.1.1 Development Team Communications

The day-to-day management of the 3MRA modeling system development required communication methods that bridged the geographic distribution of team members on a regular basis. A combination of e-mail, tele- and video- conferencing, and face-to-face meetings were used to satisfy the communication requirements. Rapid reporting of problems and transfer of the science modules was facilitated by the e-mail communications. Regular periodic and on as-needed basis teleconferences were scheduled as e-mail traffic indicated the need for a team consultation. During the critical stages of development, teleconferences were held as often as twice a week. A detailed agenda was developed and distributed to team members before each call. Project status, technical problems, and technical decisions were discussed.

Periodically (i.e., on the order of two to three times per year), an all-hands meeting was held to address issues that required extensive and focused discussion. For example, early in the development process, after the system design had been documented, teleconference discussions indicated inconsistent interpretations of the design. Attempts to resolve these issues through teleconferences were deemed unsuccessful when efforts to link the first components failed due to data interchange conflicts. Therefore, an all-hands meeting was held when multiple groups were ready to attempt linkages between their modules. The convergence to a common understanding of the system design with respect to the proper operation of the system was facilitated by the intense discussions occurring during attempts to link modules.

3.1.2 Top-Down Design Approach

The foundation of the technical approach was the "software system life cycle" process applied with modern object-oriented system design principles. Two elements applied early in the process proved to be critical to the success of the effort. First was the documentation of the system design, especially the specification of the science modules and databases. Second was the relationship among these modeling components, in the form of data representation and interchange. The use of an Applications Programming Interface (API) that both provided a standard data representation scheme and established a required protocol for data interchange proved to be critical. The API, in addition to minimizing the occurrence of data conflicts between modules, also served as a focal point for technical discussions.

3.1.3 Quality Assurance and Testing Strategy

The objectives of software testing are three-fold and include the following:

1. To uncover errors in requirements, design, and programming;
2. To identify or confirm limitations of the system; and
3. To verify the capabilities of the system.

The single most significant factor in the successful development of the 3MRA modeling system was the establishment and steadfast adherence to a rigorous testing strategy. Given the technically diverse and geographically dispersed nature of the 3MRA modeling system development team and the size of the software system to be developed, it was imperative to establish a rigorous software testing strategy. The strategy for testing the 3MRA modeling

system included a procedure for components in a standalone mode and a procedure for systems integration testing.

The software development occurred at the component level first. When sufficient infrastructure and science-based components (modules and databases) were available, system-level integration was initiated. When component developers had completed a first version of the software, they could test it both as a standalone executable and also in the context of the system software. Often, component software that ran without error in a standalone mode would experience significant difficulty when integrated into the system. Typically, this was due to data conflicts with other components that were either sending data to the module or receiving outputs from the module.

As components were developed, the developers also established and documented formal test plans. Software testing for the 3MRA modeling system was requirements based; that is, specific tests were designed to ensure that each of the requirements associated with the software design was correctly implemented. While the developer had primary responsibility for the test plan and its successful execution, it was also required that the test plans be reviewed and the tests re-executed by independent developers (i.e., software engineers and modelers not directly involved in developing the component software). Thus, all 3MRA modeling system software was required to undergo two levels of formal testing. Figure 3-2 illustrates the testing protocol for the developer and Figure 3-3 illustrates the protocol followed for independent testing, at the component level. To facilitate the independent testing, the developers constructed test packages that included all documentation, source code, and test files associated with a component. As can be seen in Figure 3-3, the independent tester first reviewed the test plan for completeness, to determine if sufficient tests had been designed to verify the implementation of all requirements. The independent tester was free to add tests to the test plan. Once the test plan was approved, the independent tester executed all the tests using the developer's executable version of the software. When this was successful, the independent tester then recompiled the component software and re-executed the tests a second time. This second level of independent testing proved invaluable in identifying issues related to compilation and also ensured that the complete set of software related to the component was provided.

After the 3MRA modeling system components satisfied all tests, it was necessary to place them into the complete 3MRA modeling system to confirm their functionality in this context. The system integration tests required that components operate error free while executing within the full system context (i.e., running the full set of site/WMU combinations for the contaminants of interest and the iterations of the Monte Carlo simulation). System-level testing uncovered not only programming errors such as data conflicts, but also several science-based errors. The 3MRA modeling system representative national dat set of 201 sites executed within a Monte Carlo simulation provided a testbed that stressed the numerical solutions of science models in a manner not previously possible. For example, even legacy codes that had more than a decade of wide use experienced environmental conditions that resulted in unstable numerical solutions.

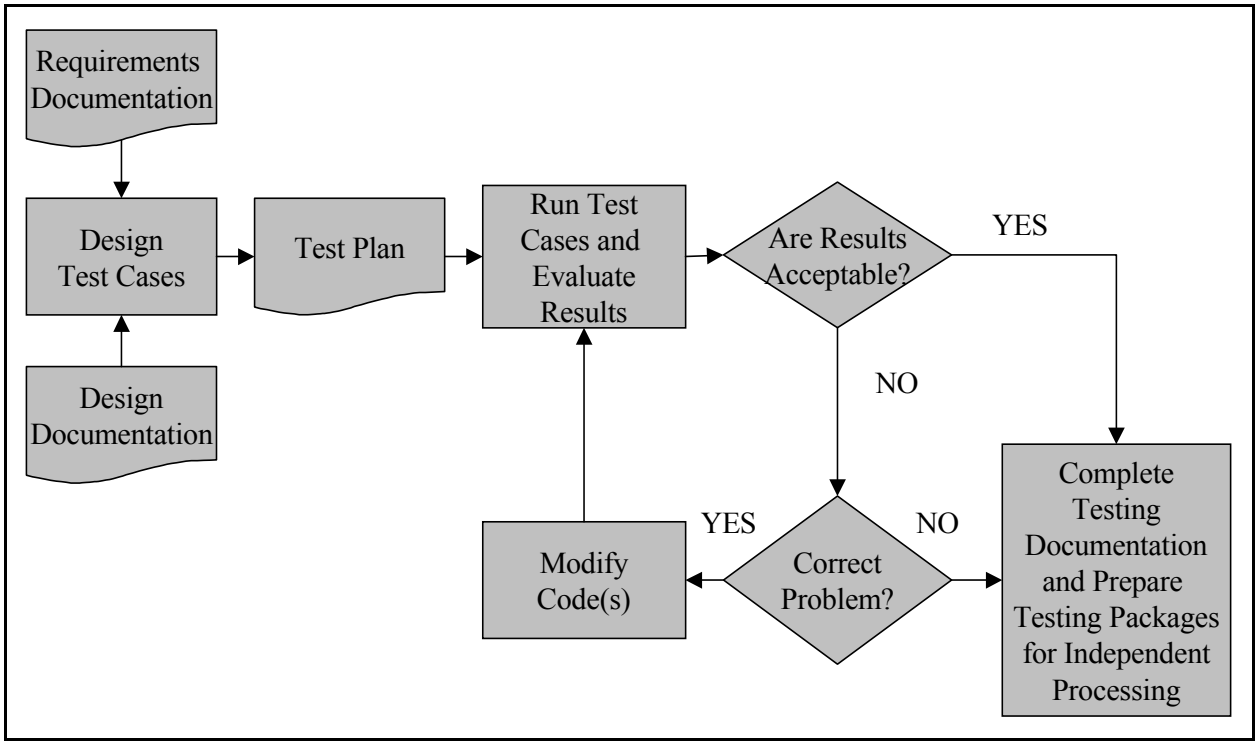

Figure 3-2. Developer testing process for the 3MRA modules.

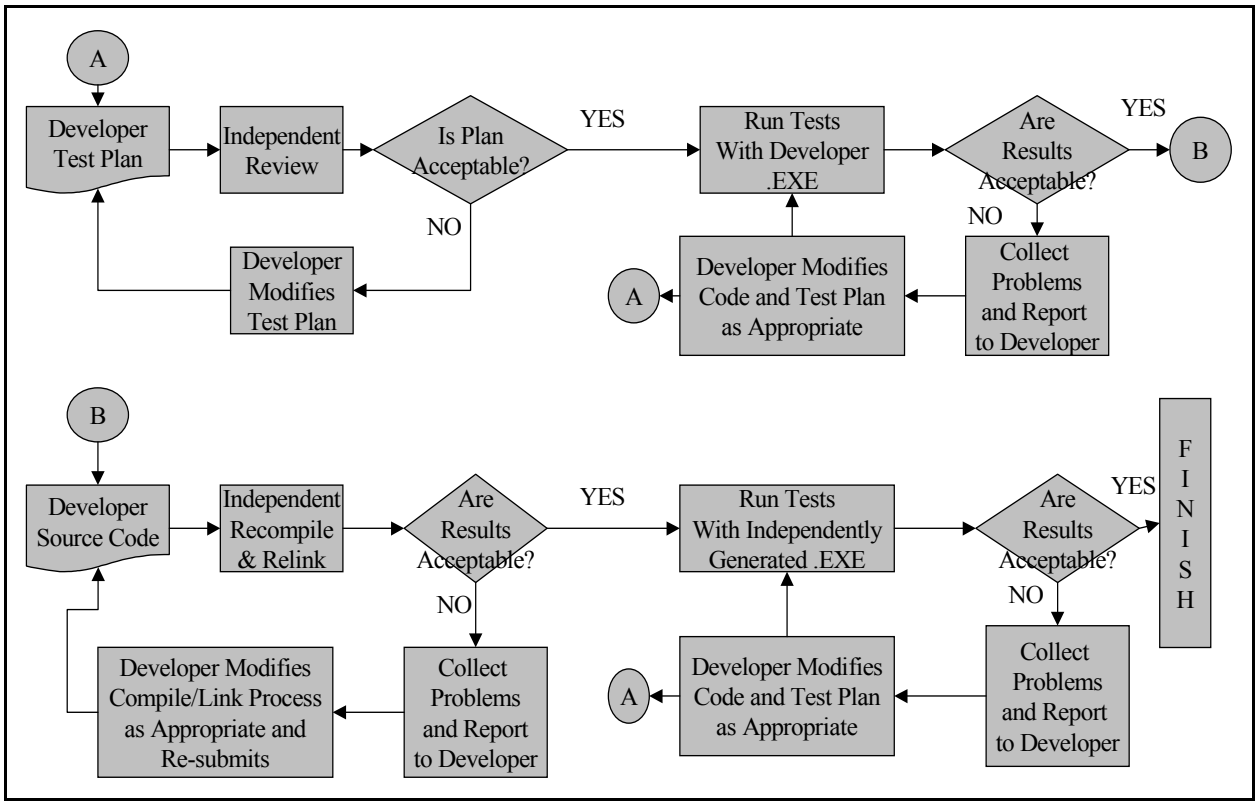

Figure 3-3. Independent testing process for the 3MRA modeling system.

The system integration tests were initially conducted on single PCs. Computation 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 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. Recently, EPA has constructed a PC-based cluster that includes approximately 160 PCs networked together and developed software for distributing the computational load across this network and retrieving output files. While this configuration of PCs (named the Super-computer for Model Uncertainty and Sensitivity Evaluation [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 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.

3.1.4 Software Archiving and Distribution

The 3MRA modeling system is a large and complex software system. It is composed of over 100 binary, configuration, and data files. In addition, the test packages included over 200 source code files and numerous files. More than 15 software engineers and scientists from five geographically distributed groups contributed to the development of the 3MRA modeling system and it is likely that additional software engineers will contribute to its future development. Coordinating all the changes among these entities in order to assure the quality and reproducibility of the final release required formal archiving and release procedures.

The first step to establishing these procedures was to set up a version control system. Version control software is used to archive files and track changes. Several commercial software packages that could handle this task were reviewed. Microsoft's Visual SourceSafe was selected because it provided a robust functionality, licenses were available, and the internal development team had previous experience using it. The Visual SourceSafe software runs locally on a user's machine. However, the actual file repository is kept on a network drive. This drive is fully backed up every week and incrementally backed up each evening. Two of the primary functions of the software package are keeping track of file versions and preventing multiple developers from modifying the same file at the same time. When a developer wants to update a file, the file is "checked out," which locks the file and prevents others from updating it. The file is modified and then "checked backed in." This updates the file in the version control system. The previous version of the file is not lost, as all versions are archived. This allows the reconstruction of any version of the components or the entire system.

Individual projects in Visual SourceSafe were created for each system component (e.g., science module). The baseline version of all components and the system in general is referred to Version 1.0.

The initial compilation of the Version 1.0 archive was actually the last step of the testing protocol. For reference, a system component is compiled in the form of a binary file such as an executable file or a dynamic link library (dll) file. On the Microsoft Windows platform, an

executable is a file that has an ".exe" extension. A dll file has a ".dll" extension. Each developer was required to provide a package of files that were to be associated with the Version 1.0 release. The package was to include the following:

- All necessary source code and libraries needed to compile the specified module;
- All test packages, including test data and auxiliary files (e.g. batch files, script files) required to run the test suites; and
- All documentation describing the purpose of each test case and how to execute it and the expected results.

As the individual module packages were received, they were then compiled. Compilation is the step whereby source code, computer instructions written in higher-level languages such as FORTRAN or C++, is converted into machine-readable binary files. There are a wide variety of compiler types, brands, and versions available. For instance, to compile C++ code, EPA used the compilers included with Borland C++ Builder and Microsoft Visual C++. Each of these has six or more versions in existence. The compiler originally used by each developer was used whenever possible. When not possible, a version as close to the developer's version as possible was used. This resulted in a standard set of compilers now used by EPA for archiving.

All tests included in the packages were then executed. Accompanying documentation provided step-by-step instructions on how execute the individual test suites. In cases where tests were not successfully executed, the developer was informed and required to resolve any issues (e.g., out-of-date test package, errors in source code).

After successful completion of all tests, the resulting materials were entered into Visual SourceSafe. This completed the component level testing and verification process. The next step was to perform system testing. The PCs in the SuperMUSE are currently configured with different versions of Microsoft Windows. SuperMUSE has custom software that allows it to run stand-alone models such as the 3MRA modeling system on the PC cluster. The software allows for the distribution of various scenarios and subsequent data collection. Running the software on SuperMUSE enables EPA to complete hundreds of thousands of runs. This would not be feasible if all system testing were done on individual PCs. Any component-specific errors that were discovered were referred back to the developer as described above. The development team addressed system-level errors and the system was retested. Any file changes that were required to fix component or system errors were updated into Visual SourceSafe.

After final testing was completed and the archive was populated with a complete set of system software and related documentation, the materials were made available to the public. Procedures are under development for distributing the software to the public, providing technical assistance, and accepting new or updated models. It is not currently clear how version control will work when the 3MRA modeling system is distributed to the public. All materials, including source code, will be made available. EPA is currently reviewing various open-source licensing agreements and anticipates including such an agreement requirement whenever the source code is requested. It is understood that EPA is the designated owner of the "official" 3MRA modeling

system software. EPA keeps all the files necessary to compile, test, document, and execute the 3MRA modeling system. Although the public will be free to modify the software, the altered software will not be considered official unless it is processed by EPA through the procedures described above.

3.2 Validation of the System

In the context of a national regulation, a complete approach to demonstrating that the 3MRA modeling system produces results consistent with field observations would necessarily require field data comparisons of the 3MRA modeling system for numerous contaminant release scenarios covering the range of environmental conditions where waste disposal is possible. However, as pointed out earlier, no such data are currently available to validate the system. Therefore, EPA had to resort to alternative approaches to ensure the quality of the modeling system.

The approach undertaken here, as a first step, involves the application of the 3MRA modeling system to a single site and the comparison of results with (1) available field observations, and (2) compare with the results of the application of a second modeling system to the same site.

This approach was implemented through a collaborative effort with the modeling team developing the Total Risk Integrated Methodology (TRIM), a multimedia model designed to serve a similar purpose in support of EPA's Office of Air Quality Planning and Standards (OAQPS). Although TRIM supports the development of air regulations, as opposed to the 3MRA modeling system's focus on land-based disposal of solid wastes, the two models share a need to simulate the fate and transport of contaminants in all media, not just the media in which a contaminant is first released. The 3MRA modeling system and TRIM take very different approaches to simulating the multimedia system of physical/chemical/biological processes and thus a model comparison study provides an opportunity to gain experience applying each approach and confidence that model predictions are reasonable.

There are five primary steps to modeling a site: problem definition, site conceptualization, collection/organization of modeling data, model execution, and interpretation of results. Problem definition includes site selection, a statement of an assessment problem, and specific modeling goals to be achieved. Site conceptualization is the process of delineating the physical features of a site in a manner consistent with model design. The inter-connectivity of the features must also be specified (e.g., watershed connectivity to stream segments). Data representing contaminant source terms, environmental conditions related to the physical features of the site, chemical properties (physical/chemical/biological constants/rates), and contaminant distribution in each of the media must be collected and organized for use by the model. Model execution is a mechanical step that applies the model to achieve the stated modeling goals. Interpretation of results for this study includes both a comparison of results with available field observations as well as an inter-model comparison. The following sections provide a more detailed description of these steps for this model comparison study.

3.2.1 Problem Definition

3.2.1.1 Site selection. Establishing criteria for site selection is fundamentally a function of model purpose and design. The purpose of both the 3MRA modeling system and TRIM is to estimate the potential human and ecological exposure and associated health risks associated with the release of contaminants from regulated industrial sources. As such, a site selected for this study must contain a source of contaminant released to the environment. The contaminant, at least for initial comparisons, should be a multimedia contaminant, that is, subsequent to release it should be distributed throughout the environment. Further, data must be available that describe the environmental setting as it is represented in the models. In the case of both TRIM and the 3MRA modeling system, the environmental setting includes all media: air, soil, vadose zone, ground water, surface water, sediment, and biota. Data that vary as a function of time (e.g., meteorology) must be available for a time period relevant to the simulation. For example, if a facility operated for thirty years, then time series data should be available for those thirty years, and for a period of time following facility closure. The 3MRA modeling system and TRIM estimate long-term average exposures extending over periods of several years to a lifetime. Each model simulates these periods with time steps that may be as short as an hour or as long as a year; thus, time-varying data must be available for decades and at intervals as short as an hour. Finally, data must be available that reflects the impact of the source on the health of the human and ecological receptors occupying an area near the source, generally to two or more miles from the source. These data include time series of concentrations in each of the modeled media and intermedia contaminant fluxes. These concentrations and fluxes should be available at several locations within the area of interest.

In response to comments of the EPA Science Advisory Board related to a review of TRIM, an extensive review of the literature was conducted in an effort to locate data sets for use in evaluating the performance of TRIM.Fate. The conclusion reached by the TRIM modeling team is that "[N]one of the studies identified during EPA's literature review provides complete and concurrent information on contaminant concentrations in the five major environmental media (i.e., air, water, sediment, soil, biota) along with the associated source terms(s) and historical environmental characteristics (e.g., meteorology, hydrology, landscape properties)." Given this limitation it is necessary to scale back on the site selection criteria and choose a site where the amount of available information is maximized.

Of the sites reviewed, the TRIM modeling team selected the HoltraChem Manufacturing site in Orrington, Maine, and selected mercury as a case study contaminant of concern. The following description of the HoltraChem site is taken from the Maine Department of Environmental Protection website[1].

> *The HoltraChem Manufacturing Company in Orrington, Maine… is located on a 235-acre property on the banks of the Penobscot River. Approximately 50 acres are developed and include the manufacturing facility, five landfills, a surface impoundment and a waste pile. The immediate plant area is approximately 12 acres. The property is west of Route 15 and it abuts the*

[1] http://www.state.nc.us/dep/rwm/holtrachem/index.htm

PERC waste-to-energy plant on the north and west. It opened in 1967 and manufactured chlorine, caustic soda (sodium hydroxide) and chlorine bleach (sodium hypochlorite) used by paper mills. The plant also manufactured hydrochloric acid and the pesticide chloropicrin. The plant closed in September, 2000.

The plant used a chlor-alkali process to separate sodium and chlorine from salt water. In this process, elemental mercury was used as a cathode to collect the sodium from the water. The chlor-alkali process is an older technology and has been replaced by mercury-free production techniques at newer plants and some converted older plants. When it stopped operations last fall, HoltraChem was one of 13 chlor-alkali plants left in the country. There were as many as 30 chlor-alkali plants in the United States at one time.

A site investigation determined that the HoltraChem property, including parts of the Penobscot River, is contaminated with mercury, chloropicrin and several volatile organic compounds. Additional investigation will be done into the presence of additional areas of mercury contamination and polychlorinated biphenols (PCBs).

Specifically, the following contaminants at a minimum are present on site:

- *Soils: chloropicrin, ethylbenzene, xylenes, arsenic, barium, cadmium, chromium, lead and mercury.*
- *Ground water: 1,1 dichloroethane, acetone, bromodichloromethane, bromoform, carbon disulfide, carbon tetrachloride, chlorobenzene, chloroform, chloromethane, chloropicrin, dibromochloromethane, methylene chloride, trichloroethene, mercury, potassium, and sodium.*
- *Surface Water: carbon tetrachloride, chloroform and mercury.*
- *Sediment: mercury*
- *Biological samples: mercury*

The developed part of the property can be subdivided into three physiographically distinct areas: 1, the bedrock ridge, 2, the plant area, and 3, the river area. The northeast trending bedrock ridge is north and northwest of the plant area and separated from the plant by an abrupt scrap. The elevation of the crest of the ridge varies from 80 ft. to 145 ft. The plant is constructed on a relatively flat surface about 65 ft. elevation, about 500 feet east of the Penobscot shoreline. The river area slopes steeply from the plant area to the river. The northwest side of the bedrock ridge is drained directly to the river by a small intermittent stream. The western part of the plant area drains west through the river area by way of the Northern Stormwater Drainage Ditch. The eastern part

of the plant area is drained south to the Penobscot by the Southerly Stream. The Northern Stormwater Drainage Ditch and the Southerly Stream are perennial streams that flow all year long and derive some of their water from ground water discharge.

The overburden deposits at the site can be grouped into four types. Glacial till is a silty sand that contains abundant clay and gravel as well. Till is deposited directly from glacial ice without appreciable sorting by water. Glacial outwash is made up of moderately sorted sand and gravel that tends to be poor in silt and clay. Outwash is quite permeable, and where thick deposits occur below the water table it can be an excellent aquifer resource. Fine grained marine sediments in coastal Maine are referred to as the Presumpscot Formation. The Presumpscot Formation is made up largely of silty clay that was carried out of the glacier by meltwater and settled out in the ocean. Finally, there are deposits of fill on the site that include till, outwash and marine sediments that were redistributed during construction at the plant, and brine and wastewater sludge stabilized with sand in the hazardous waste landfills.

The geology of the site varies from place to place. The bedrock ridge is made up of tough metamorphic rock covered by a thin layer of glacial till. There are thick deposits of man-made fill on the ridge, including three hazardous waste landfills. The plant area is developed on thick overburden that is mostly compact glacial till, but a shallow wedge of sandy outwash occurs all along the southern edge of the bedrock ridge. The shallow sandy outwash thickens west toward the river so that the river area is underlain by a thick sequence of sand and gravel.

Ground water flows in bedrock fractures on the bedrock ridge. It flows north directly to the Penobscot on the north side of the ridge, but it flows south toward the plant on the south side of the ridge. The thick compact glacial till under the plant area is not very permeable, so most of the ground water under the plant area flows in shallow fill and outwash sand over the top of the till surface. Ground water from the southern part of the plant area discharges to the Southerly Stream. Ground water from the rest of the plant area flows west to the Penobscot River through the river area.

While ownership has changed several times, Mallinckrodt, Hanlin and HoltraChem have each worked to advance the cleanup. Several of the actions which HoltraChem and Mallinckrodt have taken to control and clean up pollution at the plant are listed below:

- *Relined a lagoon to stop waste from discharging to ground water which flows into the Penobscot River;*
- *Installed riprap on the riverbank next to one of the plant landfills to prevent erosion and river contamination;*

- *Installed a ground water collection system to capture a portion of contaminated ground water discharging from the site for treatment, and*

- *Instituted measures to prevent contaminated sediment from reaching the river.*

3.2.1.2 Problem statement and modeling goals. As described, the HoltraChem site includes a host of contaminant release problems, ranging from chemical spills to disposal of waste in landfills, a surface impoundment, and a waste pile to fugitive emissions from chemical processing. Contaminants present at the site include several metals, volatile organic compounds, and PCBs.

Mercury will serve as the initial focus of model application and comparison because (1) mercury is a contaminant of concern to both OAQPS and OSW, (2) mercury is a pollutant whose fate, transport, and bioaccumulation involve all media, and (3) mercury levels have been monitored in a number of media and locations at the HoltraChem site. Table 3-1 summarizes the available mercury monitoring data.

Various limitations in data availability and differences between TRIM and the 3MRA modeling system constrain the application and the interpretation of results. With respect to data availability the following limitations exist:

- The source term for mercury emissions is based on based on the characteristics of the chlor-alkali facility operations and not specific measurements at HoltraChem;

- Monitoring data provides more of a snapshot of mercury in the surrounding environment than a continuous measure of its presence during the period of HoltraChem operations; and

- Contributions from other sources of mercury (both on-site and off-site) are not explicitly accounted for in this initial assessment.

With respect to differences between the 3MRA modeling system and TRIM the following limitations in the model comparison are noted:

- Currently, TRIM simulates only multimedia fate and transport; human and ecological exposure and risk are currently being added.

- The 3MRA modeling system does not simulate subsurface fate and transport for atmospherically deposited contaminants. Thus, no vadose zone or aquifer simulation of mercury movement is conducted for the 3MRA modeling system runs.

- TRIM does not simulate land-based disposal units and thus the landfills, surface impoundment, and waste pile are not simulated.

Table 3-1. Site Sampling Data for HoltraChem Facility and Nearby Areas and Water Bodies

All data sampled between 1993 - 1997	Minimum	Maximum	Mean	Std Dev	Median
On-site					
Surface Soil (THg* mg/kg, dry wgt)	0.18	10.3	5.05	3.47	4.8
Surface Soil (THg mg/kg, dry wgt)	0.14	310	30.1	47.6	13
Surface Soil (THg mg/kg, dry wgt)	0.2	310	5.37	11.4	1.2
Surface Soil (THg mg/kg, dry wgt)	4.5	126.9	23.8	41.8	
SubSurface Soil (THg mg/kg, dry wgt)	0.1	80	12.4	16.3	6.2
Deer Mouse (THg mg/kg, ww, whole body) 75% moisture	0.06	0.198	0.1	0.063	
Earthworm (THg mg/kg, ww, 85% moisture)	0.087	2.82	0.982	0.79	
Off-site					
Ambient Air (THg ng/m3) [1500m SE]	0.834	157	9.96	15.52	
Ambient Air (THg ng/m3) [4300m NNW]	0.993	25.8	2.46	2.15	
Ambient Air (THg ng/m3) [6400m NNW]	0.565	14.8	1.85	1.66	
Surface Water (THg ug/L unfiltered Upstream of Facility	0.00359	0.00529	0.004	0.001	0.004
Surface Water (THg ug/L unfiltered Downstream of Facility	0.000646	0.0703	0.034	0.033	0.027
Surface Water (THg ug/L unfiltered River Adjacent to Facility	0.0041	0.173	0.015	0.0377	
Sediment Swetts Pond (THg mg/kg dw)	0.319				
Sediment Thurston Pond (THg mg/kg dw)	0.157				
Sediment Brewer Lake (THg mg/kg dw)	0.201				
Sediment Fields Pond (THg mg/kg dw)	0.132				
Juvenile Loon Swetts Pond (blood THg conc ppm ww)			1.3		
Loon Egg Brewer Lake (Hg conc ppm ww)	1.6	1.8	1.73	0.11	
Deer Mouse Dorethea Dix Park (THg mg/kg, ww, whole body) 75% moisture	0.016	0.087	0.0515	0.05	
Earthworm Dorethea Dix Park (THg mg/kg, ww, 85% moisture	0.044	0.044	0.044		

(continued)

Table 3-1. (continued)

All data sampled between 1993 - 1997	Minimum	Maximum	Mean	Std Dev	Median
Short Tail Shrew Dorethea Dix Park (THg mg/kg,			0.064		
Eel (THg mg/kg ww 80% moisture River Upstream of Facility)	0.271	0.876	0.53	0.2	
Eel (THg mg/kg ww 81% moisture River Downstream of Facility)	0.259	0.678	0.46	0.14	
River Minnow (THg mg/kg dw whole body Downstream of Facility)			0.447		
White Perch Swetts Pond (mg/kg ww)	0.5	1.31	0.98	0.25	
White Perch Fields Pond (mg/kg ww)	0.28	0.72	0.45	0.14	
White Perch Thurston Pond (mg/kg ww)	0.6	2.2	1.07	0.43	
White Perch Brewer Lake (mg/kg ww)	0.32	0.53	0.41	0.08	
State of Maine averages					
State Avg Loon Egg Hg Conc (ppm ww 43 samples)			0.93	0.55	
State Avg Juvenile Loon THg BloodConc (ppm ww 52 samples)			0.22	0.29	
State Avg Adult Male Loon Hg Conc (ppm ww 6 locations)	0.61	3.71	2.62	1.23	
State Avg Adult Male Loon Hg Conc (ppm ww 67 samples)			2.5	1.1	
State Avg Adult Female Loon Hg Conc (ppm ww 64 samples)			2.1	1.5	

*THg = Total mercury.

For these reasons, the initial model simulations for comparison focus only on the fugitive emission of divalent mercury over the thirty year period of facility operations (3MRA simulates divalent mercury, while the surface water module of 3MRA does speciate mercury. The monitoring data is for total mercury). The criteria for selecting specific endpoints, locations, and times are designed to ensure that each media is included, as well as a representative cross section of terrestrial and aquatic species as a function of both food source and trophic level. Locations are a function of both model site conceptualizations (e.g., habitat delineation) and locations where monitoring data have been collected. Table 3-2 lists the endpoints for the initial model runs.

Table 3-2. Model Estimation Endpoints for Initial HoltraChem Simulations

Medium	Endpoints	Hg Species	Locations	Times
Atmosphere	ambient concentrations (in breathing air), deposition rates	divalent	Location of ambient air monitoring stations, lakes/ponds for deposition, selected watersheds/habitats	Annual average time series (30 years)
Soil	average surface soil concentrations	divalent	on site, across river just south of facility, selected watersheds/habitats	Annual average time series (30 years),
Surface Water (water column)	average water column concentration	divalent, methyl	River (north/south of facility), Swetts Pond, Brewers Lake, Fields Pond, Thurston Lake	Annual average time series (30 year)
Surface Water (sediment)	to be determined (3MRA has 2 sediment layers, TRIM ?)	divalent, methyl	River (north/south of facility), Swetts Pond, Brewers Lake, Fields Pond, Thurston Lake	Annual average time series (30 years)
Biota (terrestrial)	terrestrial vegetation, White-tailed Deer {terrestrial herbivore}, Deer Mouse {terrestrial herbivore}, Short-tailed Shrew {terrestrial invertebrate feeder}, earthworm	divalent, whole body	to be determined based on TRIM/3MRA site conceptualizations	year 30
Biota (aquatic)	Largemouth Bass, white perch	methyl, whole body	Swetts Pond, Brewers Lake, Fields Pond, Thurston Pond	Year 30
Biota (terrestrial/aquatic)	Common Loon {semi-aquatic piscivore}, Mink {semi-aquatic piscivore}, Raccoon {semi-aquatic omnivore}	divalent, whole body	in proximity of Swetts Pond, Brewers Lake, Fields Pond, Thruston Pond	Year 30

- The 3MRA modeling system simulates mercury speciation only in the surface water while TRIM simulates mercury chemistry in all media.

3.2.2 Site Conceptualization

Figures 3-4, 3-5, and 3-6 show aerial photographs of the HoltraChem facility and the surrounding area. Figure 3-7 displays the land use patterns and waterbodies in the modeling area of interest. The site conceptualization task requires that site layout features relevant to the models be delineated and that logical connections between the features (watershed drainage to surface water) be specified.

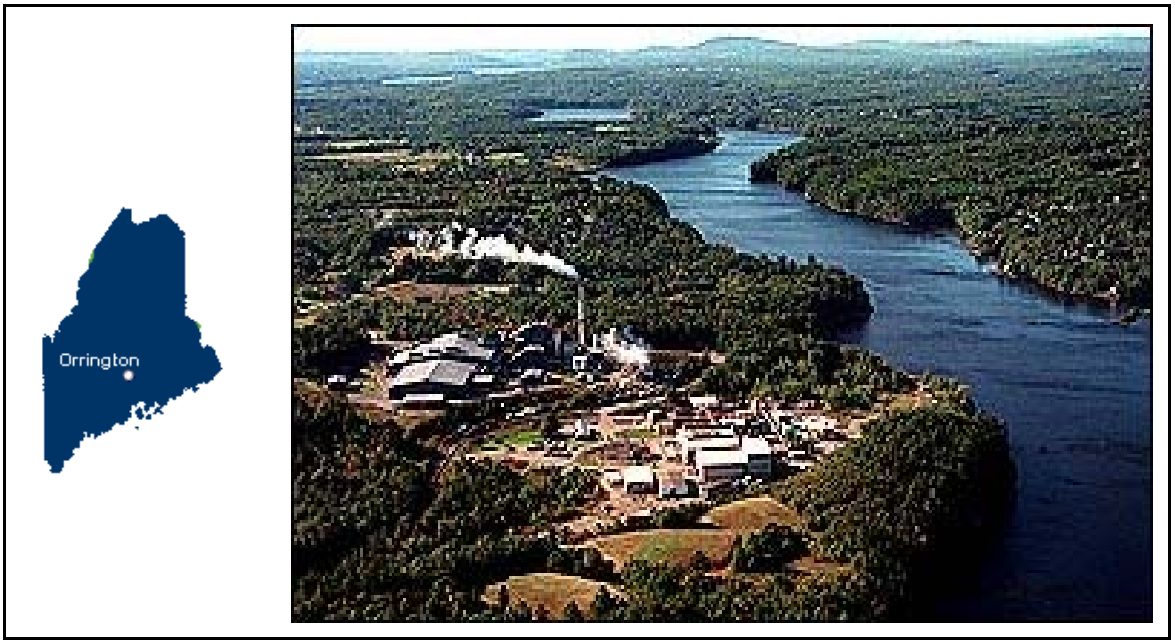

Figure 3-4. HoltraChem manufacturing site.

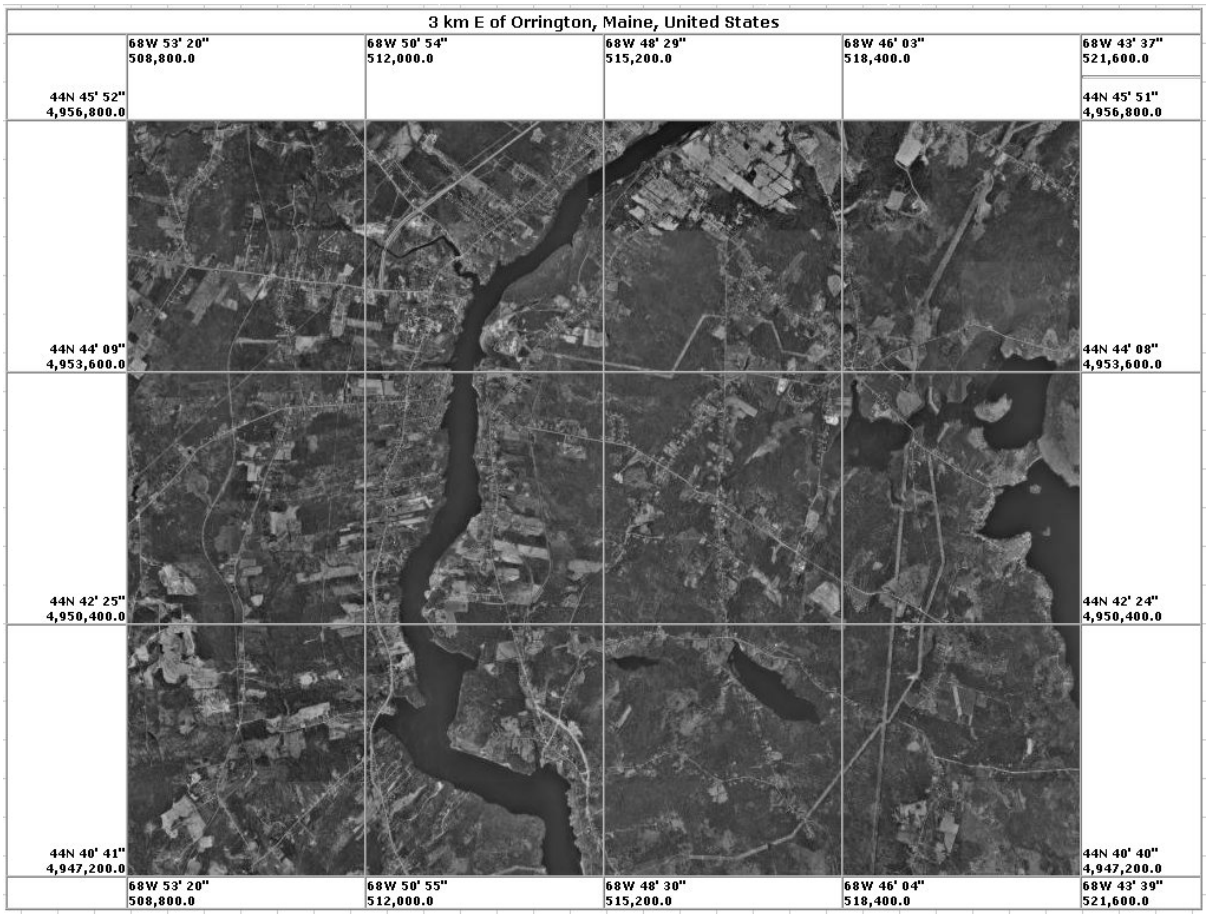

Figure 3-5. HoltraChem area photo.

Figure 3-6. Aerial view of HoltraChem facility.

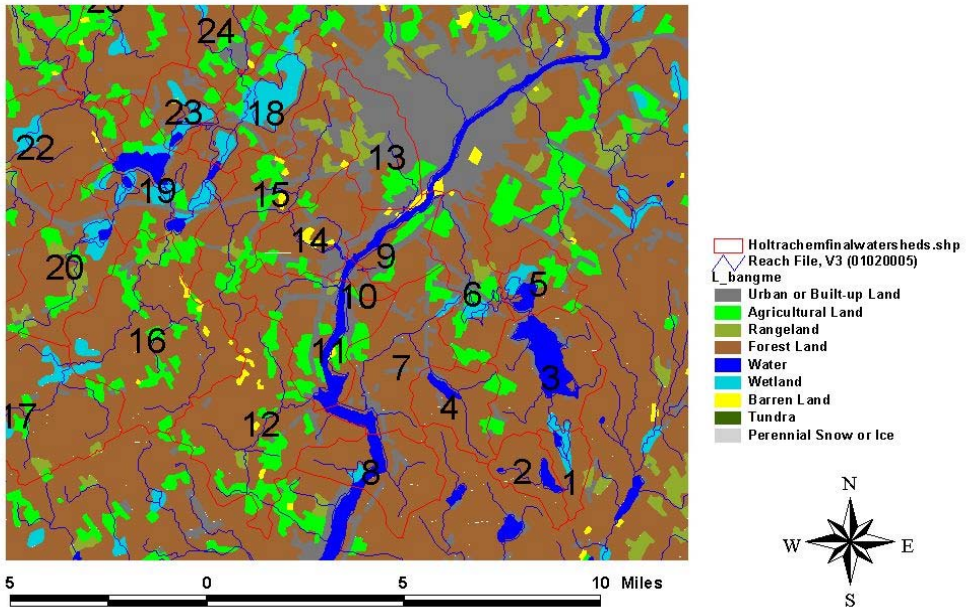

Figure 3-7. Land use and surface water around HoltraChem facility.

The number and extent associated with each of the site features depends on the initial problem statement, which specifies endpoints of concern. In the case of the HoltraChem site there is interest in the potential transport of mercury to lakes southeast of the site (Brewers Lake, Thruston Lake, Fields Pond) because these lakes lie in the primary downwind direction from the facility. The interest in potential mercury impacts in these lakes defined the aerial extent for the modeling for each model. Within the area of interest, each model simulates contaminant fate and transport in all media, including watershed soils; streams, rivers, ponds, and lakes; airsheds; unsaturated zone; aquifer; and biota associated with the terrestrial and aquatic foodwebs. The delineation of aerial extent and depth associated with each of these features is conceptualized differently between the two models.

TRIM conceptualizes a site as a set of surface parcels and air parcels. The parcels are 2-dimensional areas of assumed homogeneous environmental conditions. The air parcels are placed such that they conform first to a need to estimate ambient air concentrations and depositions as a function of radial distance from the source and, secondly, to the degree possible, so they align with the surface parcels. The surface parcels are placed considering together the combination of watersheds, habitats, surface water segments, vadose zone, and ground water aquifer. When depth is assigned to each of the parcels, the result is a volume element that represents the unit of analysis for the TRIM model. Figures 3-8 and 3-9 illustrate the surface and air parcels that define the basis of the site conceptualization for the HoltraChem surrounding area.

The 3MRA modeling system conceptualizes a site by delineating the actual 2-dimensional area associated with each unit of the physical features. Site conceptualization is achieved by delineating areas directly from GIS-based maps of the site. For the HoltraChem site, the site features considered in 3MRA modeling system runs include several watersheds, a surface water network, a single airshed, and several ecological habitats. The unsaturated zone below the root zone and the ground water aquifer were not modeled.

Figure 3-10 illustrates the surface water network that is modeled by the 3MRA modeling system for the HoltraChem site. The surface water network consists of the Penobscot River, tributaries in the vicinity of the HoltraChem facility, wetlands, and lakes. For modeling purposes, the network was configured as a interconnected series of fourteen reaches. Directly connected to specific surface water network reaches are individual watershed subbasins. Watershed subbasins that drain to the segment of the Penobscot river lying between the extents of the tributaries containing the lakes of interest are included. Figure 3-11 illustrates the eighteen watershed subbasins included in the 3MRA modeling system runs for the HoltraChem site. Figure 3-12 illustrates the ecological habitats that are delineated principally as a function of land use. Twelve habitat areas are defined, including two cropland habitats, two forest habitats, four lake habitats, one residential habitat, two wetland habitats, and one river habitat. Within the 3MRA modeling system, each habitat type includes a list of species that are both of interest and native to the area of the country being modeled. Each species within a habitat is assigned a home range, specifying the sub-area extent occupied by the species.4

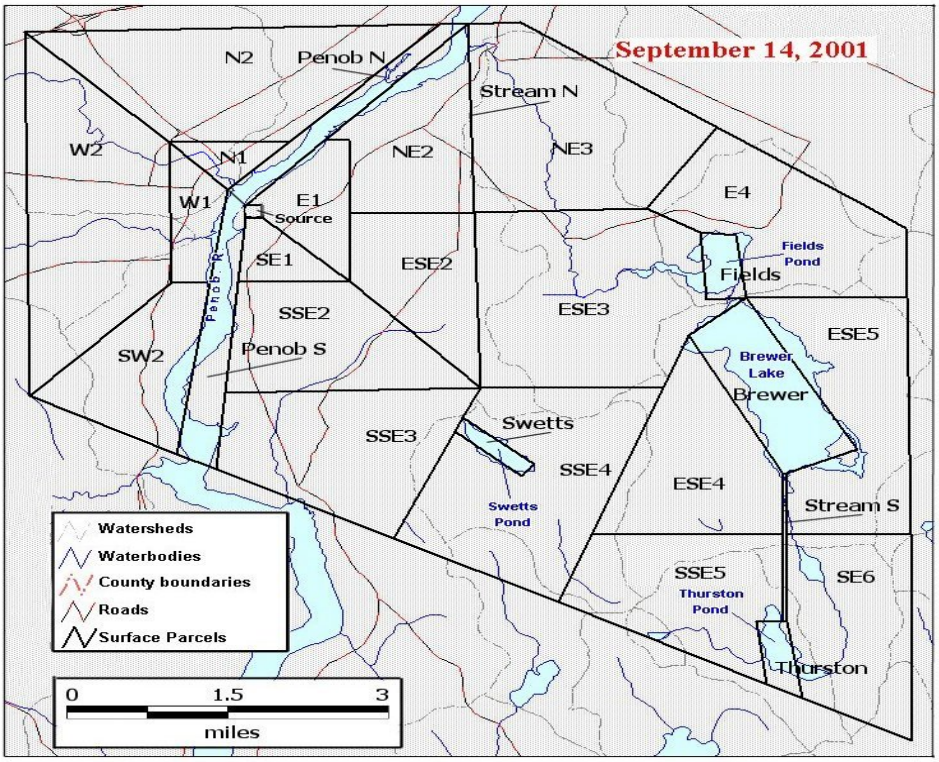

Figure 3-8. TRIM surface parcels for HoltraChem facility.

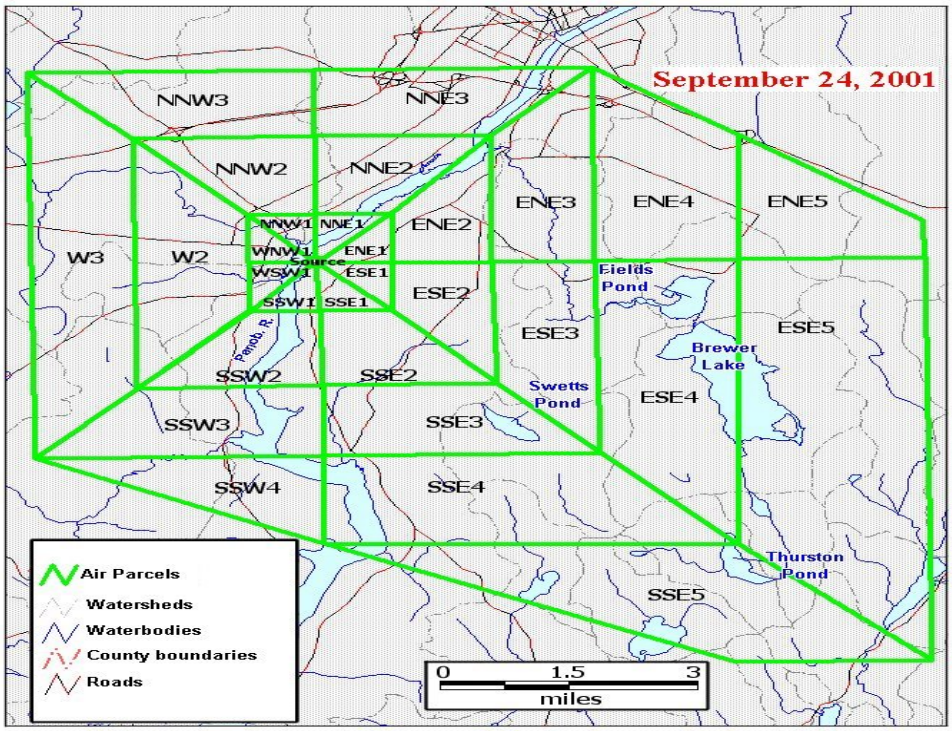

Figure 3-9. TRIM air parcels for HoltraChem facility.

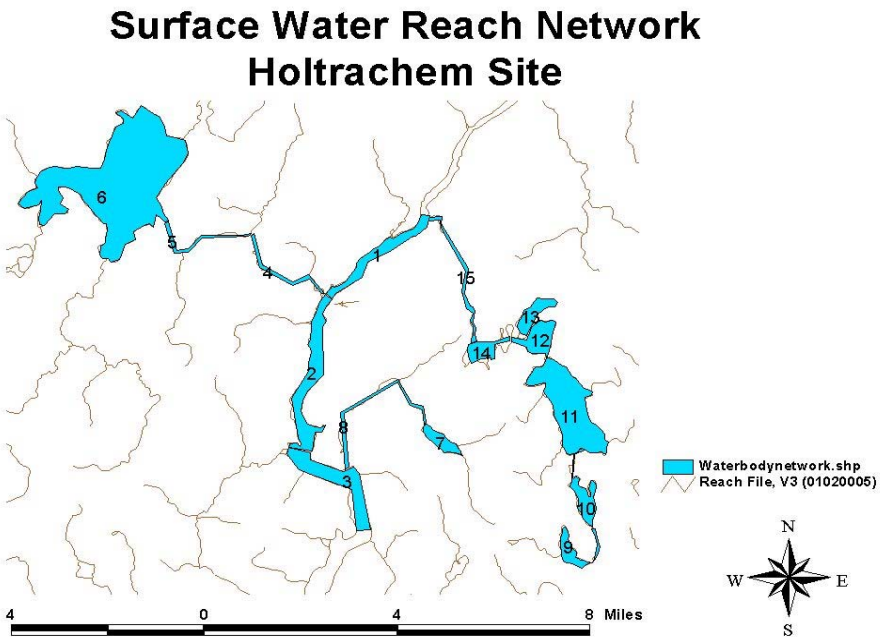

Figure 3-10. 3MRA modeling system surface water reach network for HoltraChem facility.

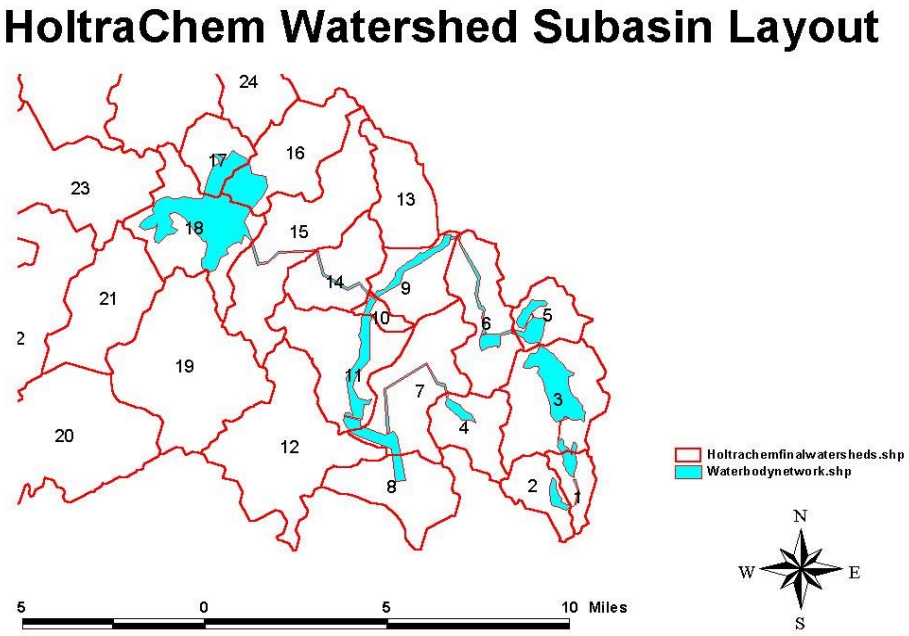

Figure 3-11. 3MRA modeling system watershed subbasin delineation for HoltraChem facility.

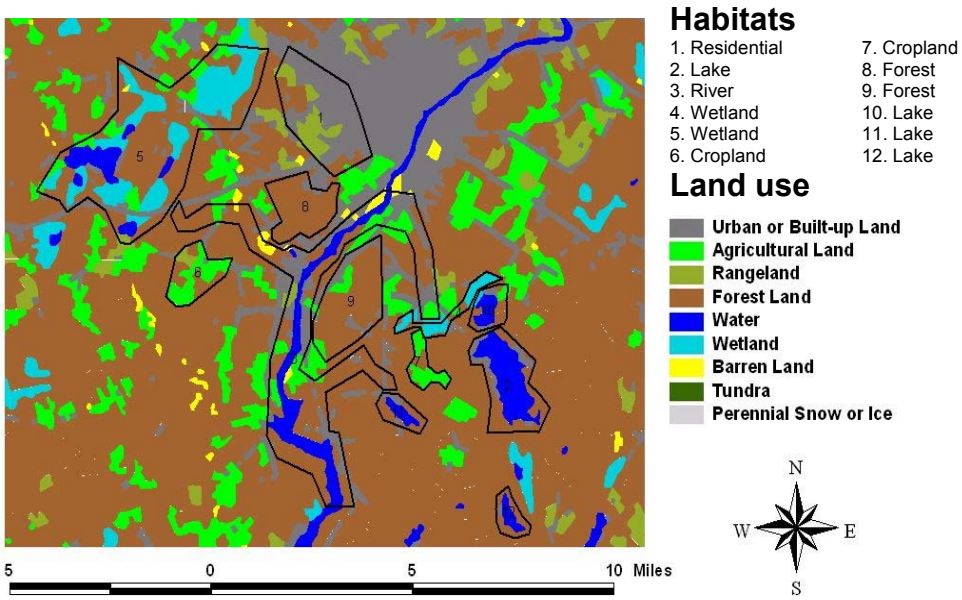

Figure 3-12. 3MRA modeling system land use and ecological habitat delineation for HoltraChem facility.

3.2.3 Data Collection

The data collection effort for the TRIM comparison is on-going.

3.2.4 Model Execution

The TRIM comparison has not yet been executed.

3.2.5 Interpretation of Results

The TRIM comparison has not yet been executed.