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4.0 Overview of 3MRA Version 1.0 Technology

A modeling-based methodology entitled *Framework for Multimedia, Multipathway, and Multireceptor Risk Assessment (3MRA)* (Marin *et al.*, 1999) was originally developed with the goal of facilitating the establishment of national regulatory limits related to “safe” constituent concentration levels in waste streams entering land-based solid waste management units (WMUs). The 3MRA methodology is a conceptual approach to “site-based” regulatory risk assessment problems. Site-based regulatory problems and assessments, in this context, refer to national-scale regulatory decisions that are based on risk assessments conducted at individual sites, where the modeled set of sites was statistically determined to be representative of the total population of actual sites that occur across the nation for some given (present and future, conditioned upon a practical perspective of a given, finite time frame). In its construction (constituent models and data), the 3MRA modeling system embodies a regionalized, site-based approach to estimate risks from waste management units on a regional or national basis.

The actual implementation of that science methodology (i.e., the Technology; 3MRA Version 1.0) for site-based risk assessment of hazardous waste disposal is described in detail in Volumes I, II, and III and the *3MRA Modeling System: Technology Design and Users Guide*. A brief, summary description of the 3MRA Methodology and data sets used to drive the modeling system were presented in Section 3 to introduce the basis for describing the 3MRA Technology and uncertainty in associated input data sets. The full description of the underlying science methodology (Marin *et al.*, 1999, 2003) is found in Appendix A; Volume I provides a summary of the 3MRA “system-level” aspects of the technology (i.e., system level processors, execution management, wastestream concentration “exit level” post-processing schemes, etc.). Volume III introduces and discusses aspects of module-level and system-level verification and validation activities undertaken to date for 3MRA Version 1.0. These cited background documents provide crucial information to the reader in understanding the methodology and the technology underlying the 3MRA Version 1.0 modeling system.

The presentation that follows in this section is intended to provide a brief overview of salient features of the 3MRA Version 1.0 modeling system to facilitate the discussion of model evaluation tasking, and more specifically, activities related to uncertainty and sensitivity analysis of 3MRA. This context is also needed to describe implementation of 3MRA Version 1.0 in a Windows-based parallel supercomputing environment, which is needed to implement various uncertainty and sensitivity analysis experiments in a timely manner for the national assessment strategy.

4.1 Models and Modeling Systems Within a Technology Framework

During the past five years, USEPA's Office of Solid Waste and Office of Research and Development (ORD) have sponsored, along with other U.S. Federal Agencies, the development of the Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) (see Figure 1-1), a Windows-based modeling infrastructure that supports both model development activities and model applications. The Multimedia, Multipathway, Multireceptor Risk Assessment (3MRA) modeling system comprises a unique set of simulation models concurrently developed within FRAMES. While design elements and issues underlying the framework technology (i.e., FRAMES) development is important to place in perspective future model development and application activities, the discussion herein is focused primarily on the first implementation of such a modeling system within FRAMES, i.e., 3MRA Version 1.0. To place into perspective the dichotomies of "Technological Framework", "Modeling System", and "Applications", these concepts are presented in Figures 4-1 and 4-2.

A point briefly emphasized while recognizing "FRAMES", is that many, if not all, of EPA's models require greater attention to the tasks of building and coding them, and performing model evaluation investigations. The concepts of uncertainty and sensitivity analysis represent a generic requirement of such tasking. The capabilities developed for evaluation of 3MRA, described throughout this Volume IV, can eventually be lent to evaluation of other models and modeling systems used by EPA, most readily within the FRAMES technology currently underlying 3MRA. In FRAMES, generic needs in modeling system development (i.e., I/O exchange, execution management, etc.) and model evaluation tasking (e.g., uncertainty and sensitivity analysis) embodied a core software design philosophy in: (1) building 3MRA Version 1.0; and (2) delivering software solutions for conducting uncertainty and sensitivity analysis of 3MRA. The FRAMES design elements imparted to 3MRA represent a continuing recognition by ORD of the need to achieve economies of scale in model development and model evaluation, and the need to improve communication of uncertainty in risk analysis to decision-makers.

4.2 3MRA Version 1.0 Modeling System

Principally designed and developed by staff at the USEPA's Office of Solid Waste and Office of Research and Development (ORD), in collaboration with the U.S. Department of Energy's Pacific Northwest National Laboratory (PNNL, 1999), the FRAMES 3MRA Version 1.0 modeling system includes a set of 17 science modules that collectively simulate release, fate and transport, exposure, and risk associated with hazardous solid waste constituents disposed of in various land-based waste management units. System-level layout of the 3MRA Version 1.0 modeling system is conceptualized in Figure 4-3. Detailed in Volumes I, II, and III and briefly introduced in Section 3.3, the 3MRA modeling system has undergone extensive quality assurance testing throughout its design and development, including module-level and system-level peer-reviews, and independent module and system processor component compilation and test plan execution.

Table 4-1 presents the dimensions of the 3MRA output as it is utilized in deriving “safe” exit levels for chemicals and metals in industrial wastes. These dimensions include 9 major categories:

- Chemicals and metals in the 3MRA database,
- Sources (i.e., waste management units or WMUs),
- Transport and fate processes, and intermedia contaminant fluxes,
- Food chain/food web components,
- Human receptors and exposure pathways,
- Ecological receptors and exposure pathways, and
- Human and ecological risk measures.

4.2.1 Multimedia Multipathway Simulation Processor

The 3MRA modeling system encompasses 966 input variables derived from national, regional, site-based, and chemical properties databases; system level processing control variables; and 45 meteorological model inputs. Over 185 are explicitly stochastic (i.e., represented as stochastic distribution functions). 3MRA also preserves 372 module-level output variables. These model outputs are further distilled and summarized via exit level post-processing routines shown in Figure 4-3. Attributes of 3MRA module-level inputs and outputs are delineated in Section 8. 3MRA starts with a waste stream concentration in a waste management unit (landfill, waste pile, aerated tank, surface impoundment, or land application unit), estimates the release and transport of the chemical or metal throughout the environment, and predicts associated exposure and risk. 3MRA simulates multimedia (air, water, soil, sediments), fate and transport, multipathway exposure routes (food ingestion, water ingestion, soil ingestion, air inhalation, etc.), multireceptor exposures (resident, gardener, farmer, fisher, ecological habitats and populations; all with various cohort considerations), and resulting risk (human cancer and non-cancer effects, and ecological population and community effects).

Processes, intermedia fluxes, parameters, and exposure pathways considered in 3MRA are more fully outlined in Table 4-1. Figures 4-4 and 4-5 show the interconnected flow of downstream module execution associated with the Multimedia Multipathway Simulation Processor (MMSP), relating the system’s formal data consumption and production scheme and connections between the various science modules in the modeling system. In Figure 4-5, the watershed module proper is actually driven only by the airshed module, where the “local” WMU-based watershed is handled directly within the source term modules, where appropriate.

For each particular site and simulation description, appropriate modules are serially executed by the system. Science modules available include those to simulate: contaminant release from sources (i.e., WMUs); contaminant movement through the air, groundwater, soil, watersheds, rivers, lakes, ponds, and wetlands; direct contact of humans, plants, and animals with the waste contaminants; contamination of drinking water wells, farms (through irrigation water or direct atmospheric deposition), plants, and animals (both on land and in waterbodies); ingestion by humans and animals of contaminated materials such as food and soil; and risks to humans, plants, and animals from all potential methods of exposure being modeled.

4.3 Modeling System Execution Flow in 3MRA

For the 3MRA stand-alone PC application (Figure 4-3), the user begins the simulation procedure by activating the System User Interface (SUI). Details of 3MRA Version 1.0 stand-alone (i.e., single PC) model installation and execution are laid-out in the *3MRA Modeling System: Technology Design and Users Guide*. In the SUI, the user selects the sites, source types, chemicals and/or metals, and wastestream concentration ranges (defined as C_w) of interest. Upon launching the simulation set, the SUI generates a header file that contains all of this information specified by the user. The Site Definition Processor (SDP) reads-in the header file information to determine the next scenario to be simulated, and creates a complete set of flat-ASCII “site simulation files” (SSFs). Table 4-2 presents a brief summary of SSF input and GRF output dictionary information, and associated acronyms used in file-naming conventions and internal model representations.

In Figure 4-3, the innermost looping order for a given scenario set selected in the SUI is in order of: (1) wastestream concentrations first, (2) then chemicals/metals, (3) Monte Carlo stochastic iteration # (i.e., realization #), (4) sources, and (5) sites. The *Users Guide* provides more detail on how a user defines scenario sets, and various selection options with the SUI. Generically, the term chemical used in various figures and tables throughout this discussion, infer the collection of 43 organic chemicals and metals evaluated in 3MRA, where notably, Mercury, as a single metal of concern, is represented by 3 separate species.

The term “iteration” and “realization” are used interchangeably throughout this discussion. As well, were convenient, the term model may be used occasionally and usually implies the 3MRA modeling system, where the term “module” implies a constituent model in the integrated modeling system (e.g., ecological exposure model).

4.3.1 Site Definition Files For a Given Scenario

The SSFs represent the input data files for the 17 science-based modules, along with definitions for site layout, chemical properties and the SUI header data. These are created by extracting information from existing databases, or by randomly generating data using distribution information (parameterized in the databases) and statistical subroutines. Various databases represent different levels of data: site-based, regional, and national. These data are constant or stochastic, with rank-ordered cross-correlation data associated with certain variables. The MET database contains five meteorological datasets describing various national monitoring stations (i.e., representing hourly, daily, monthly, annual, and long-term climatic data). The chemical properties database contains needed data related to all chemical-dependent variables. Per model run, 9 different chemical properties files are actually created by the SDP providing module-specific information. These 9 files contain the same list of model inputs defined by the chemical properties dictionary file, where some input values are the same across all 9 files, some are the same within certain files, and some may be different for each file. Separate chemical properties SSF files per model run are broken down by:

1. cpsr.ssf (source),
2. cpws.ssf (watershed),

3. cpvz.ssf (vadose zone),
4. cpaq.ssf (aquifer),
5. cplake.ssf (lake),
6. cpstream.ssf (stream),
7. cpwetlnd.ssf (wetland),
8. cpff.ssf (farmfood), and
9. cphe.ssf (human exposure).

For each site, using a hierarchical scheme, the site-based database is first accessed to acquire actual site data that are constants, and then available stochastic site data are sampled. Regional data are next accessed to fill-in data not in the site-based database, for both constant and then stochastic data. Finally, the national data are used to fill-in any remaining missing data. Whenever possible, data collected at actual waste management facilities are used to fill the databases from which site information is defined. However, when such data are not available, the system selects appropriate information from either regional or national data of the same type. For example, if a site in Georgia were missing data related to rainfall, the system would select a distribution of regional rainfall data. If regional data were not available, the system would select a distribution of national rainfall data.

4.3.2 Model Output and System Level Error and Warning Management

Like the other processors shown in Figure 4-3, the SDP reports any processor-specific warnings or errors to the SUI. The Multimedia Multipathway Simulation Processor (MMSP), which executes each site simulation, uses the generated SSF files and upstream GRF files to create appropriate command line arguments to launch each science module. The SSF file set includes information describing chemical properties, site layout, sources, air data, vadose zone data, aquifer data, watershed data, waterbody network data, farm, terrestrial, and aquatic foodchain data, human and ecological exposure data, and human and ecological risk data.

Like SSF files, each modeling system run (i.e., model run) produces a new set of “global results files” (GRF), one GRF file for each science module, and contains all the key MMSP output data generated during a given site simulation. The Exit Level Processor I (ELP1) output database summarizes and stores key risk results (i.e., as a “risk summary output file” or RSOF) for the entire simulation set (i.e., the set of model runs or scenarios defined by the user in the SUI). The Exit Level Processor II (ELP2) interprets ELP1 output data, and presents final protection summaries of risk in graphical and tabular form (tabular data is stored in “protective summary output files” or PSOFs).

4.3.3 Data Management For Uncertainty and Sensitivity Analysis

As will be detailed in later sections, scenario-specific data represented in the input files (SSFs), output files (GRFs), and scenario set data found within the ELP1 database form the body of information upon which uncertainty and sensitivity analysis are conducted. For conducting sampling-based uncertainty and sensitivity experiments, this entails a system level approach to extraction of individual scenario-specific data (i.e., SSF and GRF files) and management (i.e., aggregation or disaggregation) of ELP1 data across various sets of scenarios.

Aggregated Versus Disaggregated Exit Level Processing

The term “aggregation” used here simply refers to the concept that risk-based receptor protection results, for a given exposure profile in 3MRA Version 1.0, are normally summed in risk bins in the ELP1 database across sites and realizations, where one database is created for each chemical-WMU combination in the scenario set. In 3MRA Version 1.0, the term “disaggregation” implies the separation of such data by archiving individual ELP1 databases by realization (or site) as shown in Figure 2-9 and 2-10. The term “segregation” is used here judiciously to indicate the standard internal disaggregation of risk results in the ELP1. This internal segregation is used in keeping data separated for various exposure profiles (e.g., in preserving risk results by subpopulation, or by chemical and WMU type).

Described in Sections 4.5.6 and 6.4, the term “disaggregation” is also applied in describing concepts facilitated in 3MRA Version 1.x, where a single ELP1 database, with an enhanced data structure design, can be used to preserve risk results through use of separate records for each realization or site. For example, to conduct a pseudo 2nd-order analysis of output sampling error (OSE) (Figure 2-10) requires the segregation or disaggregation of national realizations by realization (i.e., where a single national realization represents a set of model runs conducted across all sites in the site-based database. In summary, the term “disaggregation” is used herein to describe the concept of the segregation of input and output data by deterministic model run, or between sets of deterministic model runs.

Equally important in the simulation design and evaluation stages of 3MRA, the approach to managing raw model data for conducting uncertainty and sensitivity analysis must also be extended to management of system-level warnings and errors across scenario sets. This allows for accurate assessment by the model user of any runtime problems that may have been encountered in execution of the experimental design.

4.3.4 3MRA Pseudo-Random Number Generator

The 3MRA Stat.dll, or Statistical Dynamic Link Library, represents a modular set of routines that facilitates calculation of statistical parameters for several system processors. The HwirMC.dll, or Monte Carlo Dynamic Link Library, is a modular set of routines that simplifies the interface between the Statistical Dynamic Link Library, and the system components, and allows the Stat.dll to run with various compilers. The Stat.dll is statically linked within the HwirMC.dll file. Together, the HwirMC.dll and Stat.dll are responsible for generating random numbers needed for the Monte Carlo Simulation experimentation. The basic approach for a given model run is to seed the Stat.dll using an internal “SDPSeed” value, and request a large list of uniformly distributed random numbers from the Stat.dll. For each stochastic parameter the SDP samples in generating SSF input files, the list of random numbers is used, in order without replacement, to calculate a distribution-specific random value, as described in Section 2.5.2.

In addition to organizing the needed calls to the HwirMC.dll and Stat.dll to obtain random numbers for a variety of distributions used in 3MRA (see Section 8), the SDP is also responsible for providing seed values to initialize the Stat.dll. A critical feature in facilitating system-level testing and evaluating software code changes over time is to provide an ability to

use the same SDP seed value for certain scenario-specific descriptions (i.e., defined by site, source, chemical, initial seed, and realization #), regardless of the order that model runs are executed by the SUI (or SUI Tasker; see Section 6.2.2). Comparative consistency over time in this approach is, of course, lost whenever a new stochastic parameter is introduced into the modeling system. Ideally, the approach should also provide an ability to further randomize seed assignment over sets of multiple model runs to facilitate testing of the overall randomness of the system, and precision in the underlying random processes. The algorithm currently used by the SDP for generating seed values in 3MRA Version 1.0/1.x facilitates both approaches. The latter is facilitated through the user's ability to modify the "SiteIDSeed" field in the Facility table contained within the site-based database. For example, this field can be randomly populated using a uniform distribution returning integers ranging between 1 and 9999.

For the national assessment, 3MRA cycles over sites, WMUs, chemicals, and C_w 's, for a number of iterations or realizations (Figure 4-3). In 3MRA, three model inputs are actually used to establish an internal "SDPSeed" value for any given model run: (1) the SUI "Initial Seed" value specified by the user (an integer ranging from 1 to 32,767; i.e., up to a maximum 2-byte signed integer value); (2) the SiteIDSeed value defined in the site-based database "Facility" table; a unique integer value assigned per site (ranging from 1 to 9999) that can be modified by the user; and (3) realization #. Thus, for a given WMU and chemical, for a given initial seed, SiteIDSeed, and realization #, the SDP will always use the same list of random numbers to populate SSF input files. This would occur, regardless of the actual looping order employed. This feature becomes useful, for example, in sensitivity analysis of exit levels using the disaggregated data structure approach described in Sections 4.5.8 and 6.4.5, where a given set of model runs at a specific site essentially calculates a site-specific % of population protection criteria across 5 C_w 's using the same input vector. The approach is also providential in facilitating precision testing in parallel computing environments.

SDP Seed Algorithm for Random Sampling

The actual algorithm used to create the "SDPSeed" value is described as follows:

1. The SUI writes the variable named initial "Seed" in the header file. The initial Seed value is input by the user in the System User Interface (SUI).
2. The SDP reads this Seed value from the header file and converts it to a 5-character string.
 - a. Leading 0's are added as needed to fill all 5-digit positions of the maximum value possible (i.e., 32,767).
 - b. For example, if Seed = 1019, the string created is "01019"
3. The SDP software reads the "SiteIDSeed" value directly from the "Facility" table using the SiteID value read from the header file.
 - a. Leading 0's are also added as needed to fill all 4-digit positions of the maximum value possible (i.e., 9999).
 - b. For example, if SiteIDSeed = 201, the string created is "0201"
4. The two strings created from Seed and SiteIDSeed are next concatenated.
 - a. The concatenated string is subsequently prefixed by the string "1".
 - b. For example, the string "1010190201" is created.

- c. This concatenated string is next converted to an integer.
 - d. Using "1" at the beginning of the concatenated string preserves the significance of any leading "0" characters, and guarantees the converted integer will be less than the maximum value of a standard integer.
 - e. An interim SDP seed value is thus generated (e.g., 1010190201).
5. The SDP next initializes the statistical package with this interim SDP seed value.
 6. The SDP then reads the current realization # from the header file (e.g., 3)
 - a. If realization # (R) = 1, the final "SDPSeed" value is set to the interim seed value (e.g., 1010190201).
 - b. If realization # (R) > 1, the SDP samples R-1 values from a discrete uniform distribution, returning a minimum value of 1 and a maximum value of 99,999,999.
 - c. The Rth-1 value in this sampling series is then used as the final SDPSeed.
 7. The SDP ultimately initializes the statistical package for subsequent random number generation using the final SDPSeed value.
 8. At the end of this process, the value finally used to seed the statistical package each model run is written out to the "messages.all" file in the GRF directory as the "SDPSeed".

In testing of the original SDP seed generation routine used in 3MRA Version 0.98r, the January 2002 3MRA Developers Version 1.0, and beta Versions of 3MRA Version 1.0, non-random number generation patterns were eventually detected across scenarios (but never within a given model run). Essentially, despite the use of quite different SDPSeed values generated for multiple realizations within a given site using the older approach, seeds used effectively resulted in sampling from the same uniform list of random numbers.

The original approach actually used the SUI Initial Seed value and the SiteID Setting value (i.e., the WMU-SiteID string) in two random number generation sequences, with use of the first returned value to reseed the second sampling from the "IntUniform" distribution. The problem was apparently attributed to a previously unknown Stat.dll behavior associated with using large randomly generated seed values that were slightly smaller than the maximum 4-byte integer return value allowed of 2,147,483,647. While the problem appeared to be solved by specifying a maximum return value of 99,999,999 for the second interim seed in the original approach, the final algorithm described here avoids the potential linkages in use of two randomly generated seeds to arrive at the final SDPSeed value. Other problems were noted in the original approach with respect to the non-uniqueness of the concatenated string being used for the initial seed. The final approach was tested and was found thus far to consistently generate trains of random numbers for various distribution types.

4.4 Use of 3MRA In National Risk Assessment Strategies

The development of 3MRA was originally driven by its initial intended application to provide a nationwide risk assessment for USEPA's Hazardous Waste Identification Rule (HWIR, 1995), described in Section 3. The 3MRA modeling system was designed, for example, to handle the question of identification of waste streams that can safely be released from existing

hazardous waste disposal requirements. Providing an integrated, quantitative, risk-based probabilistic assessment approach for regulatory decision-making, hazardous solid waste with constituent chemical and metal concentrations less than "exit" levels calculated by 3MRA could be reclassified as nonhazardous solid waste.

3MRA application for national assessment strategies, such as for HWIR, is currently based on data collected from 419 representative industrial waste management units, located at 201 sites across the contiguous United States. To eventually expand to hundreds of waste constituents, a dataset for 43 metals and organics was initially developed. The probabilistic national exposure and risk assessment design entails calculating risk for various receptor groups, and addressing specific questions posed via the 3MRA model using its randomly stratified, sampled site-based database. Bayesian inference establishes the risk estimates from this modeling exercise as representing the actual risk of the target population of all national industrial nonhazardous waste management units.

4.4.1 Cross-Sections of Data Analysis Possible

Figure 4-6 shows the spatial extent of the existing national, regional, and site-based data collection approach, and is further summarized in Table 4-3. Table 4-3 represents the actual set of site-WMU facility combinations (419) established through the final site-sampling plan. For assessment of a given risk analysis problem statement, focus is normally placed on evaluating a single WMU-chemical combination (Section 3.2). Risk estimates are always segregated in 3MRA Version 1.0 ELP1 data structures by both chemical of concern and WMU type, along with segregated subpopulation risk analyses preserved for ecological versus human receptors, cohort distinctions within these receptor groups, ring distances from the facility, risk type (cancer, health hazard), risk level, and contact media and exposure pathway (see Table 4-1). There are currently facility descriptions for 56 landfills, 61 waste piles, 28 land application units, and 137 surface impoundments (and 137 aerated tanks), spanning 201 physically distinct waste management facilities across the United States, representing the total of 419 site-WMU combinations. Three ring distances for human concerns are examined by 3MRA (<500m, <1000m, <2000m), representing areas of interest (AOI) portrayed in Figure 4-7. Ecological rings are constructed slightly differently (<1000m, 1000m to 2000m, <2000m).

Based on sensitivity analysis results for the air module, EPA defined the AOI for the 3MRA modeling system as the area encompassed by a circle defined by a 2 km radius extending from the corner of a square WMU. Many Industrial D sites have multiple WMU types; when this occurs, multiple AOIs and "settings" are defined. A setting is the basic modeling unit for the 3MRA modeling system and is defined as each unique WMU type/site combination. Thus, a site with a landfill and a wastepile would constitute two settings.

Because of inherent segregation of data maintained within the ELP1 database(s) during runtime and post-processing, a user can conduct Monte Carlo sampling-based simulation experiments, concurrently, preserving the ability to query upon all of the above internal distinctions. Thus, for example, a single scenario set can be constructed to calculate risk estimates for all WMUs and chemicals in a single simulation experiment on a subset of sites, or

on all sites. A user can later query the system for various exposure profiles of concern, for total populations or subpopulations of receptors, and for various target risk levels and ring distances.

One can also create the same output data constituency iteratively, for example, by partitioning sites in two experiments, or through use of different initial random seeds (as defined by the user through the SUI) used in the data generation and collection approach for large samples of the output distribution. The ELP1 database(s) simply accumulates the results of model runs across multiple experiments, until it is deleted or otherwise archived.

4.4.2 National Site Sample Selection

The following discussion on construction of the site-based database in 3MRA represents a summary of information presented in Volume I. This discussion compliments the discussion presented in Section 3.4 regarding sources of data and associated uncertainties. The material is germane to formulation of national risk assessment questions under investigation, and is important to reflect upon in designing uncertainty and sensitivity analyses to evaluate the model.

The sites in the 3MRA database were selected to be representative of facilities managing nonhazardous waste found in EPA's 1985 *Screening Survey of Industrial Subtitle D Establishments* (Westat, 1987). As discussed in Volume I and Section 3.4, one objective of this survey was to develop a list of representative industrial establishments generating industrial Subtitle D solid waste and managing it onsite. An associated objective was to estimate the number of such facilities, nationally and by industry, as well as to collect data on the size and number of landfills, surface impoundments, land application units, and waste piles at these sites.

To implement the conceptual 3MRA model, a 201-site random sample was selected from the 1985 Subtitle D survey of 2,850 facilities. These facilities represent a population of nearly 150,000 facilities across 17 industrial sectors that managed waste onsite, and had one or more of four types of waste management units—landfill, waste-pile, land application unit, or surface impoundment. The survey was stratified by establishment size and by the 17 standard industrial sectors. To maintain the industry sector stratification, the samples picked for the 201 facilities were chosen from each of the 17 industrial sectors in the same proportion as each sector appeared in the Subtitle D survey. For example, if the organic chemicals industry sector had 3 percent of the facilities in the survey, then 3 percent (that is, six facilities) of the 201 facilities were selected from the organic chemicals industry sector.

4.4.3 Representation of the Site-Based Sample of Subtitle D Facilities

EPA believes that the 201-site sample adequately represents the location and size of waste management units across the industries included in the survey. In terms of geographic representativeness, the locations of the 201 sample facilities with respect to the 2,850 facilities with onsite WMUs in the Industrial D screening survey indicated that the sample provides good geographic representation, and also good ecosystem diversity, as shown in Figure 4-6, where these 201 locations are overlain on Bailey's ecoregion divisions. The spatial coverage of the 201 sample sites, in terms of basic physiographic/climatic regions, as determined by Bailey's ecoregions and the meteorological stations being used, appears to be in good agreement with the

complete sample. Figure 4-6 presents the sample population of 201 facilities that populate the 3MRA site databases; their distribution nationally reflects the distribution of in-scope subtitle D facilities that manage industrial waste nationwide. As suggested by the overlay with Bailey's ecological regions, the sample population represents considerable variability with respect to environmental settings in the contiguous United States.

The basic assumption for the national risk assessment is that these data are representative of the types, characteristics, and locations of nonhazardous industrial WMUs. Overall, one of the most significant general uncertainties within the 3MRA spatial data is the accuracy of facility locations and its impacts on the site-based data collected around each site. Uncertainties in location designation are likely to be significant only in terms of a site-specific analysis at certain sites. The 3MRA Version 1.0 modeling system is site-based, not site-specific. EPA believes that the location review and adjustment efforts conducted in final data processing resulted in site locations representative of current and future locations of Industrial D WMUs, and, as such, these locations are adequate and appropriate for a nationwide site-based analysis. EPA emphasizes that the site-based data collected for the 3MRA example data set are not intended for site-specific risk assessments at any of the 201 facilities.

4.4.4 Representation of Meteorological Data Assignment

Meteorological data were collected regionally by meteorological station, with each of the 201 Industrial D sites assigned to the nearest station with similar weather conditions and adequate weather data for the risk analysis. In making these assignments, EPA considered all available data from 218 meteorological stations across the United States to find the best data for each site. This process resulted in 99 meteorological stations being matched to the 201 industrial sites.

To ensure that Industrial D facilities were modeled with the correct meteorological data, sites were first assigned to the meteorological data stations most representative of conditions at meteorological stations with adequate surface data. Subsequently, the country was divided into an equal number of Thiessen polygons surrounding each station, whose boundaries are equidistant from the site. As a first step in this assignment, a GIS was used to produce a map containing all 199 adjacent meteorological stations. Next, a meteorologist conflated the polygon's boundaries based on climatic and physiographic regions of the country. Data from each meteorological station were considered representative of any Industrial D facility that fell within the surrounding conflated polygon.

4.4.5 National Risk Assessment Problem Statement Formulation

Revisited from Section 1.2.1, a key question 3MRA is capable of answering may be stated as follows: At what waste stream concentration (C_w) will wastes, when placed in a non-hazardous waste management unit over the unit's life, result in:

- Fewer than A% of the people living within B distance of the facility with a risk/hazard of C or less, and

- Fewer than D% of the habitats within E distance of the facility with an ecological hazard less than F,
- At G% of facilities nationwide?

A probability (H) may also be assigned to empirical input uncertainty (e.g., SME, ISE, ME, sampling from non-target populations, etc.) associated with the derived protection profile for percentiles of the target population or subpopulations (e.g., uncertainty in C_w). Furthermore, a probability (I) may be assigned to the simulation-based empirical output uncertainty (i.e., OSE) associated with the derived protection profile for percentiles of the target population or subpopulations. Defining the assessment profile (A, B, C, D, E, F, G, H, I), 3MRA embodies an integrated, probabilistic risk assessment strategy for protection of both ecological and human health. Terminology “A” to “I” is used for simplicity herein, and represents a departure from the indexing employed in the statement of the science methodology of 3MRA by Marin *et al.* (1999).

The above construct, (A, B, C, D, E, F, G), imparts a statement of variability in the output, (H) imparts uncertainty due to lack of knowledge and data, and (I) imparts uncertainty due to computational limitations that may be imposed in describing variance in the output. Discussed in Section 2.5.3, OSE can be reduced completely given enough random “samples” of the model output distribution. Notably, the above 9-tuple description of a given model output of the ELP1 represents the compression of enormous amounts of individual calculations, possibly constructed over 100,000s to 1,000,000s of deterministic simulations for a given national assessment strategy question. 3MRA version 1.x (discussed in Section 6) is equally capable of drilling down into the system, to module-level outputs contained in GRF files, to ask similar questions, and can do this, and all of the above, on a regional or site-specific basis as well. The later is needed, for example, to facilitate sensitivity analysis of exit level calculations.

4.4.6 Waste Stream Concentration Exit Level

An identified waste stream concentration C_w that satisfies the posed assessment profile question is referred to as the exit level or $C_{w_{\text{exit}}}$, indicating the exit threshold for transition from hazardous to nonhazardous waste classification. For the 3MRA assessment strategy, in addition to the values for A, B, C, D, E, F, G, H, and I, $C_{w_{\text{exit}}}$ will also depend on the chemical of concern and waste management unit type (e.g., landfills (LF), waste piles (WP), aerated tanks (AT), surface impoundments (SI), or land application units (LAU)).

While 3MRA facilitates derivation of $C_{w_{\text{exit}}}$ for use in regulatory rulemaking, determinations of actual values A through I in a final assessment by-and-large represent policy decisions, albeit greatly informed by 3MRA simulations. Exposure pathway, receptor group, and cohort group also can be used to further define an assessment profile. One can thus evaluate which subpopulations are at greatest risk, and which pathways drive that risk, elucidating alternative strategies that might be employed in a given regulatory process. Using this robust capability, a decision-maker can, for example, even quantitatively examine issues of environmental justice.

Per 3MRA simulation, the ELP1 (Figure 4-3) calculates risk, receptor by receptor, if a site meets various pre-selected, discrete risk criteria (C, F), at various discrete distances (B, E), for various population protection percentiles (A, D). After all simulations are completed, the ELP2 extracts information from the ELP1 output data, based on a given user-selected profile (A, B, C, D, E, F), providing interpolation capabilities to derive $C_{w_{exit}}$ for a user-selected site protection level G. Currently in 3MRA Version 1.0, graphical display of uncertainty probabilities, H and I, are constructed outside the ELP2. There is also no existing capability in 3MRA to easily facilitate two-dimensional (i.e., 2nd-order) analysis of empirical input uncertainty, although 3MRA Version 1.x (Section 6) has the ability to more easily construct a pseudo 2nd-order analyses for separation of empirical uncertainty and variability, while considering output sampling error (OSE) due to Monte Carlo sampling imprecision (Section 2.6.6 and Section 6).

4.5 Science Module Overview - 3MRA Version 1.0

The following information summarizes basic information on 3MRA reviewed earlier in Volume I and briefly outlined in Section 3.3. The first purpose of the discussion immediately following is to more clearly set out perspectives on temporal variability, which in 3MRA exit-level calculations is always “rolled-up”, and spatial variability. The second purpose is to quickly review the role of each module, and assign familiarity in acronyms used to identify various modules and their inputs (Table 4-2). Regarding empirical uncertainty due to constituent science module error (ME), discussions are presented in Volume I covering: (1) strengths and advantages; and (2) uncertainty and limitations, on a science module-by module basis.

4.5.1 Model Temporal Scale

The 3MRA model operates on an annual average time scale, with individual module results being reported as a time series of annual average concentrations or fluxes. Individual modules may operate on different time scales, depending on what is appropriate for the modeling objectives for a given model run. Reasons for departures from annual average conditions include the need for shorter time scales to accurately estimate waste constituent release or fate and transport in media sensitive to fluctuations in meteorological data. For example, the surface impoundment module needs monthly data to capture seasonal temperature extremes that can impact volatilization. The land application unit (LAU) and watershed modules require daily precipitation data to accurately estimate precipitation-driven runoff and erosion events.

The modeling time frame for exposure and risk depends on the migration times of the waste constituents in the receiving media. For most media (i.e., air, surface water, soil), the exposure and risk occur in the same time frame as the release from the impoundment. For media such as groundwater, where both the media and chemical properties attenuate the migration process, the exposure and risk time frame can be tens to thousands of years after the release. The modeling time frame, therefore, varies for each chemical and environmental medium considered, for each specific facility and WMU. The maximum time limit for considering exposure and risk in 3MRA is defined as 10,000 years. This value was assumed to capture the significant impacts of most chemicals included in the analysis.

A given receptor will be considered subject to exposure from various, but not necessarily all, pathways simultaneously. The aggregate risk to any individual receptor is defined as the sum of the risks from each pathway over a given time period. Given that the exposure in the different media can occur over significantly different times, aggregation of risk is performed for exposures that occur at the same time. For instance, exposures and risks due to contaminated air occurring in the first 10-year time frame is not aggregated with exposures and risks due to contaminated groundwater occurring in the hundredth year time frame. Risks are aggregated across different exposure routes (i.e., ingestion, inhalation) considering current EPA guidance with regard to similarity of toxicological endpoints.

4.5.2 Source Modules

Waste management units modeled by 3MRA are listed in Table 4-1 along with release pathways and directly impacted media. The landfill, waste pile, surface impoundment, and land application units were selected for modeling in 3MRA because, according to an EPA industrial waste screening study, they are the most likely destinations for industrial nonhazardous waste (Westat, 1987). Aerated tanks were modeled because there has been a shift away from surface impoundments to aerated tanks for managing liquid hazardous waste since the screening study was done. If hazardous waste managed in an aerated tank becomes exempt, it is likely that it would still be managed in the same aerated tank.

Landfill (LF)

The landfill module simulates the gradual filling of an active landfill and the subsequent long-term releases during its active life, and after closure. The module assumes that the landfill is composed of a series of vertical cells of equal volume that are filled sequentially, with each cell being filled in 1 year. The landfill module is based on the assumption that the contaminant mass in the landfill cells may be linearly partitioned into the aqueous, vapor, and solid phases. The module simulates chemical and metal behavior during the active lifetime of the landfill (30 years), and continues simulating their releases until less than 1 percent of the initial mass is left, or for a total of 200 years, whichever occurs first. The 3MRA landfill has minimal controls (e.g., no liner) and is constructed below grade.

Wastepile (WP)

The waste pile module simulates the management of wastes in a storage pile situated on the ground (i.e., above grade). Wastes are removed from the pile after its active lifetime (30 years), and chemicals and metals are released only during the operating lifetime of the pile. Waste pile height and area are set and constant, and the waste in the pile is replaced annually.

Land Application Unit (LA or LAU)

The land application unit module simulates the disposal of wastes in an open field for the purpose of degradation or treatment of chemicals. The module assumes that waste is applied to the surface soil periodically, and then tilled into the top layer of the soil during each of 40 years of operation. Chemicals and metals are released during active operation, and up to 200 years

after the land application unit has been closed (releases stop when less than 1 percent of the total mass remains). The module simulates annual releases of: leachate to the unsaturated zone; volatile and particulate emissions to the air; dissolved chemicals in runoff; and chemicals absorbed to eroded particles in runoff.

Surface Impoundment (SI)

The surface impoundment module simulates liquid waste disposal in an earthen material pit, and chemical and metal releases during the lifetime of the unit. The impoundment does not receive runoff from or contribute runoff to the watershed. No liner other than native soils is assumed to be present, and there is no cover to reduce volatile emissions. The surface impoundment module simulates annual release of leachate to the unsaturated zone and volatile emissions to air.

Aerated Tank (AT)

The aerated tank module simulates releases from aerated tanks used for the treatment of wastewaters. 3MRA models aerated tanks (versus storage or other types of treatment) because aeration increases volatilization and potential air emission risks. The primary source for aerated tank data was EPA's National Survey of Hazardous Waste Treatment, Storage, Disposal, and Recycling Facilities (TSDR Survey) (EPA, 1987). These surveys were used to populate the database of unit characteristics. 3MRA assumes that an aerated tank would operate as long as the surface impoundment (50 years). However, each aerated tank has a maximum lifetime of 20 years, and, therefore, the operating lifetime includes a tank replacement every 20 years. The aerated tanks are assumed not to fail or leak liquids to soil or surface runoff. While physical characteristics of the other four source modules are measured or directly estimated, site-based data for facility layout of aerated tanks (e.g., tank size characteristics) are selected randomly from a discrete distribution of 624 possible source configuration profiles.

4.5.3 Transport, Fate Processes, and Intermedia Contaminant Fluxes

Air Module (ar)

The purpose of atmospheric modeling in 3MRA is to estimate, at various receptor points in the area of interest, the annual average air concentration of dispersed waste constituents (particles and vapors), and the annual deposition rates for vapors and particles. The area of interest is defined by a 2-km radius measured from the edge of the largest area source (WMU) at the site. For a given facility and its association with a given meteorological data station, unit concentration contaminant deposition profiles need only be created once if site layout characteristics do not vary. These profiles are stored in "LFO" files. For aerated tank configurations, which are randomly varied from realization to realization, there are 624*137 possible combinations, and thus 85,488 possible aerated tank LFO profiles.

Watershed Module (ws)

Fate and transport processes simulated by the watershed module are volatilization, leaching, runoff, erosion, and biological and/or chemical degradation. Chemicals are transported by runoff and erosion into adjacent waterbodies. Because the surface transport processes are hydrologically related, the land areas surrounding the surface impoundment are disaggregated into watershed subbasins. A watershed subbasin can vary in size from a portion of a hillside, similar to the local watershed construct of the land application unit module, to much larger areas encompassing regional stream or river networks. In all cases, a watershed is modeled as a single, homogeneous area with respect to soil characteristics, runoff and erosion characteristics, and chemical concentrations in soil. No spatial disaggregation below the watershed level is made.

Groundwater (Vadose and Aquifer) Modules (aq, vz)

The 3MRA vadose and aquifer modules simulate the fate and transport of waste constituents released from land-based waste management units through the underlying unsaturated or vadose zone (soil) and saturated zone (surficial aquifer). The approach considers: (1) the formation and transport of transformation products; (2) the impact of groundwater mounding on groundwater velocity; (3) finite source as well as continuous source scenarios; and (4) metal transport.

The composite vadose/aquifer model consists of a one-dimensional (1-D) vadose zone module that simulates infiltration and dissolved waste constituent transport from the bottom of the waste management unit through the unsaturated zone to the water table, which is coupled with a pseudo 3-D saturated zone module. The saturated zone module consists of a 1-D groundwater flow submodel and pseudo 3-D transport submodel. The saturated zone groundwater flow submodel accounts for the effects of leakage from the land disposal unit and regional recharge on the magnitude and direction of groundwater flow. The saturated zone transport submodel also accounts for pseudo 3-D advection and dispersion, and linear or nonlinear equilibrium sorption. The modules are based on computationally efficient solutions ideally suited for use in Monte Carlo frameworks. The modules are part of EPA's Composite Model for Leachate Migration with transformation products (EPACMTP).

The vadose zone module receives infiltration and solute mass fluxes from the source modules. The migration of chemicals and metals in the vadose zone is terminated at the water table where chemical and metal fluxes, in the form of concentrations, are transferred to the aquifer module. The aquifer module also receives areal recharge from the watershed module. The aquifer module provides time-dependent, annual average chemical concentrations at receptor wells and annual average chemical fluxes at an intercepting stream located in the AOI.

Surface Water Module

The 3MRA surface water module models streams, lakes, ponds, and wetlands. Chemical and metal mass released from a WMU can enter a nearby surface waterbody network in runoff and eroded particles directly from the WMU, from atmospheric deposition to the water surface, in runoff and on suspended sediment from adjoining watershed subbasins, and by interception of

contaminated groundwater. The chemical or metal is then subject to transport and transformation processes occurring within the waterbody network, resulting in variable chemical or metal concentrations in the water column and in the underlying sediments. These chemical and metal concentrations are the basis for direct exposure to human and ecological receptors, and indirect exposure through uptake in the aquatic food web.

The surface water module estimates annual average total and dissolved chemical concentrations in the water column, and in the underlying sediments, at various receptor points within the affected waterbody. Transport/transfer processes modeled include advection, vertical diffusion, volatilization, deposition to the sediment bed, resuspension to the water column, and burial to deep sediments. Transformation processes modeled include hydrolysis and biodegradation as pseudo-first-order reactions influenced by temperature and pH. Outputs from the surface water module include water column and sediment concentrations that are used by the aquatic food web module and the ecological exposure module.

4.5.4 Food Chain/Food Web Components

Farm Food Chain Module (ff)

The farm food chain module calculates the concentration of a chemical or metal in homegrown produce (fruits and vegetables), farm crops for cattle (forage, grain, and silage), beef, and milk. The concentrations in homegrown produce, beef, and milk are inputs to the human exposure module and are used to calculate the applied dose to human receptors who consume them. The module is designed to predict the accumulation of a contaminant in the edible parts of a plant arising from uptake of contaminants in soil, and through transpiration and direct deposition of the contaminant in air.

Concentrations are predicted for three main categories of food crops presumed to be eaten by humans: exposed fruits and vegetables (i.e., those without protective coverings, such as lettuce), protected vegetables (i.e., those with protective covering, such as corn), and root vegetables (e.g., potatoes). In addition, the module estimates the contaminant concentration from the biotransfer of contaminants in feed (i.e., forage, grain, and silage), soil, and drinking water to beef and dairy cattle through ingestion.

The module contains two separate programs. One predicts the concentration of contaminants in produce grown by home gardeners, and the other predicts the concentration of contaminant in food crops, beef, and milk produced on farms. The methodology for home gardeners uses point estimates of air and soil concentrations at the residential receptor location assigned to each census block. In contrast, the methodology used for farms calculates an area-weighted average soil concentration for the farm, and uses an interpolation subroutine to estimate the average air concentration across the area of the farm. Thus, the predicted concentrations in farm food crops reflect the spatial average for the farm. Similarly, the feed concentrations for the cattle are derived using spatial averages. In predicting concentrations in beef and milk, the contribution from contaminated drinking water sources, such as farm ponds or wells on the farm, is also considered. However, irrigation of crops and home gardens is not modeled.

Terrestrial Food Web Module (tf)

The terrestrial food web module calculates chemical concentrations in soil, terrestrial plants, and various prey items consumed by ecological receptors, including earthworms, other soil invertebrates, and vertebrates. These concentrations are used as input to the ecological exposure module to determine the applied dose to each receptor of interest (e.g., deer, kestrel). The module is designed to calculate spatially averaged soil concentrations in the top layer of soil (i.e., surficial soil), as well as deeper soil horizons (i.e., depth-averaged over approximately 10 cm). The spatial averages are defined by the home ranges and habitats that are delineated within the area of interest at each site. Once the average soil concentrations are calculated, these values are multiplied by empirical bioconcentration factors (for animals) and biotransfer factors (for plants) to predict the tissue concentrations for items in the terrestrial food web.

The conceptual approach used in developing the module was designed to predict a range of concentrations in plants and prey items to which a given receptor may be exposed. The predator and various prey are represented in the site layout by allowing the respective home ranges to overlap. For plants and soil fauna, this module estimates concentrations based on the spatially averaged soil and air concentrations across each home range. Receptors that ingest plants and soil invertebrates as part of their diet are presumed to forage only within that part of the home range that is contained within the AOI at a given site. Consequently, home range defines the spatial scale for concentrations in soil, plants, and prey (both mobile and relatively immobile) to which a given receptor is exposed.

Aquatic Food Web Module (af)

The aquatic food web module calculates chemical and metal concentrations in aquatic organisms that are consumed by human and ecological receptors (e.g., fish file, aquatic macrophytes). These concentrations are used as input to the human and ecological exposure modules to determine the applied dose to receptors of interest. The module is designed to predict concentrations in aquatic organisms for both coldwater and warmwater aquatic habitats. The methodology uses an internal probabilistic algorithm that cycles through the database on prey preferences to select dietary fractions for TL3 and TL4 fish for predicting tissue concentrations (TL - trophic level).

4.5.5 Human Receptors and Exposure Pathways

Human Receptors

Human receptor types include residents, gardeners, farmers, and fishers, each divided into five age cohorts. Contaminated foodstuffs are considered only for resident gardeners and farmers. EPA is concerned with the potential risk to the exposed population within a 2-km radius of the surface impoundments at a facility. Census and land use data are used to identify receptor types and populations that are potentially exposed in the AOI for each site.

Human Exposure Pathways

The human exposure assessment predicts the type, timing, and magnitude of exposures that receptors may experience due to contact with the chemicals and metals of potential concern (these exposures are calculated using the human exposure module). Exposures are evaluated for potentially complete exposure pathways. An exposure pathway describes the course that a waste constituent takes from a source to an exposed individual. An exposure pathway is complete when there is a route by which a human receptor takes-up a chemical or metal that was released from the source of concern.

Exposure routes include uptake mechanisms such as ingestion and inhalation. When modeling human exposure, the exposure routes considered are:

- Direct ingestion of soil,
- Direct ingestion of contaminated groundwater (private groundwater wells only),
- Inhalation of contaminated shower air (private groundwater wells only),
- Inhalation of volatile emissions from impoundments,
- Inhalation of particulate emissions from sludge (post-closure in place),
- Indirect exposure through ingestion of produce (gardeners, farmers) and meat and dairy products (farmers only) contaminated from air deposition or erosion/runoff to soil and subsequent plant uptake and consumption, and
- Indirect exposure (all recreational fishers) through ingestion of TL3 and TL4 fish contaminated through the aquatic food web from air deposition onto, or erosion/runoff into, surface waterbodies surrounding each WMU.

In addition to these, as shown in Table 4-1, summaries are also calculated for all ingestion routes, all inhalation routes, and all ingestion plus inhalation routes.

Because human health benchmarks are pathway-specific, pathways and routes are combined in the analysis. The evaluation of human exposure must include evaluation of both spatial and temporal variability in exposure across a site, and also variability and uncertainty in exposure factors for each receptor type. The exposure for each of these receptor types is estimated at each receptor location across the study area to capture spatial variability in exposure, and, for every year over the modeling time frame, to capture temporal variability at each location. In addition, each receptor type has distributions for all exposure factors for each of the age groups. In 3MRA, these age cohort-specific distributions were derived from percentile data for contact rates, body weight, etc. Exceptions include fixed values assumed for exposure duration (set to 9 years) and medium or food-specific estimates of fraction contaminated.

Human Exposure Module (he)

The human exposure module calculates the applied dose (milligram of constituent per kilogram of body weight) to human receptors from media and food concentrations calculated by other modules in the 3MRA methodology. These calculations are performed for each receptor, cohort, exposure pathway, and year at each exposure area.

The human exposure module calculates exposures for two basic receptor types: (1) residential receptors (residents and home gardeners); and (2) farmers. Residential receptors may also be recreational fishers in addition to being a resident or home gardener. Farmers may be beef farmers or dairy farmers, and either type of farmer may also be a recreational fisher. Within each of the two basic receptor types, the human exposure module calculates exposures for five age cohorts: infants (ages 0-1 year), children ages 1-5 years, children ages 6-11 years, children ages 12-19 years, and adults (ages 20 years and up).

Human Risk Module (hr)

The essence of the 3MRA approach for human health is an evaluation of total risks to receptors incurred as a result of simultaneous exposure from different pathways. To calculate risks from multiple pathway exposures, the 3MRA human risk module considers the same two basic human receptor types: (1) residential receptors (residents and home gardeners); and (2) farmers. In total, there are eight categories of human receptors:

- Resident,
- Home gardener,
- Resident fisher,
- Home gardener fisher,
- Beef farmer fisher,
- Dairy farmer fisher,
- Beef farmer, and
- Dairy farmer.

The human exposure module models each of these eight categories and provides outputs for each. The human risk module uses these outputs to calculate cancer risks and/or hazard quotients (HQs) for each category. However, to maintain output storage at reasonable levels, it aggregates results into four composite receptor categories (resident, resident gardener, fisher, and farmer) to develop the cumulative population frequency histograms and critical years. These three basic human risk module functions (calculating risk/HQ, building cumulative frequency histograms, and determining critical year) are performed for each radial distance in a series of nested loops. Seven (7) risk bins are utilized for cancer, and four (4) are utilized for human health hazards.

4.5.6 Ecological Receptors and Exposure Pathways

Ecological Receptors

EPA developed a representative habitat scheme for 3MRA, intended to capture the variability in ecological systems, as well as to provide explicit spatial boundaries for the exposure and risk calculations. This scheme provides the basis for incorporating the unique characteristics of each site into the risk assessment methodology. That is, the habitat was chosen as the ecological unit of interest that provides the context for the assessment endpoints and ecological receptors included in the 3MRA database. Within the AOI for each of the 201 sites,

representative habitats were delineated depending on the site data relevant to exposure, such as land use and the presence of surface waterbodies and/or wetlands.

A simple food web structure was constructed for each of the three major habitat groups, and the representative habitats were populated by ecological receptors that cover a broad range of feeding strategies along the trophic continuum. These simple food webs include many common characteristics (e.g., producers, soil biota); however, there are differences for each of the representative habitats related to the particular region, site location and the type of habitat.

Ecological Exposure Pathways

Various combinations of media and exposure routes are evaluated by the ecological exposure module for each group of ecological receptors, and are presented in detail in Volume I.

Ecological Exposure Module (ee)

The ecological exposure module calculates the applied dose (in mg/kg-d) to ecological receptors that are exposed to contaminants via ingestion of contaminated plants, prey, and media (i.e., soil, sediment, and surface water). These dose estimates are then used as inputs to the ecological risk module. The ecological exposure module calculates exposures for each receptor placed within a terrestrial or freshwater aquatic habitat (as defined in the site layout). Thus, exposure is a function of the:

- Habitat to which the receptor is assigned,
- Spatial boundaries of the species' home range,
- Food items (plants and prey) that are available in a particular home range,
- Dietary preferences for food items that are available, and
- Media concentrations in the receptor's home range.

In essence, the module estimates an applied dose for birds, mammals, and selected herpetofauna that reflects the spatial and temporal characteristics of the exposure (i.e., exposure is tracked through time and space).

The conceptual approach in developing the ecological exposure assessment for 3MRA was to reflect the major sources of variability in ecological exposures. In particular, the approach considers variability through:

- Development of representative habitats,
- Selection of receptors based on ecological region,
- Recognition of opportunistic feeding and foraging behavior using probabilistic methods,
- Creation of a dietary scheme specific to region, habitat, and receptor, and
- Application of appropriate graphical tools to capture spatial variability in exposure.

Depending on the type of habitat and chemical-specific uptake and accumulation, animals may be exposed through the ingestion of plants (both aquatic and terrestrial), soil invertebrates, aquatic invertebrates, fish, terrestrial vertebrates, media, or any combination that is reflected by the dietary preferences of the particular species. The ecological exposure module also includes an algorithm to construct a unique, randomly selected diet for each receptor species at each site where it occurs. This algorithm reflects the variability in receptor species' dietary composition. Dietary preference data required by the ecological exposure module includes a list of potential diet items for each species and the maximum and minimum proportion of the species' diet that each item can comprise. Diet items are categorized as one of 17 types of prey recognized by the 3MRA modeling system.

Ecological Risk Module (er)

The ecological risk module calculates hazard quotients for a suite of ecological receptors assigned to habitats delineated at sites. These receptors fall into eight receptor groups: mammals, birds, herpetofauna, terrestrial plants, soil community, aquatic plants and algae, aquatic community, and benthic community. The spatial resolution of this module is, to a large degree, determined by the home ranges and habitats delineated at each site.

The habitat area is important in assessing risks to several receptor groups (e.g., benthic community). Exposures and associated risks are considered across the entire habitat rather than for one or more home ranges. The temporal resolution is based on annual average applied doses or media concentrations. The HQs for all receptors assigned to the study site are calculated and placed into one of five risk bins developed to assist decision-makers in creating appropriate risk metrics. Five (5) HQ risk bins are used in developing cumulative distribution functions of risk.

In addition to spatial variability across a site, particular attributes considered relevant to ecological risks and regulatory decision-making include the following:

- Habitat type (e.g., grassland, pond, permanently flooded forest)
- Habitat group (i.e., terrestrial, aquatic, and wetland)
- Receptor group (e.g., mammals, amphibians, soil community)
- Trophic level (i.e., producers, TL1, TL2, TL3, top predators).

In calculating receptor-specific HQs, the ecological risk module does all of the necessary accounting to develop distributions based on the specific receptor and habitat groupings of interest. The ecological risk module: (1) reads-in information about the chemical concentrations that each receptor is exposed to; (2) calculates hazard quotients based on the ecological benchmark (EB) or chemical stressor concentration limit (CSCL), and the chemical exposure information; and (3) provides summaries of ecological risk information developed for the simulation to determine when the critical years, i.e., those with the maximum HQs, occur. For any given year, the set of HQ data is stored as a series of distributions along with their attributes. The cumulative frequency distributions are composed of a series of bins for different ranges of HQ values. The bins are populated based on the number of simulated receptors with HQ values in the range defined for the given bin.

Outputs are generated for three areas of the site relative to the distance from the edge of the waste management unit. These distances are termed EcoRings and depict the following: (1) habitats that fall within 1 km of the WMU; (2) habitats that fall between 1 and 2 km from the WMU; and (3) habitats within 2 km of the WMU (i.e., across the entire site's AOI). The HQ results for habitats that intersect both EcoRings are attributed to the risk results for both of those distances. In other words, the habitat risks are not apportioned by distance; they are reported as though they are positioned entirely within each distance ring. Because the fundamental unit of this analysis is the representative habitat (not distance to the waste management unit), it was considered inappropriate to truncate risks by distance.

4.5.7 Risk Metrics

Described in more detail in Section 6 (see Figure 6-8), risk metrics represent the outputs of the risk analysis and the information that is needed to support the decision-making process. The 3MRA system uses the exit level processor (ELP) to store (i.e., ELP1), and then process and display risk metrics (i.e., ELP2). The 3MRA Version 1.0 ELP processor group contains three components:

- The ELP1 reads the human health and ecological risk/hazard results from the human risk and ecological risk modules, aggregates key risk results for certain receptor exposure profiles across modeling system runs, by chemical, by WMU, by C_w , by target risk bin, and by population percentile, and stores these results in a series of Risk Summary Output Files (RSOFs).
- The ELP2 provides chemical-specific exit level wastestream concentrations for selected exposure profiles (i.e., risk summary scenarios) that meet a user-specified level of protectiveness, in tabular and graphical formats.
- The Risk Visualization Processor (RVP) graphically displays exit level wastestream concentrations, and is contained within the ELP2 module.

The excess human cancer risk and human and ecological health hazard quotient bins currently used in the 3MRA system include:

- **Excess Human Cancer Risk (7 bins):**
 - $< 10^{-8}$,
 - 10^{-8} and $< 5 \times 10^{-7}$,
 - 5×10^{-7} and $< 10^{-6}$,
 - 10^{-6} and $< 5 \times 10^{-5}$,
 - 5×10^{-5} and $< 10^{-5}$,
 - 10^{-5} and $< 10^{-4}$, and
 - $> 10^{-4}$.
- **Noncancer Human HQ (4 bins):**
 - < 0.1 ,
 - 0.1 and < 1 .

- 1 and < 10, and
- >10.
- **Ecological HQ (5 bins):**
 - < 0.1,
 - 0.1 and < 1,
 - 1 and < 10,
 - 10 and < 100, and
 - > 100.

Human Health Risk Summary Output

For human risk, the current MS-Access-based 3MRA Version 1.0 ELP1 stores and maintains, by chemical and WMU type, the number of “site and iteration” pairs that protects at least some percentile of the human population (0%, 5%, 25%, 50%, 75%, 85%, 90%, 95%, 98%, and 99%) for each “risk bin/ C_w ” or “hazard-bin/ C_w ” pair by distance, pathway, receptor, cohort, and critical-year (T_{crit}) method. The ELP2 determines the Protective Summary Output File (PSOF) that specifies which wastestream concentrations will provide risks below the target risk level for the user-selected percentage of receptors due to exposure at a user-specified percentage of the sites. The population risks estimated across facilities can be summarized by exposure pathway, by receptor type, and by chemical.

Ecological Risk Summary Output

For ecological risks, the current MS-Access-based 3MRA ELP1 data structure similarly uses the ecological hazard quotient bins to store, by chemical and WMU type, the number of “site and iteration” pairs that protects at least some percentile of the population for each critical-year method and “hazard-bin/ C_w ” pair by distance and habitat group, distance and habitat type, distance and receptor group, distance and trophic level, receptor group and habitat group, or trophic level and habitat group.

Thus, for the human health and ecological risk summary outputs, the “risk-bin/ C_w ” and “hazard-bin/ C_w ” fields in the ELP1 data structure store integer numbers, where each model run either a “1” or a “0” is added to bins applicable for the given site-based scenario considered (see Figure 6-8). The updating of individual “risk-bin/ C_w ” or “hazard-bin/ C_w ” fields in the ELP1 data structure reflects the basic determination per model run that the given population percentile was (i.e., add 1) or was not (i.e., add 0) protected for the given exposure profile. For some chemicals, various risk factors are not applicable. In such a case, associated exposure profiles are not actually updated, in effect adding a “0” to all associated “hazard-bin/ C_w ” fields. The last risk/health bin for each C_w and 0% population protection stores the number of model runs that have been considered for a given exposure profile, by chemical and WMU-type, allowing calculation of the % sites protected for the global scenario set considered.

4.5.8 Aggregation Versus Disaggregation of Risk Metrics

Using tools described in Sections 6.4.4 and 6.4.5 for 3MRA Version 1.x, ELP1 data can also be maintained in a more resolved, disaggregated form (via MySQL data structures) by either: (1) creating a different ELP1 database for each site and/or iteration (using the “aggregated” data structure approach); or (2) alternatively using a single database that preserves site and iteration indices (using the “disaggregated” data structure approach; see Table 6-14). In the former case, it is impractical to maintain different databases across sites due to data storage requirements, but is quite manageable for across iterations. For the same reasons, the latter case will not allow full preservation of every “exposure profile” calculated by 3MRA. To better interpret the 3MRA Version 1.0 ELP1 descriptions given directly above for human and ecological risk summaries, the reader is referred to Table 6-8, which provides the ELP1 data structure in MySQL database format. The field “tableName” describes the various “exposure profiles” considered by 3MRA. In 3MRA Version 1.0, a separate Access table is actually maintained for each exposure profile,, where a separate Access database is maintained for each chemical-WMU combination.

A basic approach in 3MRA sensitivity analysis will be to first use aggregated data structures for consideration of a set of sites, determine the dominant pathways, media, and receptors with the greatest risk, and then use the disaggregated ELP1 approach to evaluate more in depth those inputs that drive output sensitivity. In keeping with the underlying science-based methodology (Section 3.2), this would be done on a chemical-WMU basis. One of the driving forces behind development of the fully disaggregated data structure across sites and iterations is the current destruction of the mapping between individual modeling system input vectors and risk summaries currently saved in the aggregated ELP1 data structure. In the aggregated ELP1, many input vectors (the set describing all sites and iterations sampled for a given experiment) are all mapped to a single exit level calculation for each exposure profile of interest (i.e., mapped to a set of exit levels representing various exposure profiles of interest as calculated by the ELP2).

In addition to population protection outputs generated by exit level processing (ELP) performed by 3MRA Version 1.0, with the input/output (I/O) extraction capabilities in 3MRA Version 1.x (see Section 6), one can also examine any relationship within and between any 3MRA inputs (i.e., in SSFs) and any of the outputs of 3MRA’s underlying science modules (i.e., in GRFs), for a single site or set of sites, across multiple realizations. As an example, exposure and risk from a particular wastestream can be quantified for a specific type of aquatic biota (e.g., periphyton) in a given foodweb (coldwater stream habitat) at a given site (e.g., site #0113456) in a specific local watershed (e.g., waterbody network #1), in a specific reach (e.g., reach #2 of waterbody network #1), at a specific time (e.g., $t = 30$ years; relative to initiation of waste disposal activities).

4.6 Calculation Flow and Outputs

Figure 3-1 (Section 3.3.3) illustrates how the 3MRA model conceptually executes a given scenario set defined by the user through the System User Interface (SUI). In implementation of 3MRA Version 1.0, the basic “internal” model looping order (Steps 5 to 17 in Figure 3-1) is

always the same, where the SUI initiates individual deterministic model runs by looping first through C_w , then through chemicals, then through random iterations, next through sources, and finally through sites, as shown in Figure 4-3. The actual “internal” and “external” model looping order (Steps 1-4 and 18-21) would be immaterial to the ELP2 calculation outcome, but the final procedure, as outlined in Section 4.6.1, offers efficiencies in SSF file generation for sets of multiple scenarios in stand-alone PC execution mode.

The parallel execution mode procedure (3MRA Version 1.x; see Sections 5 and 6.2) offers a slightly different looping order (i.e., C_w , chemical, source, site, and iteration), moving the iteration loop to the outside, since it takes advantage of abilities to disaggregate existing 3MRA Version 1.x ELP1 data structures (see Table 6-8) by site and iteration to preserve dimensions of uncertainty and/or to calculate OSE. Another reason for this different paralleling loop structure is the need to ensure quality assurance in ELP1 data for large sets of runs (e.g., 100,000's to 1,000,000s) across several computers. A limiting feature of the existing aggregated ELP1 data structure in (see Table 6-8) is that once a run has been aggregated, it cannot be removed. As an example, issuing sets of C_w 's to a single machine parallel execution mode (Section 5) is problematic if the machine does not complete the entire C_w loop. Efficiency in SSF generation by the SDP is sacrificed for this increased demand for quality assurance in the output sample set sought. This is only a concern for the aggregated ELP1 (Table 6-8), not the disaggregated ELP1 (Table 6-14).

4.6.1 Model Execution Steps for Stand-Alone PC Applications

A more detailed presentation of model execution steps is presented in Volume I and in science-based methodology outlined by Marin *et al.* (1999, 2003). The basic steps of modeling system runtime execution implemented in 3MRA Version 1.0 are listed below, and were previously laid out in Section 3.3.3:

- Step 1 → Select Facility/Environmental Setting from Representative Sample
- Step 2 → Select WMU/Source Type (and effectively waste type; e.g., liquid)
- Step 3 → Select Chemical Constituent
- Step 4 → Select Concentration of the Constituent in Waste, C_w
- Step 5 → Read Data Files
- Step 6 → Select Receptor Location or Habitat
- Step 7 → Calculate Contact Media Concentration at Receptor Location
- Step 8 → Select Receptors
- Step 9 → Select Receptor Age Cohort
- Step 10 → Select Pathway
- Step 11 → Calculate Risk or Hazard
- Step 12 → Select Next Pathway
- Step 13 → Select Next Age Cohort
- Step 14 → Select Next Receptor
- Step 15 → Select Next Receptor Location

Once the risk or hazard calculations are completed, the model generates the risk distribution across a site for each exposure period in the time series. Given the resulting time

series of pathway-specific, receptor-type/cohort-specific, and location-specific risks, HQs, or margin of exposure (MOEs), a time series of frequency histograms is constructed. The histogram for any given year is constructed as a series of risk bins defined by risk or HQ ranges. For any given year, the histogram contains the pathway-specific risk or HQ distribution of the number of people (corresponding to a given receptor type/cohort) across locations. Figure 4-8 shows an example of such a cumulative frequency histogram for one pathway, one receptor type, and one time period at one setting.

Each histogram shows the variability of risk to receptors across a setting. When the time series of similar histograms for this pathway and receptor type is examined, the variability in risk from year to year can be assessed. When these histograms are examined across pathways, the different contributions to exposure and risk for each pathway can be determined.

- Step 16 → Find the Critical Time Period for Evaluation
- Step 17 → Output Risk/Hazard at T_{crit}

Inner and Outer Loops

The 3MRA system currently has the capability to implement a pseudo two-stage Monte Carlo analysis as described in Figure 2-9 and Section 2.6.6. The 3MRA system also has the capability to implement a general two-stage Monte Carlo analysis (Figure 2-9) by incorporation of a Distribution Statistics Processor (see Section 6.5.1) that has not yet been constructed. The latter would be needed, for example, in evaluating ISE uncertainty. The first stage would, as indicated in Figure 3-1 and Figures 2-9 and 2-10, cycle through all the sites. This is referred to as the inner loop in the system (the dimension of variability) and provides a quantitative measure of variability across sites with regard to the many input variables. To address OSE in the general 2-stage Monte Carlo, several iterations through the inner loop, using the same distribution specifications for the various stochastic variables, would be needed. In this case, each iteration in the inner loop would require a new selection of values from the unique instance of specified distributions. For the pseudo 2-stage Monte Carlo, which cannot address ISE in stochastic distributions, only a single loop through all sites would be conducted.

In the general 2-stage Monte Carlo, the second stage is designed to generate new instances of distributions for all the input variables, and therefore a new set of iterations must be conducted, as described directly above. In the pseudo 2-stage Monte Carlo, the second stage is designed to preserve instances of empirical uncertainty by national realization, for example in dealing with constant but uncertain quantities or sampling from non-target populations. In both 2-stage techniques, this is referred to as the outer loop (the dimension associated with empirical input uncertainty) in the system, and provides a measure of empirical uncertainty with regard to the input variables used. In dealing with ISE, the general 2-stage Monte Carlo procedure has not been implemented in 3MRA due to its extensive data requirements, and a pragmatic need to first evaluate sensitivity of the modeling system for the current “best estimate” parameterization of each stochastic model input described by a probability distribution function.

Appending previous comments on looping order, as shown in Figures 2-9 and 2-10, any looping order on C_w , chemical, and WMU can be entertained, as long as the inner and outer loop are placed outside of the site facility loop, if site variability is of interest. It is critical to also ensure that the “inner loop” be used for assessing OSE in either 2-stage analysis technique.

- Step 18 → Select Next C_w
- Step 19 → Select Next Chemical
- Step 20 → Select Next WMU
- Steps for Uncertainty Analysis → Insert Inner and Outer Loops
- Step 21 → Calculate Exit Levels

Calculation of Exit Levels

Once sampling is completed and the output from the set of deterministic modeling system runs is collated in the ELP1 (automatically done on the fly), using the ELP2, chemical-specific results, for example for human health, can be generated for three distances from the source (see Table 6-8j) and for the 13 exposure pathways considered (see Table 6-8p): total ingestion and inhalation combined, total ingestion, total inhalation, total groundwater ingestion and shower inhalation combined, air inhalation, shower inhalation, groundwater ingestion, soil ingestion, fruit and vegetable ingestion, beef ingestion, dairy ingestion, fish ingestion, and breast milk. In addition, the results are available for separately evaluating five receptor types (see Table 6-8r): all receptors, residents, gardeners, farmers, and fishers. Results can also be queried for four age cohorts (see Table 6-8h): infants, children age 12 and under, all ages 13 and over, and all ages. Appropriate selections can also be made for ecological risk calculations.

In general, the following exposure profiles are offered for ELP2 analysis and are described in the *3MRA Modeling System: Technology Design and Users Guide*, where the reader is referred to Table 6-8 for specific category descriptions available (see also Section 3.4):

- **Human** (21,840 total possible permutations)
 - Distance (3 categories),
 - Method Used for Critical Year (currently only one category; maximum),
 - Exposure Pathway (13 categories),
 - Receptor Type (5 categories),
 - Cohort Type (4 categories),
 - Risk Level (7 categories), and
 - Hazard Quotient (4 categories)
- **Ecological** (645 total possible permutations)
 - Hazard Quotient (5 categories), and
 - Roll-up Option (6 categories; 129 total permutations)
 - By Ring and Habitat Group (9 permutations)
 - Radius Distance Ring (3 categories)
 - Habitat Group (3 categories)
 - By Ring and Habitat Type (36 permutations)

- Radius Distance Ring (3 categories)
- Habitat Type (12 categories)
- By Ring and Receptor Group (27 permutations)
 - Radius Distance Ring (3 categories)
 - Receptor Group (9 categories)
- By Ring and Trophic Level (15 permutations)
 - Radius Distance Ring (3 categories)
 - Trophic Level (5 categories)
- By Habitat Group and Receptor Group (27 permutations)
 - Habitat Group (3 categories)
 - Receptor Group (9 categories)
- Habitat Group and Trophic Level (15 permutations)
 - Habitat Group (3 categories)
 - Trophic Level (5 categories)

4.6.2 3MRA Output Vector Dimensionality

In considering all permutations of hazard quotients and roll-up options for a chemical that has ecological health concerns, for each chemical and WMU-type across various C_w 's, 645 (i.e., $5 \cdot (9+36+27+15+27+15)$) separate exit levels could be calculated for a given population percentile (i.e., 10 additional possible selections) and % sites protection level. This would, of course, assume all elements above were active within the site scenarios defining the experiment used to create the underlying ELP1 database. In considering all permutations for a chemical that has human health concerns and imparts both cancer and health hazard risks, for each chemical and WMU-type across various C_w 's, 21,840 (i.e., $3 \cdot 1 \cdot 13 \cdot 5 \cdot 4 \cdot 7 \cdot 4$) separate exit levels can be calculated for a given population percentile and % sites protection level. The two figures together would represent, from the perspective of exit levels and a chemical with all three risk factors present (human cancer and hazard, and ecological hazard), $n_y = 10 \cdot (645 + 21,840) = 224,850$ possible modeling system-level outputs (i.e., elements of y ; Section 1.3.1) normally captured by the ELP1 and ELP2 calculation schemes.

Described in the following sections, however, the decision-maker's focus typically would be placed on a smaller set of exit levels. OSW is primarily interested, for example, in evaluation of 2 target risk levels for each risk factor, and two population percentiles. For human health risk assessment, assuming one active risk factor is present for a given chemical, for the three distance criteria and considering only all cohorts, all receptor types, and the summation of inhalation and ingestion pathway, focus would be placed on evaluating 12 (i.e., $3 \cdot 2 \cdot 2$) exit levels. For ecological risk assessment, assuming one ring distance (e.g., <2000m) and one trophic level (e.g., communities), focus would be placed on evaluating 220 (i.e., $2 \cdot 2 \cdot (3+12+9+1+27+3)$) exit levels. Concern would be typically focused on the most limiting exit level group determined by either human or ecological health concerns. Selection of which exit level constructions to focus upon, of course, is a matter of policy decision that can be greatly informed by the flexibility provided by 3MRA output processing capabilities, and preliminary analyses which would determine the driving concerns per chemical and WMU-type.

In the above analysis, one would generally double all of the estimates provided to account for 2 specific % sites protected levels that are of interest to OSW.

4.6.3 Protection Criteria

The 3MRA assessment strategy uses five different risk protection criteria to generate wastestream concentration exit levels: (1) risk level; (2) human health hazard quotient; (3) ecological hazard quotient; (4) population percentile; and (5) probability of protection. By setting a value for each of these criteria, the chemical-specific waste concentrations are identified that are protective at those values. Each of these risk criteria is explained in more detail below.

Cancer Risk Level

Risk level refers to a person's increased chance of developing cancer over a lifetime due to exposure to a specific chemical. A risk of 1×10^{-6} translates as an increased chance of one in a million of developing cancer during a lifetime. EPA generally sets regulations at risk levels between 10^{-6} and 10^{-4} (in other words, from one in a million to one in ten thousand increased chance of developing cancer during a lifetime). In the RCRA hazardous waste listing program, a 10^{-6} risk is usually the presumptive "no list" level, while 10^{-5} is often the presumptive list level; 10^{-5} was the level chosen in setting the toxicity characteristic (TC) levels for constituents (see Section 3.1).

OSW is primarily interested in understanding 10^{-5} and 10^{-6} risk levels. As indicated, 3MRA offers the flexibility to assess variability in cancer risk level selection across seven (7) different cancer risk intervals (i.e., the human cancer risk bins).

Human Hazard Quotient (HQ)

The HQ refers to the likelihood that exposure to a specific chemical would result in a noncancer health problem (e.g., developmental effects). The hazard quotient is developed by dividing the estimated exposure to a chemical or metal by the associated reference dose (RfD) or reference concentration (RfC) (the highest dose or concentration that might be considered safe). A HQ of 1 or lower indicates that the given exposure is unlikely to result in adverse health effects. Some programs, such as the drinking water program, set the HQ target at less than 1 to provide a safety factor against exposure to a chemical from other sources.

OSW is primarily interested in understanding HQ's of 0.1 and 1. As indicated, 3MRA offers the flexibility to assess variability in human HQ at four (4) levels (i.e., the human hazard bins).

Ecological Hazard Quotient (HQ)

The ecological hazard quotient is analogous to the human health HQ, except that the estimated exposure is compared with an ecological toxicity value rather than the human health RfD or RfC. For this analysis, two types of toxicity values were developed: (1) an ecological benchmark that is analogous to the human health HQ using an RfD; and (2) a chemical stressor

concentration limit (CSCL) that is analogous to the human health HQ using an RfC. In developing ecological benchmarks for this risk assessment, the geometric mean between a no observed effects level (NOEL) and a lowest observed effects level (LOEL) was used (Human health reference doses are based on NOELs). The ecological hazard quotient protects ecological health at the population or community level and, therefore, focuses on reproductive and developmental effects rather than the mortality of individual organisms. This approach is similar to the approach used for developing Ambient Water Quality Criteria that assumes that most, but not all, of the aquatic species and animals are protected at the criteria concentrations (Stephan *et al.*, 1985).

OSW is primarily interested in understanding ecological HQ's of 1 and 10. As indicated, 3MRA offers the flexibility to assess variability in ecological HQ at five (5) levels (i.e., the ecological hazard bins).

Population Percentile

The population percentile is the percentage of the population (or subpopulation) protected at the specified risk level and hazard quotient for a single environmental setting. A setting is a specific WMU at a specific site, and is defined by combining site-based information (such as unit size and unit placement) with variable environmental information (such as rainfall and exposure rates) generated from regional and national data. OSW is primarily interested in evaluating the wastestream concentration exit levels that result from population protection percentiles of 99% and 95%.

Probability (Frequency) of Protection

The probability of protection is defined as the percentage of settings (i.e., of 419 WMU/site location combinations) that meet the selected population percentile criteria. These distributions reflect the "total" uncertainty of the underlying data required by the model. A probability of protection is described as "high end" when it focuses on individual risk to those people at the upper end of the distribution, generally above the 90th percentile. For a given WMU and chemical, this is also referred to as % sites protected.

OSW is primarily interested in evaluating the exemption levels that result from probabilities (i.e., actual frequencies) of protection of 95% and 90%.

Here, as discussed in Section 2.1.1, the interpretation of this criterion as a "probability" applies to an individual selected randomly from the population of all settings (i.e., WMU/site combinations). It represents a "frequency" of protection for all settings considered in the analysis. As described in Marin *et al.*, (1999), the use of population protection versus the use of both population protection and % sites protection is constructible under the methodology without loss of generality. Use of the dual-criteria approach ensures individual (random) sites are not unduly assigned excessive risks for local populations, on a national protection strategy basis.

Table 4-1. Conceptual Model Elements Considered in 3MRA Version 1.0.

<p>CONTAMINANTS^a Organics (28) Metals (15)</p>	<p>FATE PROCESSES Chemical/Biological Transformation Linear Partitioning (water/air, water/solids, air/plant, water/biota) Nonlinear Partitioning (metals in vadose zone) Chemical Reaction/Speciation</p>	<p>FOOD CHAIN Human (Farm) Human (Aquatic) Ecological (Aquatic Habitat) Ecological (Terrestrial Habitat)</p>
<p>SOURCE TYPES^a Aerated Tank (137 Sites) Surface Impoundment (137 Sites) Land Application Unit (28 Sites) Waste Pile (61 Sites) Landfill (56 Sites)</p>	<p>INTERMEDIA CONTAMINANT FLUXES Source ! Air (volatilization, resuspension) Source ! Vadose Zone (leaching) Source Surface Soil ! Watershed Soil (erosion, runoff) Air ! Watershed/Farm/Habitat Soil (wet/dry deposition) Air ! Surface Water (wet/dry deposition) Air ! Vegetation (deposition/uptake) Farm/Habitat Soil ! Vegetation (root uptake) Watershed Soil ! Surface Water (erosion, runoff) Surface Water ! Aquatic Organisms (uptake) Surface Water ! Sediment (sedimentation, resuspension) Vadose Zone ! Groundwater (percolation) Vadose Zone ! Air (volatilization) Groundwater ! Surface Water Soil ! Vegetation (uptake, deposition) Vegetation, Soil, Water ! Beef and Dairy (uptake)</p>	<p>RECEPTORS <u>Human</u> Resident (adult and child) Farmer (adult and child) Home Gardener (adult and child) Recreational Fisher (adult and child) Summation of Receptors <u>Ecological</u> Mammals, Birds, Amphibians, Reptiles Soil Biota, Terrestrial Plants, Aquatic Biota, Aquatic Plants, Sediment Biota</p>
<p>SOURCE TERM CHARACTERISTICS Mass Balance Multimedia/Multiphase Partitioning Source Degradation (anaerobic/aerobic)</p>		<p>EXPOSURE PATHWAYS Ingestion (plant, meat, milk, aquatic food, water, soil, breast milk) Inhalation (particulates and gases, showering with groundwater) Direct Contact (soil, water) Summation of Ingestion Summation of Inhalation Summation of Inhalation and Ingestion</p>
<p>SOURCE RELEASE MECHANISMS Erosion Volatilization Runoff Leaching Particle Suspension</p>		<p>HUMAN AND ECOLOGICAL RISK ENDPOINTS Human Cancer Risk Human Noncancer Hazard Quotient Ecological Population and Community Hazard Quotients</p>
<p>TRANSPORT MEDIA Air Soil Vadose Zone Groundwater Surface Water Sediment</p>	<p>AGE GROUPS FOR HUMAN RECEPTORS <u>Calculated</u> <u>Reported</u> Infant < 1 year Infant < 1 year Child-a 1-5 years Child 1-12 years Child-b 6-11 years Young adults and adults; 13+ years Child-c 12 -19 years Summation of Groups Adult 20+ years</p>	

^a Counts represent current database for FRAMES-3MRA Version 1.0

Table 4-2. 3MRA Version 1.0 Module Input and Output Dictionary Files.

DictCode *	Model Group	Module Description	Filename	Variable Count
grf	af	aquatic foodweb	af.dic	18
grf	aq	saturated zone	aq.dic	11
grf	ar	air	ar.dic	17
grf	ee	ecoexposure	ee.dic	3
grf	er	ecorisk	er.dic	27
grf	ff	farm foodchain	ff.dic	39
grf	hd	header	hd.dic	0
grf	he	human exposure	he.dic	78
grf	hr	human risk	hr.dic	39
grf	sl	site layout	sl.dic	4
grf	sr	source	sr.dic	38
grf	sw	surface water	sw.dic	19
grf	tf	terrestrial foodweb	tf.dic	60
grf	vz	vadose zone	vz.dic	5
grf	ws	watershed	ws.dic	14
ssf	af	aquatic foodweb	af.dic	21
ssf	aq	saturated zone	aq.dic	14
ssf	ar	air	ar.dic	23
ssf	at	aerated tank	at.dic	24
ssf	cp	chemical properties	cp.dic	142
ssf	ee	ecoexposure	ee.dic	14
ssf	er	ecorisk	er.dic	4
ssf	ff	farm foodchain	ff.dic	45
ssf	hd	header	hd.dic	63
ssf	he	human exposure	he.dic	105
ssf	hr	human risk	hr.dic	7
ssf	lau	land application unit	la.dic	51
ssf	lf	landfill	lf.dic	44
ssf	si	surface impoundment	si.dic	25
ssf	sl	site layout	sl.dic	208
ssf	sw	surface water	sw.dic	24
ssf	tf	terrestrial foodweb	tf.dic	31
ssf	vz	vadose zone	vz.dic	3
ssf	wp	waste pile	wp.dic	50
ssf	ws	watershed	ws.dic	23

* For DictCode, ssf implies module-level input and grf implies module-level output. Except for source terms, all modules also utilize outputs from other modules as module inputs. Presentation excludes 45 meteorological model inputs accessed directly from met data files.

Table 4-3. 3MRA Version 1.0 Waste Management Unit Type Distribution.

Waste Management Unit Type	201 Sample Facilities	
	Number	Percent
Landfill	56	28
Land Application Unit	28	14
Surface Impoundment	137	68
Aerated Tank	137	68
Waste Pile	61	30
Total WMU-Facility Combinations	419	-

Overview of Modeling System Infrastructure Development

FRAMES	F ramework for R isk Analysis in M ultimedia E nvironmental S ystems <i>(Underlying Software Infrastructure for all models)</i>
3MRA	M ultimedia, M ultipathway, M ultireceptor R isk A ssessment <i>(A specific set of models within FRAMES)</i>
HWIR	H azardous W aste I dentification R ule <i>(Application – National Regulatory Assessment conducted with 3MRA)</i>

Figure 4-1. FRAMES Framework Technology, 3MRA Modeling System, and Example Application.

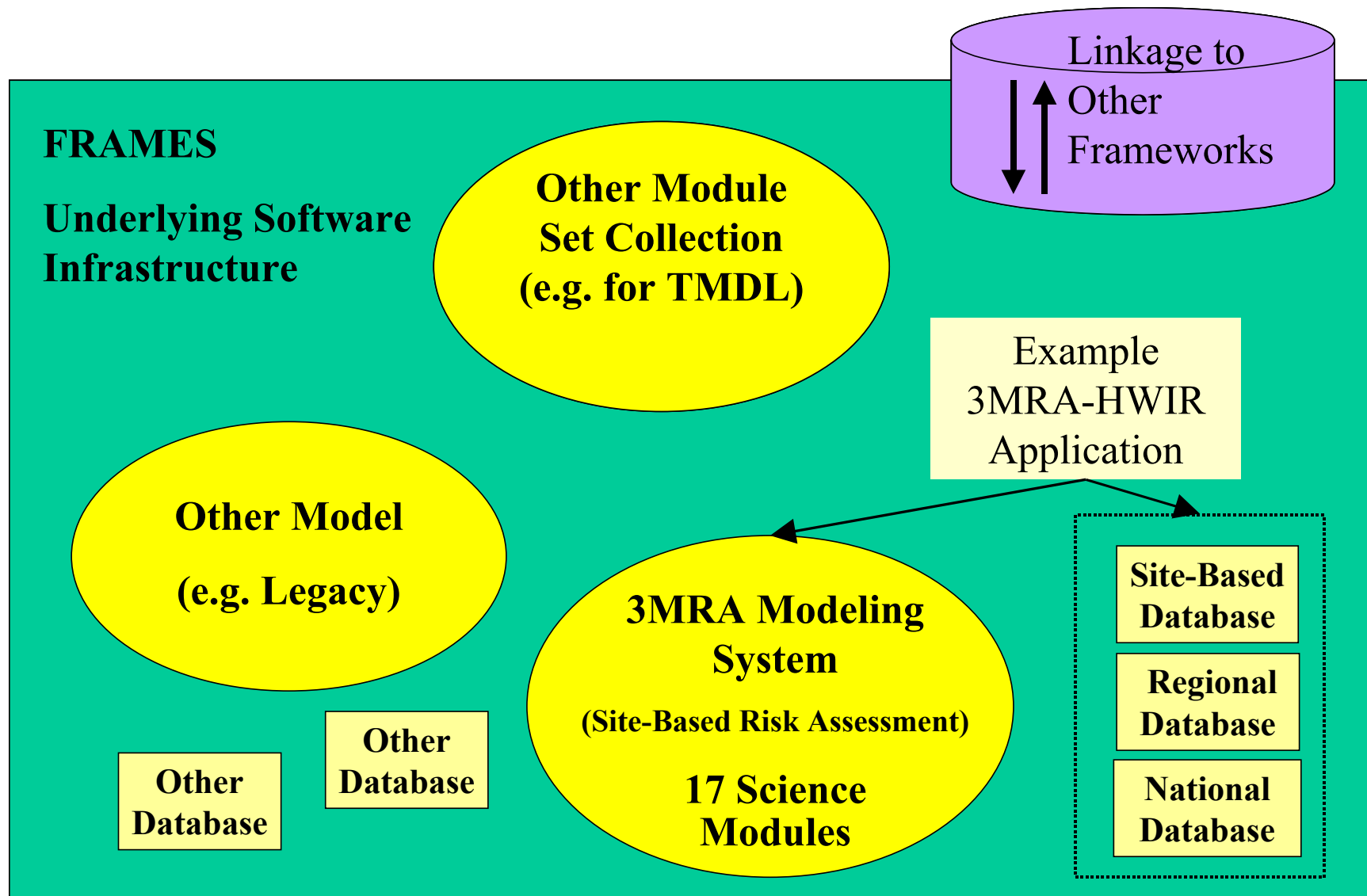


Figure 4-2. Conceptual Relationship Between Framework Technology, Models and Modeling System, and Applications.

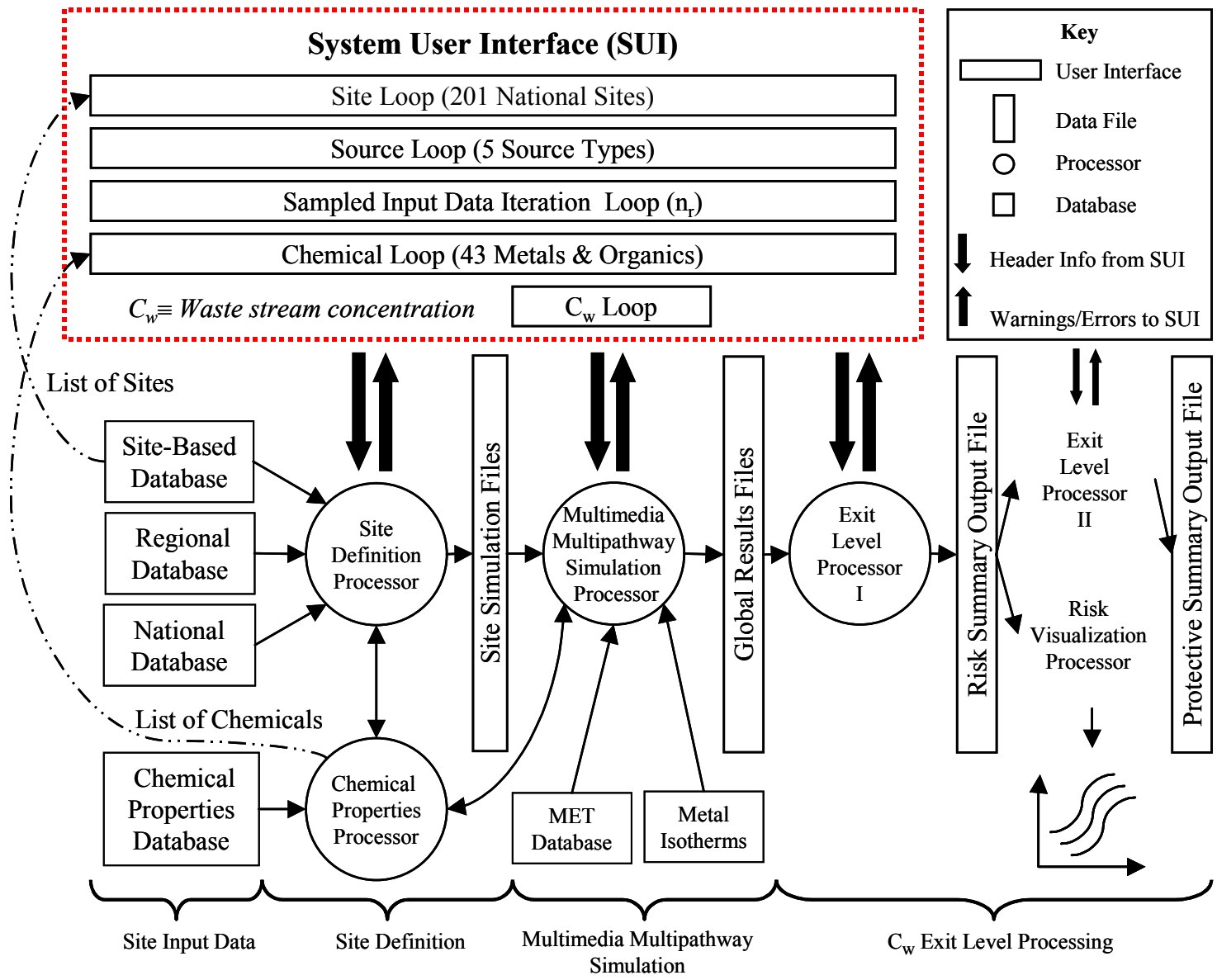


Figure 4-3. FRAMES 3MRA Version 1.0 System Design: Stand-Alone Workstation Application.

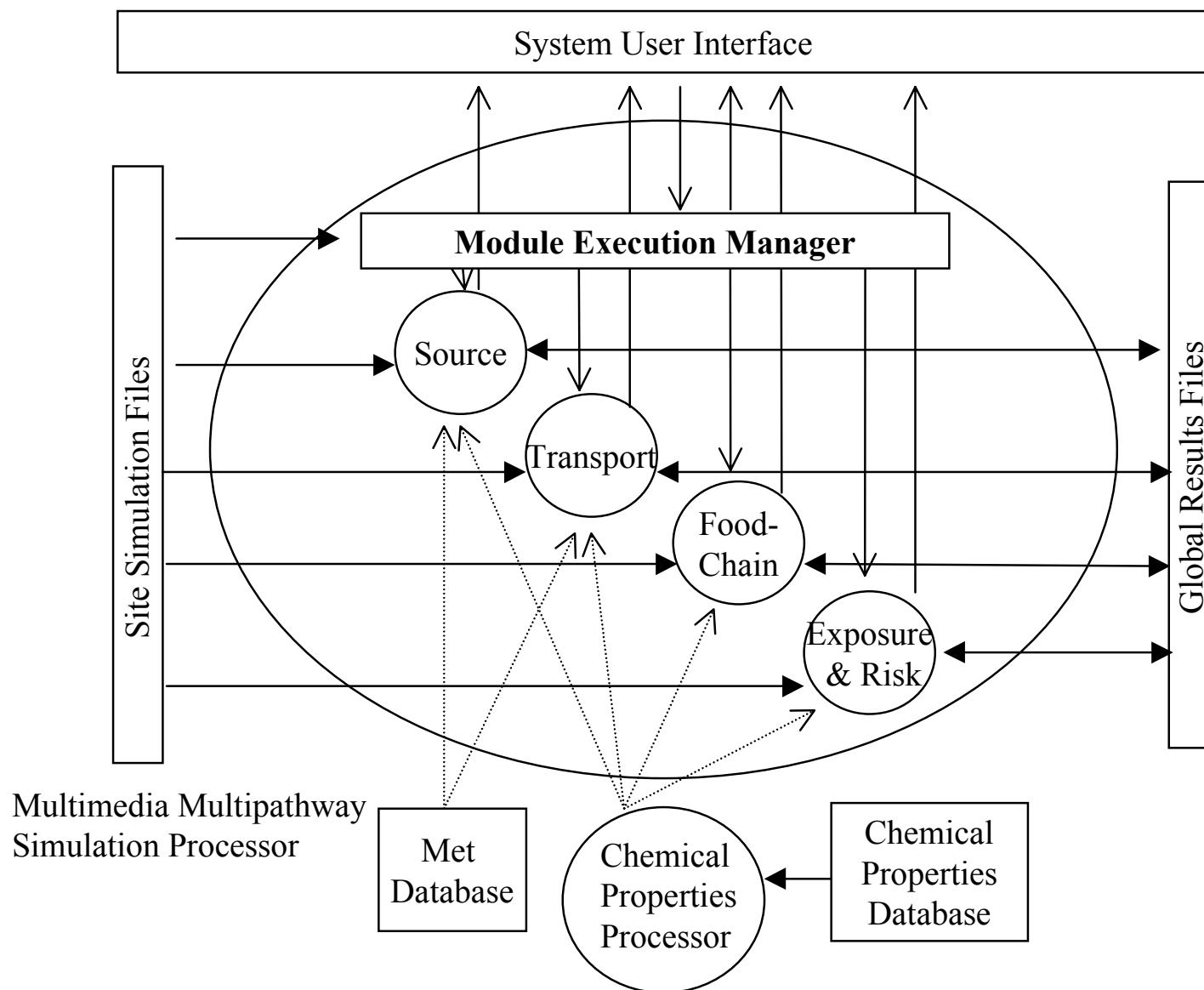


Figure 4-4. Details of the Multimedia Multipathway Simulation Processor.
 (Dashed lines indicate input from complementary components that are outside the MMSP)

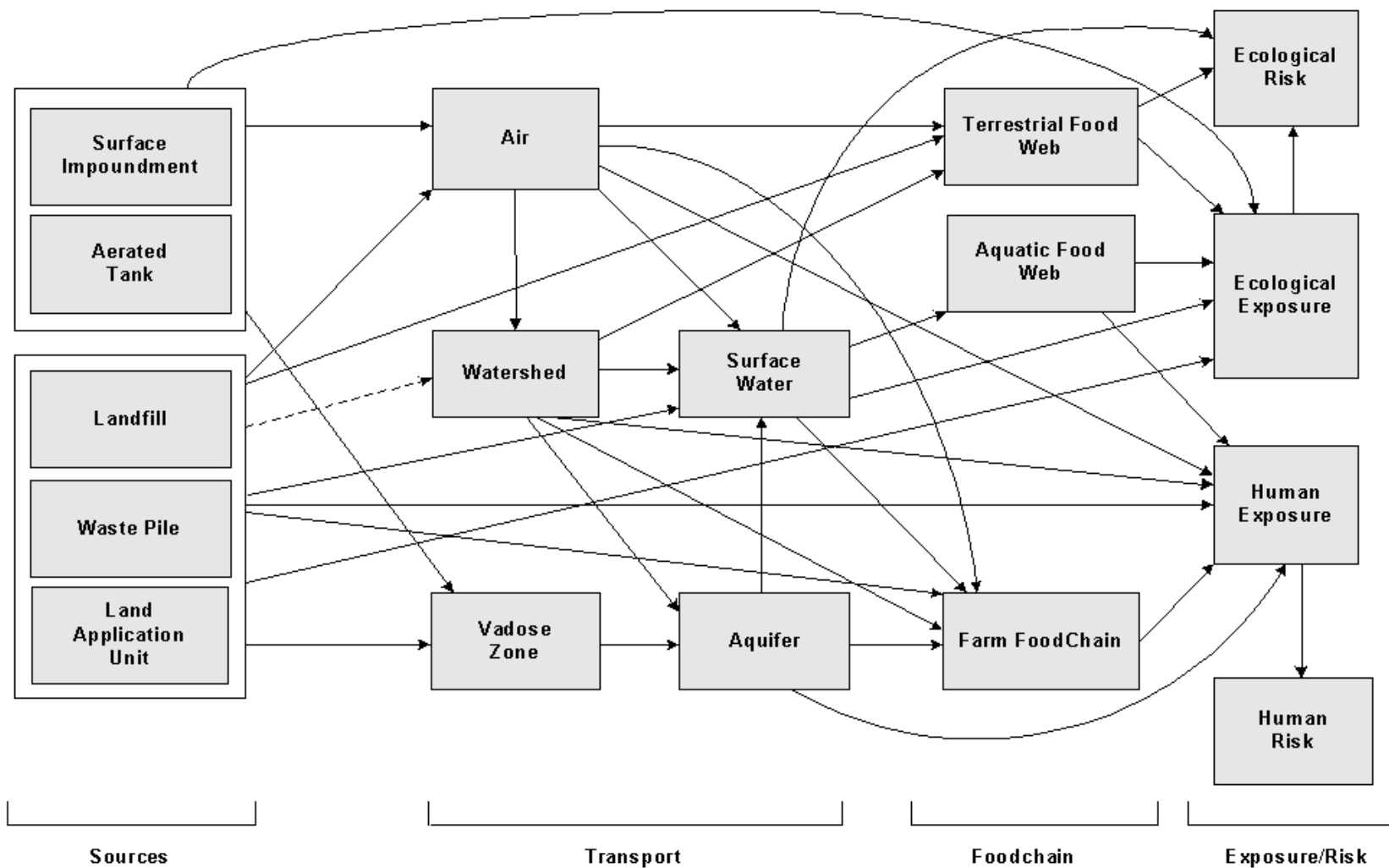


Figure 4-5. Interactions Within the Multimedia Multipathway Simulation Processor.

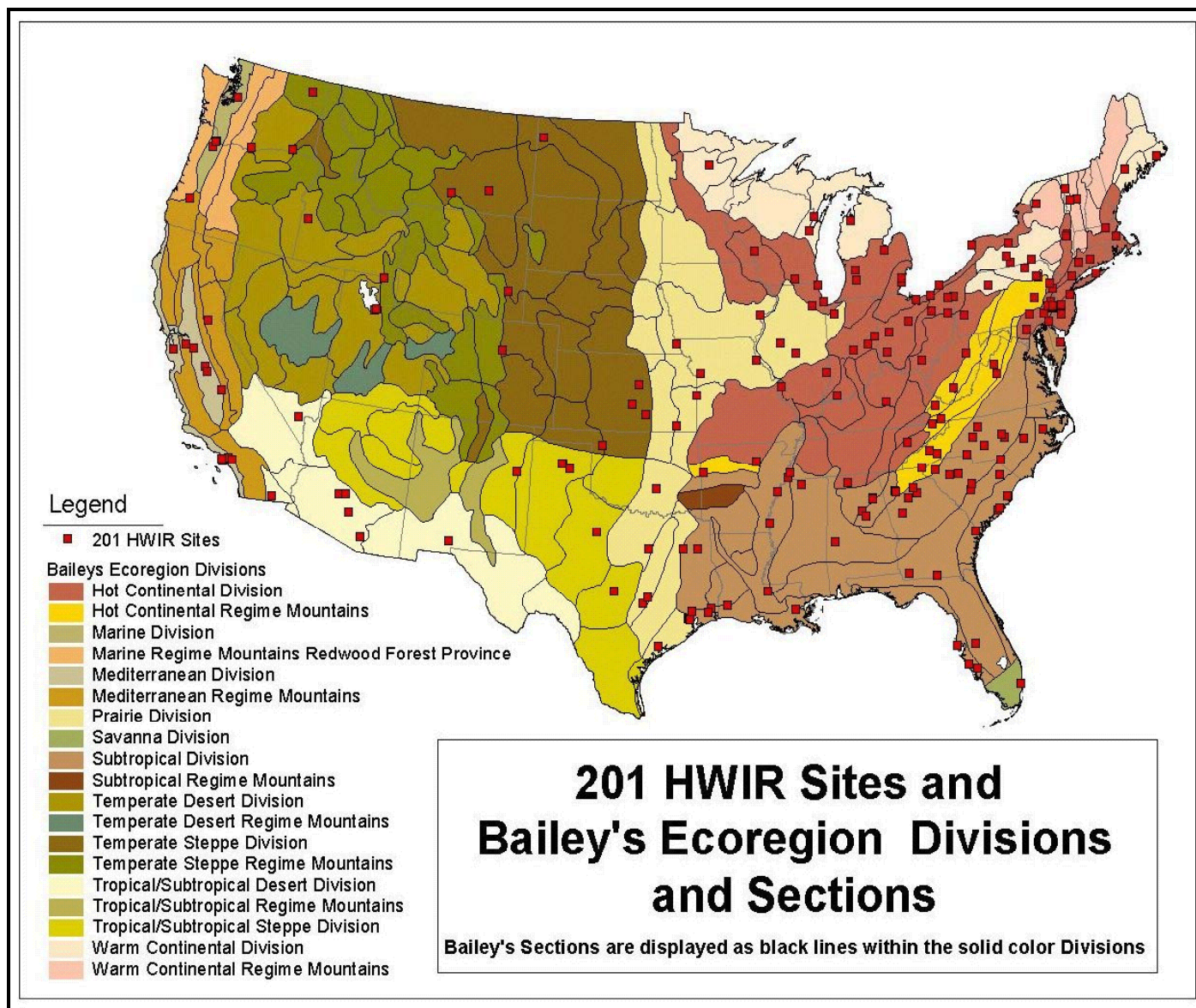


Figure 4-6. Sample Population of Facilities Across the Contiguous United States.

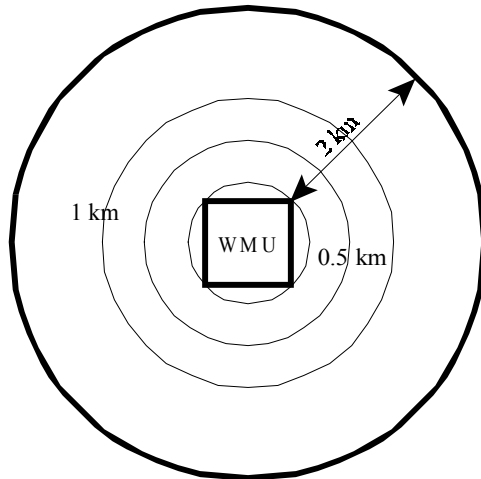


Figure 4-7. Area of Interest and Concentric Distance Rings.

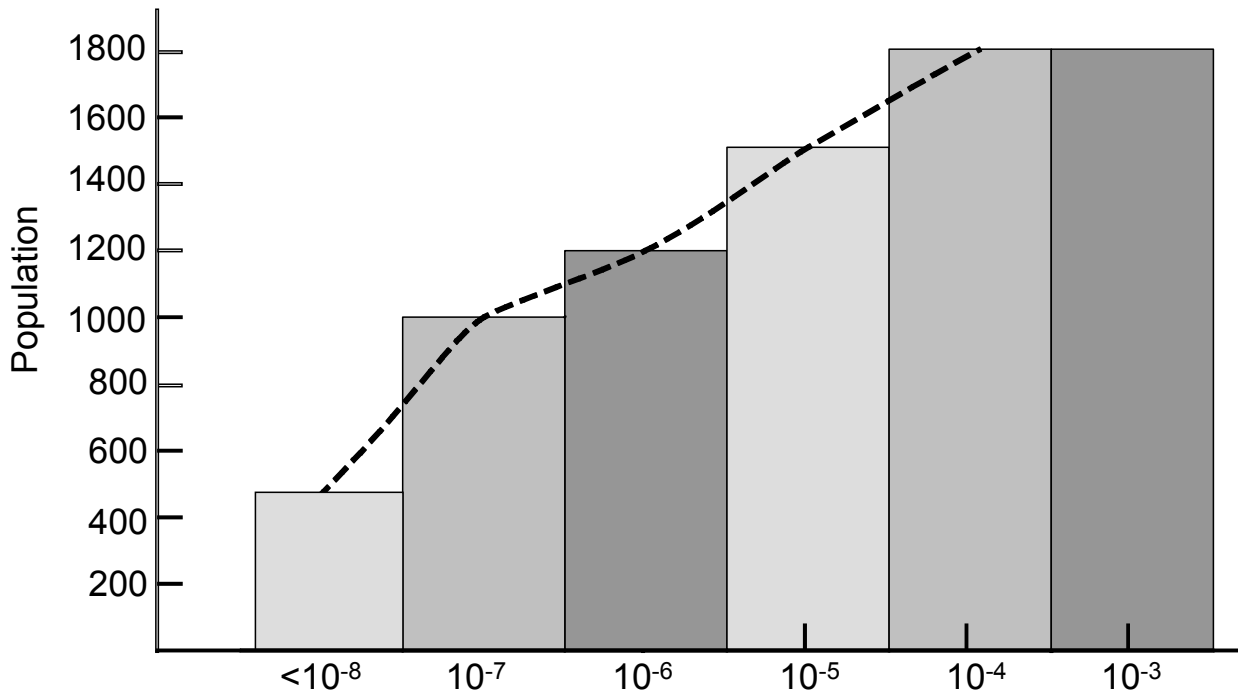


Figure 4-8. Example Cumulative Population Risk Histogram: Inhalation Pathway from Ambient Air, Single Time Period, Single Receptors.