

US EPA ARCHIVE DOCUMENT

2.0 Modeling Approach

The 3MRA modeling system is intended to be one of EPA's next generation of multimedia exposure and risk models, capable of modeling multimedia, multipathway, and multireceptor exposures. The 3MRA modeling system models multimedia exposures by simulating releases of a constituent to air, soil, and ground water, and then modeling the transport and fate of the constituent in each of these media and in the food webs associated with them. It models multipathway exposures by calculating simultaneous exposures of a receptor through multiple pathways, such as the ambient air, soil, food items, and drinking water, and summing them, when appropriate. It models multireceptor exposures by simulating a set of human receptors and a set of ecological receptors that characterize the receptor populations and behaviors of those receptors within an area of interest (AOI).

This section

- Presents an overview of the 3MRA framework—the conceptual approach and science that is implemented in the 3MRA modeling system;
- Describes the spatial and temporal scales that provide the context for the 3MRA framework; and
- Describes the design of the 3MRA modeling system as it pertains to constituents assessed and sources, exposure pathways, receptors, and human health and ecological exposures and risks modeled.

2.1 Overview and Conceptual Approach

Figures 2-1 and 2-2 illustrate the conceptual framework for human receptors and ecological receptors, respectively, in the 3MRA framework. This conceptual framework is further depicted in the flow diagram in Figure 2-3. These figures show the conceptual models for human and ecological receptors, beginning with the multimedia release of constituents from a waste management unit (WMU). Once released, constituents travel through environmental media that determine the exposure pathways for the analysis: air, ground water, watershed soils, and surface water. In addition, plants and animals take up contaminants either directly from the different media or through bioaccumulation of constituents in terrestrial and aquatic food webs. Eventually, human receptors are exposed to contaminants through inhalation or ingestion of contact media (i.e., contaminated air, soil, ground water, homegrown produce, beef and milk produced on a farm, and fish). The ecological receptors are exposed to contaminants through direct contact or ingestion of contact media (i.e., contaminated air, soil, surface water, and flora and fauna).

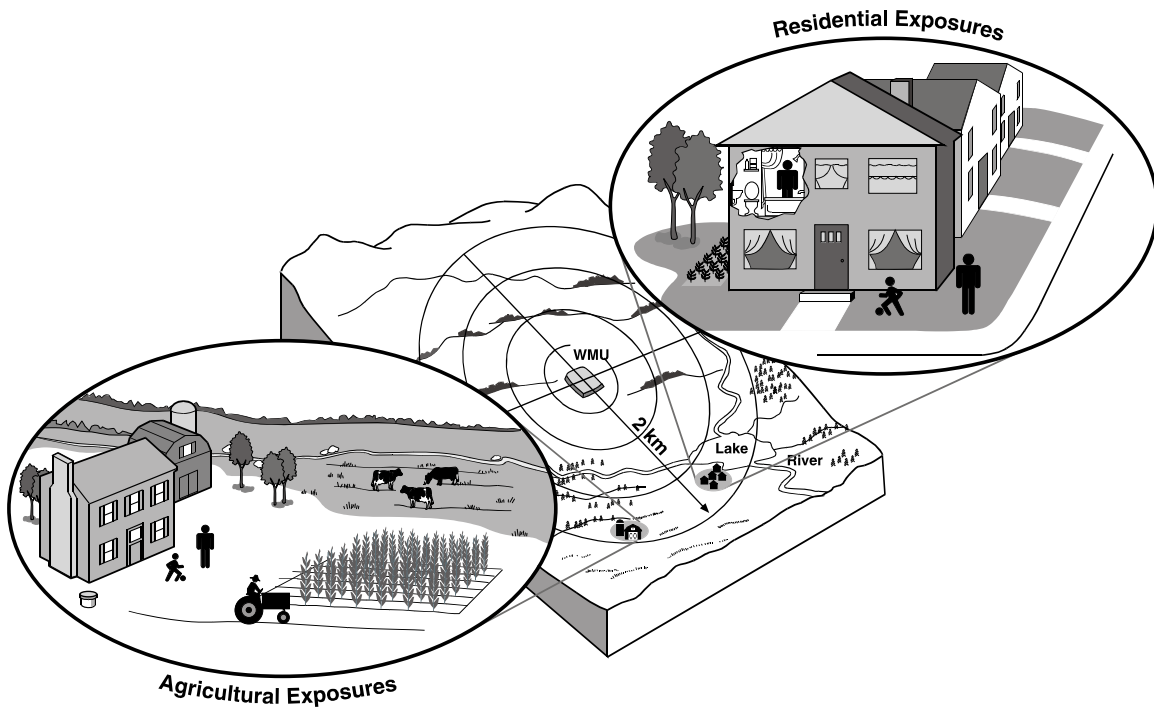


Figure 2-1. Conceptual framework for human receptors.

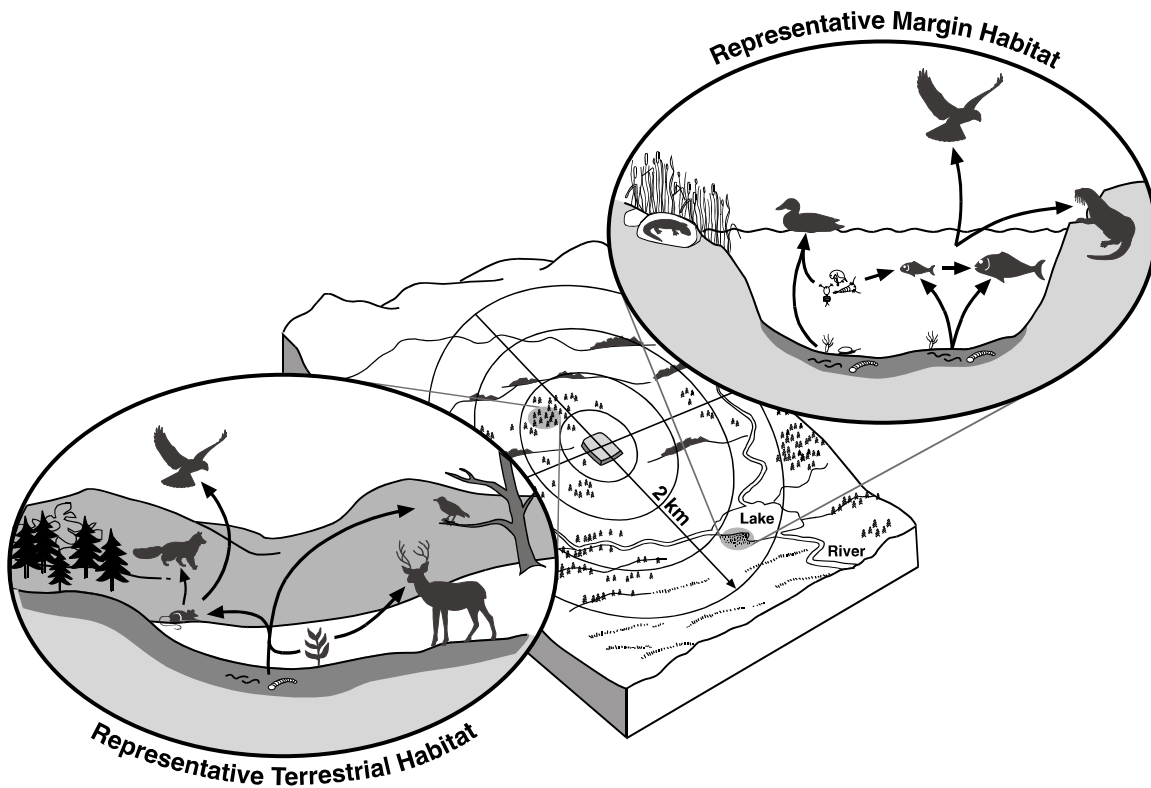


Figure 2-2. Conceptual framework for ecological receptors.

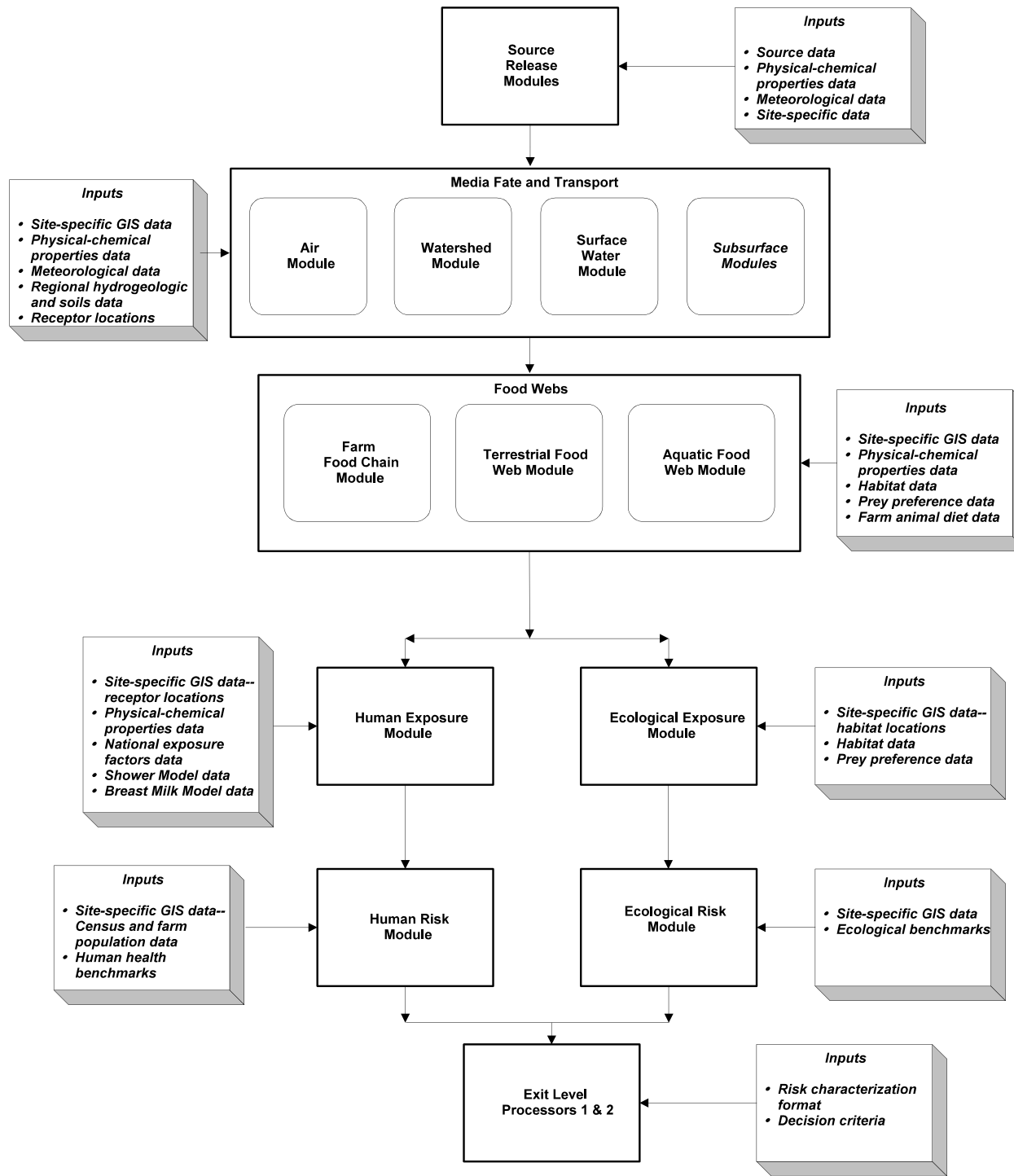


Figure 2-3. Conceptual framework of the 3MRA modeling system.

Several major strengths of the 3MRA modeling system and associated components are that they provide true multipathway functionality, maintain mass balance within the WMUs, model sorption and degradation processes, account for timing of exposures, use a regional site-based approach, and capture variability and uncertainty. These are discussed below.

True Multipathway Functionality. An overriding consideration in the development of the 3MRA modeling system was to provide a system with true multipathway functionality in which a receptor receives constituents from a source via all relevant pathways simultaneously. Constituents are released from a source to various media, depending on the characteristics of the source, the waste, and the surrounding environment. Once the constituents are in the air, soil, and ground water, they are transported through these media to the farm food chain, terrestrial food web, and aquatic food web, or they come into direct contact with a receptor via air, soil, or drinking water. At any given time, the contaminant concentrations to which a receptor is exposed in each medium or food item are evaluated simultaneously.

Mass Balance. The 3MRA modeling system maintains mass balance for a constituent within each type of WMU source. The system starts with a concentration of a constituent in the WMU and partitions the mass to vapor, liquid, and sorbed phases. The 3MRA modeling system continues this partitioning over the life of the WMU as wastes are added and constituents released. Constituent mass released via each phase is no longer available for partitioning to and release through other phases. The data used in partitioning include a range of constituent-specific partition coefficient (K_d) values representing various waste forms that are intended to reflect the full range of waste types (see Sections 4 and 5 for further discussion).

Sorption. The mobility of metals in the environment is dependent on the geochemical properties of the soil, surface water, and ground water to which they are released. To account for the metal-specific interactions with various environments modeled (wastes, soil, surface water, and ground water), the 3MRA modeling system uses nationwide distributions of key geochemical parameters, including metal sorption coefficients. See Volume II of this report for a discussion of the methods and data used to generate the sorption coefficients.

Degradation Processes. Both the source and the fate and transport modules in the 3MRA modeling system were designed to simulate biodegradation and constituent degradation. Full implementation of these processes is limited, primarily because of the limited availability of constituent-specific data on aerobic and anaerobic biodegradation rates. EPA has invested in the development of additional biodegradation rate data specifically to enhance the use of the 3MRA modeling system to support specific RCRA programs. Because of the large number of constituents regulated under RCRA, some constituents were designated as high priority because of their presence in high-volume wastes. Those high-priority constituents were addressed first. Volume II of this report provides a full discussion of the constituent-specific degradation data developed for the 3MRA model (see Sections 4 through 9 for further discussion of the degradation processes included in each of the modules).

Time Series Management. The 3MRA modeling system is designed to estimate the potential risk or hazard quotient (HQ) associated with a constituent that will be managed in a WMU throughout the WMU's operational life and beyond. Average annual exposures are specific to the constituent and environmental setting, and are estimated to occur for up to

10,000 years in some cases. The source modules simulate release of a constituent until the concentration in the WMU decreases to 1 percent of the maximum concentration or until a period of 200 years has been simulated; however, media concentrations are simulated until the constituent concentration in a particular medium (e.g., ground water) decreases to 1 percent of the maximum concentration for that medium or until a period of 10,000 years has been simulated. Therefore, modeling simulations can range from a few hundred years (for contaminants that move quickly in the environment, are not persistent, and do not bioaccumulate) to 10,000 years (for the most persistent and least mobile contaminants, such as some metals).

The risk results are evaluated over the entire modeling period, which could be up to 10,000 years. Evaluating peak doses over this time horizon allows the system to capture the slow movement of certain contaminants through the subsurface. Although the time frame for such travel may be long, such contamination could be a serious problem when the contaminant reaches the receptor wells. Particularly for contaminants that do not degrade, it is important to determine the magnitude of risk that would be experienced once the contamination does reach a drinking water well. The selection of a long time frame assumes that peaks are more likely to be considered in the assessment (see Section 2.2.1 for further discussion).

Regional Site-Based Data. The 3MRA modeling system was designed to be implemented using a site-based approach. In this approach, site-based data are used as inputs to the system when available. When site-based data are not available, data collected on a regional level, followed by data collected on a national level, are used for the evaluation. Using site-based and regional data to create data sets that represent actual site and environmental conditions ensures that implausible exposure pathways and scenarios are not included.

Detailed documentation regarding the methodology for gathering data, what data were collected, where they were obtained, how they were collected and processed, and other issues and uncertainties is provided in Volume II. Examples of the types of data collected as site-based characteristics include facility locations and the physical and environmental characteristics of the sites and surrounding areas (e.g., land use, human receptor locations, and ecological habitats). Regional data collected include meteorological data, some soil characteristics, aquifer data, and types of ecological receptors. Data collected at the national level include human exposure factors, ecological exposure factors, human health toxicity values, and ecological toxicity values.

Variability and Uncertainty Analysis. The 3MRA modeling system was designed specifically to support the analysis of uncertainty and variability in the risk outputs. The site-based approach provides a measure of intrasite variability in risk or hazard in terms of both spatial and temporal variables. With the current representative national data set, the representative sites provide a measure of nationwide intersite variability across industrial waste management sites; that is, the sites cover the range of different land-based WMU types and environmental settings. In addition, the 3MRA modeling system has been designed for a two-stage Monte Carlo analysis. For many inputs, distributions were developed to represent their variability.

2.2 Spatial and Temporal Scale

The 3MRA framework uses a site-based concept to address spatial issues. The data requirements for a multimedia modeling system that includes human and ecological receptors are considerable. Developing a realistic data set for modeling purposes requires consistency among all of the input data, such that the input data set represents a realistic, internally consistent environmental setting. To accomplish this, EPA adopted a site-based approach for the 3MRA modeling system, in which site-specific data, supplemented by regional and national data, are used to construct the environmental setting to be modeled. The inputs to the modeling system can be represented by distributions to reflect variability, and multiple distributions for selected variables can be developed to reflect uncertainty in those variables; however, the uncertainty and variability with respect to the modeling system inputs are all accounted for within the construct of a specific site. To conduct a national-scale assessment, multiple sites that either account for all relevant sites or statistically represent the population of such sites may be used as inputs to the 3MRA modeling system.

The 3MRA modeling system also manages time series data to address temporal issues. The multimedia, multipathway aspect of the modeling system results in exposures through the various pathways occurring at different times. Sometimes exposures can occur hundreds of years apart, especially when considering a ground water pathway versus an aboveground pathway. Thus, the ability to track contaminant concentrations and resulting exposures across all pathways on a common time scale is required. Although this time scale can vary depending on the needs of the analysis, a 1-year time step is used for outputs from all modules because the 3MRA modeling system was developed primarily for chronic exposures. Some of the modules use much shorter time steps to produce these annual outputs. For example, the Air Module uses an hourly time step, but provides annual averages as outputs.

2.2.1 Model Spatial Scale

The spatial scale for the 3MRA modeling system is defined in terms of the AOI surrounding a WMU or other source. The size of the AOI will depend on the goals of a particular application, as well as the ability to collect the needed data for the AOI. For most RCRA WMUs other than incinerators and other types of combustors, the AOI will be relatively constrained because of the operational nature of these sources. For the representative 201 sites in the modeling system, a distance of 2 km was selected for the AOI. If analysts or risk managers are interested in larger AOIs or in areas closer in to the WMU, site-based data sets can be created to provide additional spatial coverage or resolution for the risk results. By default, the 3MRA modeling system estimates risks for the following distance rings, as shown in Figure 2-4:

- Human risks are totaled within the 0 to 0.5 km, 0 to 1 km, and 0 to 2 km rings around the WMU.
- Ecological risks are totaled within the 0 to 1 km, 1 to 2 km, and 0 to 2 km rings around the WMU.

Within the AOI, two key spatial considerations are the location of watersheds and associated waterbodies, and the location of receptors (both human and ecological). These spatial considerations, in combination with other location-specific information, such as WMU characteristics, meteorology, hydrogeology, and land uses, constitute the environmental setting that is modeled. Figure 2-5 illustrates the delineation of watershed subbasins in the 3MRA modeling system. The watershed subbasins define the areas over which deposition rates and soil concentrations are averaged and assumed to be uniform. Although watershed size is determined mainly by the topography and hydrography at a site, the size of the subbasins within the watersheds is defined during watershed delineation. Currently, these are defined in the 3MRA modeling system so that there are generally about 10 to 12 watershed subbasins within the AOI at a site, with an average subbasin area within the AOI of about 1 million square meters. This provides the spatial resolution needed to map soil concentration gradients across the site while keeping the total number of watershed subbasins at a given site to a reasonable number.

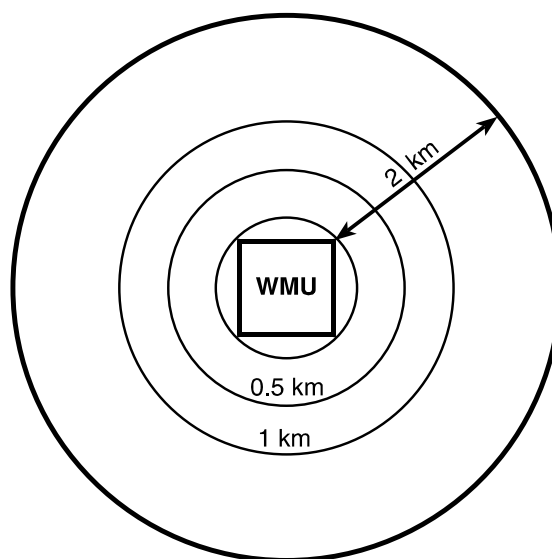


Figure 2-4. Current area of interest and concentric distance rings for human risk.

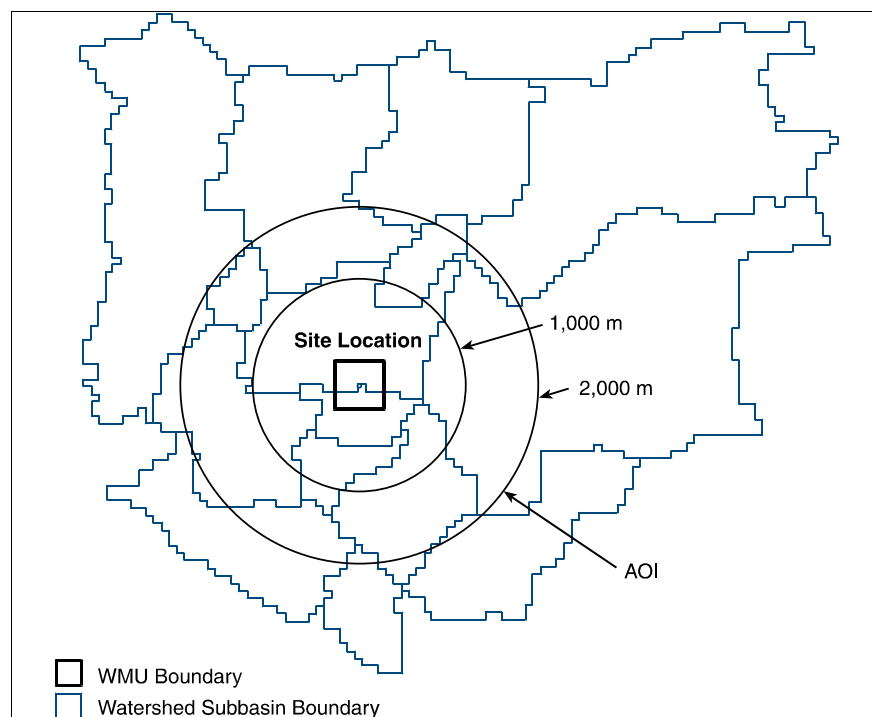


Figure 2-5. Example of watershed delineation for a typical site.

Figure 2-6 illustrates human receptor locations at an example site. Within the current representative national data set, human receptor locations at a site are defined by the centroids of Census blocks from the 1990 U.S. Census. If a distance ring crosses a Census block, then that block is divided into two components, each with a centroid, and the population associated with the Census block is apportioned to the two centroids based on the area of each of the two components. The density of receptor points varies with population density because Census blocks are sized by the population they contain.

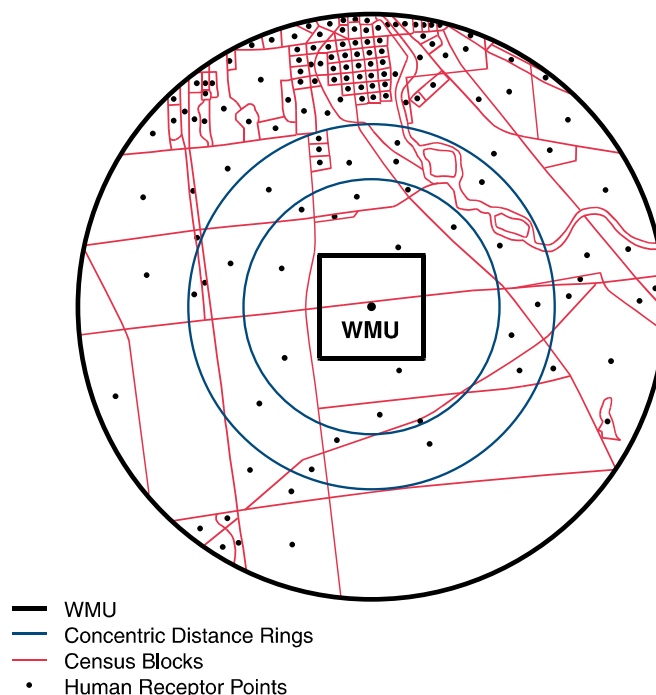


Figure 2-6. Example of human receptor placement for a typical site.

Ecological receptor locations are defined in terms of habitats and home range areas. Figure 2-7 presents a site example with five habitats delineated. The representative habitats are delineated for each site based on a variety of geographic information system (GIS) coverages of topography, land use, wetlands, and waterbodies. Within each habitat, receptor home ranges are placed at random. For each receptor, concentrations in contaminated media (soil or surface water), plants, and prey items are averaged over the home range. Various types of ecological receptors are placed within a home range, based on the available data for that particular receptor.

2.2.2 Model Temporal Scale

The 3MRA modeling system is designed to evaluate chronic exposures, with individual module results reported as a time series of annual average concentrations or fluxes. However, the time scale can be adjusted to be shorter or longer depending on the needs for a particular assessment. Individual modules may use input data on a shorter time scale to capture physical processes that vary within a year, and thus provide a more realistic estimate of the annual average. For example, annual average precipitation data do not provide details on storm events, which have a major effect on runoff and erosion processes that occur over a year. Therefore, the Land Application Unit (LAU) and Watershed Modules use daily precipitation data to more accurately estimate precipitation-driven runoff and erosion events. Similarly, for the Surface Impoundment Module, monthly temperature data can be used to capture temperature extremes across seasons, which can affect volatilization.

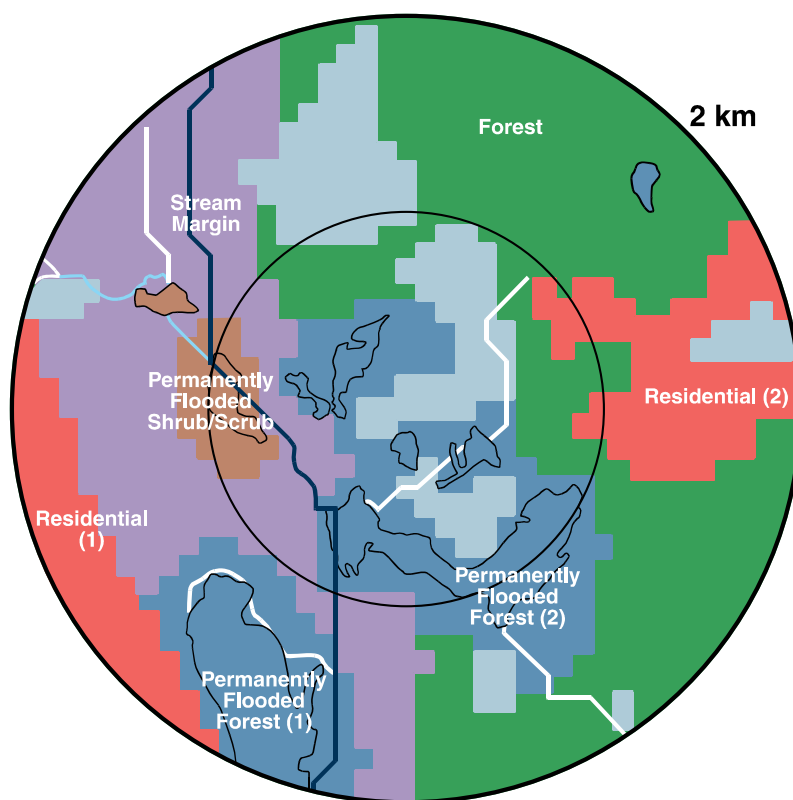


Figure 2-7. Example of representative ecological habitats delineated for typical site.

The time frame for estimating exposure and risk depends on a number of variables, including distance of receptors from the WMU, direction of receptors from the WMU, and physical-chemical properties affecting the transport and fate of contaminants 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 WMU. For ground water, where the medium and chemical properties attenuate the transport process, the exposure and risk time frame can be hundreds to thousands of years after the release. The time frame, therefore, varies for each contaminant and environmental medium considered for each specific WMU. The 3MRA modeling system calculates concentrations for each pathway for each human receptor or habitat location until less than 1 percent of the maximum contaminant concentration in the medium is left in the medium, up to a maximum of 10,000 years. This is intended to capture the large majority of exposures from most contaminants that would be included in an analysis. A few metals and dioxin-like substances may move so slowly in the subsurface that exposures within the AOI may not be fully captured even in the 10,000-year time frame.

A given receptor is subject to exposures from various (but not necessarily all) pathways simultaneously, depending on whether there is a contaminant concentration in each pathway. The aggregate risk to any individual receptor is defined as the sum of the risks from each pathway over a given time period. In the 3MRA modeling system, all exposures are calculated on an annual basis. However, the risk can be based on an exposure duration defined for the analysis. All exposure durations greater than 1 year would be the average daily exposure (or average daily dose) over consecutive years that make up the duration. For example, if there were

100 years of exposure output and the exposure duration was defined as 10 years, there would be 91 10-year averages from which to calculate risk or hazard, beginning with years 1 to 10, 2 to 11, and 3 to 12 and ending with 91 to 100.

Given that the exposure in the different media can occur over significantly different time periods for each receptor location, aggregation of risk is performed for exposures that occur at the same time. For instance, exposures and risks due to contaminated air occurring during years 1 to 10 are not aggregated with exposures and risks due to contaminated ground water occurring during years 91 to 100. Figure 2-8 illustrates how risks during the same time periods are overlaid and aggregated across exposure pathways for a given receptor and contaminant. Risks are aggregated across different exposure routes (i.e., ingestion, inhalation) only after considering current EPA practices for combining exposures through different routes.

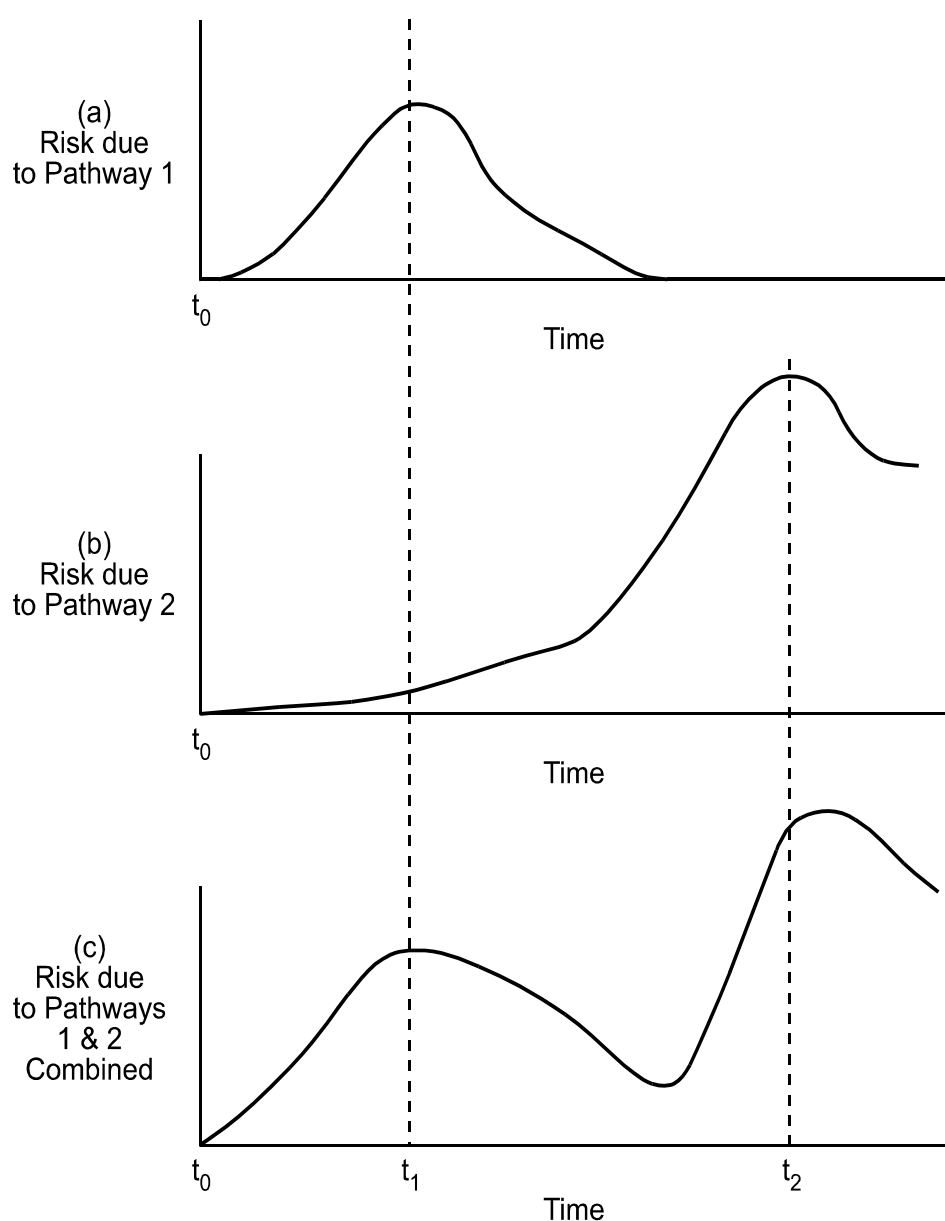


Figure 2-8. Illustration of concurrent time aggregation of risks.

Once risk estimates are calculated for each receptor at a location within the AOI, the critical time period during which the maximum risk and/or HQ occurs across the population for each receptor/cohort combination and for each exposure pathway and pathway aggregation is determined. The critical time period is determined in a similar fashion in the Ecological Risk Module for receptor types, groups, and distances. Types of outputs for the critical period include population-weighted risk or HQ; media-specific concentrations at receptor location; pathway-specific exposures for each receptor/cohort or indicator species at each receptor location; and various aggregations of media concentrations, pathways, or receptors.

2.3 Design of the 3MRA Modeling System Multipathway Modules

The design of the 3MRA modeling system takes into consideration how constituents are released to the environment, transported through various media, and result in exposure to humans and ecological receptors, and how these exposures are characterized in terms of risk measures. The major considerations in determining the design of the science modules in the 3MRA modeling system were

- Chemicals in the 3MRA database;
- Sources (WMUs);
- Transport media, fate processes, and intermedia contaminant fluxes;
- Food chain/food web components;
- Human exposure and risk; and
- Ecological exposure and risk measures.

2.3.1 Chemicals in the 3MRA Modeling System Database

The RCRA hazardous waste program covers more than 400 constituents. These constituents have a large range of physical-chemical properties, toxicological properties, and behavior in the environment. Some of these constituents are well characterized with respect to these properties and others are not. In developing the 3MRA modeling system, different approaches (e.g., algorithms) were required to appropriately model some groups of constituents versus others because of

differences in properties. Five broad categories were established to differentiate the behavior of contaminants in the environment: organic chemicals, metals, mercury, dioxin-like chemicals, and special chemicals (such as those that readily metabolize or those that are completely soluble in water). Mercury and dioxin-like chemicals are specific subcategories for which EPA has developed special approaches for modeling release and fate and transport.

Five categories used in the 3MRA modeling system to differentiate the behavior of contaminants in the environment:

- Organic chemicals
- Metals
- Mercury
- Dioxin-like chemicals
- Special chemicals (e.g., readily metabolizable)

Table 2-1 shows the 46 constituents selected to develop and test the 3MRA modeling system. These constituents were selected to ensure coverage of the range of contaminant behavior in the environment. To facilitate this selection process, all RCRA-regulated

Table 2-1. Constituents in the 3MRA Database

3MRA Constituent Type	Representative Constituent Class	Constituent Name	CASRN
organic (1)	organonitrogen (1)	Acetonitrile	75-05-8
organic (1)	organonitrogen (1)	Acrylonitrile	107-13-1
organic (1)	organonitrogen (1)	Aniline	62-53-3
organic (1)	aromatic hydrocarbon (4)	Benzene	71-43-2
organic (1)	organosulfur (7)	Carbon disulfide	75-15-0
organic (1)	chlorinated aromatic (8)	Chlorobenzene	108-90-7
organic (1)	chlorinated hydrocarbon (9)	Chloroform	67-66-3
organic (1)	chlorinated pesticide (10)	2,4-Dichlorophenoxyacetic acid	94-75-7
organic (1)	brominated hydrocarbon (11)	Ethylene dibromide	106-93-4
organic (1)	misc. halogenated (12)	Hexachloro-1,3-butadiene	87-68-3
organic (1)	chlorinated pesticide (10)	Methoxychlor	72-43-5
organic (1)	carbon/hydrogen/oxygen (6)	Methyl ethyl ketone	78-93-3
organic (1)	carbon/hydrogen/oxygen (6)	Methyl methacrylate	80-62-6
organic (1)	chlorinated hydrocarbon (9)	Methylene chloride	75-09-2
organic (1)	organonitrogen (1)	Nitrobenzene	98-95-3
organic (1)	nonhalogenated phenolic (15)	Phenol	108-95-2
organic (1)	organonitrogen (1)	Pyridine	110-86-1
organic (1)	chlorinated hydrocarbon (9)	Tetrachloroethylene	127-18-4
organic (1)	carbamate group (17)	Thiram	137-26-8
organic (1)	aromatic hydrocarbon (4)	Toluene	108-88-3
organic (1)	chlorinated hydrocarbon (9)	Trichloroethylene	79-01-6
organic (1)	chlorinated hydrocarbon (9)	1,1,1-Trichloroethane	71-55-6
organic (1)	oxoanion metal (2)	Vanadium	7440-62-2
organic (1)	chlorinated hydrocarbon (9)	Vinyl chloride	75-01-4
metal (2)	oxoanion metal (2)	Antimony	7440-36-0
metal (2)	oxoanion metal (2)	Arsenic	7440-38-2
metal (2)	cationic metal (3)	Barium	7440-39-3
metal (2)	cationic metal (3)	Beryllium	7440-41-7
metal (2)	cationic metal (3)	Cadmium	7440-43-9
metal (2)	oxoanion metal (2)	Chromium (hexavalent)	18540-29-9
metal (2)	oxoanion metal (2)	Chromium (total)	7440-47-3
metal (2)	oxoanion metal (2)	Chromium (trivalent)	16065-83-1
metal (2)	cationic metal (3)	Lead	7439-92-1
metal (2)	cationic metal (3)	Nickel	7440-02-0
metal (2)	oxoanion metal (2)	Selenium	7782-49-2
metal (2)	cationic metal (3)	Silver	7440-22-4

(continued)

Table 2-1. (continued)

3MRA Constituent Type	Representative Constituent Class	Constituent Name	CASRN
metal (2)	oxoanion metal (2)	Thallium	7440-28-0
metal (2)	cationic metal (3)	Zinc	7440-66-6
mercury (3)	organometallic (13)	Methyl mercury	7439-97-6m
mercury (3)	cationic metal (3)	Mercury (elemental)	7439-97-6e
mercury (3)	cationic metal (3)	Mercury (total)	7439-97-6
dioxin-like (4)	dioxin/furan (16)	2,3,7,8-Tetrachlorodibenzo-p-dioxin	1746-01-6
special (5)	polynuclear aromatic (5)	Benzo[a]pyrene	50-32-8
special (5)	carbon/hydrogen/oxygen (6)	Bis-(2-ethylhexyl)phthalate	117-81-7
special (5)	polynuclear aromatic (5)	Dibenz[a,h]anthracene	53-70-3
special (5)	chlorinated phenol (14)	Pentachlorophenol	87-86-5

constituents were sorted into 17 representative constituent classes with similar physical-chemical properties. Only constituents with adequate constituent-specific toxicity and physical-chemical properties data were considered for model testing.

The specific properties used to establish these 17 constituent classes included

- Degree of aromaticity (the number and arrangement of benzene rings);
- Volatility;
- Presence of halogens, such as bromine and chlorine;
- Presence of other key elements, such as oxygen, nitrogen, sulfur, and/or phosphorus;
- Use (e.g., pesticides);
- Presence of organic functional groups, such as phenols and carbamates; and
- Similarities in ionic behavior (e.g., anionic and cationic metals).

Candidate constituents were selected from each of the 17 classes by considering toxicology, fate and transport properties, waste chemistry, and other considerations, such as

- Total number of RCRA constituents within a group,
- Range of expected toxicity of the constituents within a group,
- Availability of defensible physical-chemical property data and analytical methods,

- Differences in constituent structures within a group,
- Differences in degree or type of halogenation (chlorinated or brominated),
- The mix of isomers represented in the toxicity data,
- The potential for constituents to accumulate in food or prey,
- The degradation products required to understand the toxicity for a constituent,
- The significance of constituents to other EPA programs or their representativeness of a given class of chemicals (e.g., 2,3,7,8-TCDD for halogenated dioxins and furans), and
- The frequency or expectation of finding the constituent in many process waste streams.

The chemical properties were obtained through a combination of modeling, existing databases, and literature review. Many properties were modeled using SPARC (System Performs Automated Reasoning in Chemistry) and MINTEQA2. These models are described briefly below. Table 2-2 summarizes how the various chemical property values were obtained.

Table 2-2. Methodology and Data Sources for 3MRA Chemical Properties

Property	Methodology	References
<i>Organic Chemicals</i>		
Thermodynamic properties and partition coefficients ^a	SPARC-calculated values, adjusted by CPP for temperature and pH	U.S. EPA (2003) U.S. EPA (1999f)
Hydrolysis rates	Measured or estimated rate constants adjusted by CPP for temperature and pH	U.S. EPA (1996d) U.S. EPA (1999f)
Aerobic biodegradation rates	Measured values from literature, grouped by pH and temperature regimes	Aronson et al. (1999)
Anaerobic biodegradation rates	Measured values from literature, grouped by pH, temperature, and redox regimes	U.S. EPA (1999d)
Soil/water partition coefficients	Calculated from Kow by CPP	U.S. EPA (1999f)
<i>Metals</i>		
Partition coefficients (waste, soil, surface water, sediment)	Measured or estimated values, presented as national distributions	U.S. EPA (1999e)
Sorption isotherms	MINTEQA2 model	U.S. EPA (1998, 1999c)

^a Molecular weight, density, volume, vapor pressure, boiling point, air and water diffusion coefficients, solubility, Henry's law constant, octanol/water partition coefficient (Kow), ionization coefficient.

SPARC. EPA developed the predictive modeling system SPARC to help meet the growing need for constituent-specific inputs for multimedia, multipathway, multireceptor risk assessment tools such as 3MRA. SPARC calculates a large number of physical and chemical parameters (such as solubility, vapor pressure, Henry's law constant, octanol/water partition coefficient, air diffusivity, water diffusivity, and ionization potential) from pollutant molecular structure and basic information about the environment (media, temperature, pressure, pH, etc.) For more information on SPARC, see U.S. EPA (2003).

MINTEQA2. The MINTEQA2 model was used to develop metal sorption isotherms that are contained within the 3MRA Vadose Zone and Aquifer Modules and used to provide the pH and concentration-adjusted soil/water partition coefficients needed to estimate sorption of metal contaminants in the subsurface. MINTEQA2 is an equilibrium metals speciation model that can be used to calculate the equilibrium composition of dilute aqueous solutions in the laboratory or in natural aqueous systems. The model can calculate the equilibrium mass distribution among dissolved species, adsorbed species, and multiple solid phases under a variety of conditions including a gas phase with constant partial pressure. For more information on MINTEQA2, see U.S. EPA (1998) and U.S. EPA (1999c).

The 3MRA chemical database can be expanded as applications using this modeling system require and as constituent data become available.

2.3.2 Sources (WMUs)

The WMUs included in the 3MRA modeling system represent the major management practices where wastes are put into or on the land for recycling, recovery, reuse, treatment, or disposal. The various types of WMUs manage different types of industrial waste in different ways. For example,

- **Surface impoundments** are used to treat and dispose of liquid industrial waste and generate a sludge that requires further management;
- **Aerated tanks** are used to actively treat industrial liquid waste and generate a sludge requiring further management;
- **Landfills** are a common disposal site for many nonliquid industrial wastes;
- **Waste piles** are temporary storage areas on the ground for nonliquid industrial waste, such as ash or slag; and
- **LAUs** are used to reuse, treat, or dispose of industrial waste in liquid, semiliquid, or solid form. Some wastes are used as a soil amendment, which is a reuse practice; some wastes are applied to land for treatment through biological degradation; and some wastes are applied to land as a disposal method.

As illustrated in Table 2-3, each WMU source is modeled to conserve mass. That is, the WMU source boundaries are defined, and mass balance equations are derived to describe the various transport and loss mechanisms that affect the amount (mass or concentration) of

Table 2-3. WMU Types and Source Term Characteristics

WMU Type	Source Term Characteristics			
	Mass Balance	Partitioning	First-order Degradation	Finite Source
Surface Impoundment	✓	✓	✓	✓
Aerated Tank	✓	✓	✓	✓
Landfill	✓	✓	✓	✓
Waste Pile	✓	✓	✓	✓
LAU	✓	✓	✓	✓

constituent within the defined WMU. Each of the WMU source mass balances provides and accounts for partitioning of the constituent of interest among solids (sediment or soil particles), water, and air. First-order degradation terms are also included to account for constituent losses via hydrolysis and biodegradation.

Each of the WMUs included in the 3MRA modeling system is shown in Table 2-4, along with release mechanisms and directly affected media. Surface impoundments, landfills, waste piles, and LAUs were selected because they are the most likely destinations for industrial nonhazardous waste, according to an EPA industrial waste screening study (Westat, 1987). Aerated tanks were selected because hazardous waste management has been shifting from surface impoundments to aerated tanks since the 1987 study was conducted.

Table 2-4. WMU Types and Release Mechanisms Modeled

WMU Type	Release Mechanism (receiving medium)			
	Leaching (ground water)	Volatilization (air)	Windblown dust (air)	Runoff/erosion (soil and surface water)
Surface Impoundment	✓	✓		
Aerated Tank		✓		
Landfill	✓	✓	✓	
Waste Pile	✓	✓	✓	✓
LAU	✓	✓	✓	✓

As shown in Table 2-4, constituents enter four environmental media after direct release from a WMU: (1) air, where volatile and particulate releases disperse and are deposited onto soil, plants, and surface water; (2) soil, which receives runoff and eroded solids from WMUs; (3) surface water, which receives runoff and eroded solids from WMUs; and (4) ground water, which receives dissolved constituents leached from wastes in land-based units by infiltrating precipitation.

Certain characteristics were assumed for each of the five WMU types to complete the waste management scenario and to capture the variability in management practices. These characteristics drive the design and parameterization of the 3MRA source modules; they are described briefly below and in more detail in Sections 4 and 5 of this volume.

Surface Impoundment. The surface impoundment is used for the management of liquid wastes in an earthen basin. Constituents are released during the lifetime of the unit. The impoundment does not receive 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 unit is assumed to contain two well-mixed phases: liquid and sediment. The solids in the liquid waste settle to the bottom of the impoundment over time and fill pore space in the native soils. This attenuates the transport or leaching of constituents to underlying soils and ground water. In addition, a fraction of each surface impoundment is aerated, which enhances biodegradation and increases volatilization of some constituents. Each surface impoundment is assumed to operate for 50 years and then undergo clean closure—that is, all waste is removed from the unit.

The surface impoundment releases leachate to the unsaturated zone and volatile emissions to air. The surface impoundment is assumed to have a berm to prevent overrun; therefore, runoff is assumed not to occur. However, volatilized releases can be deposited on the surrounding soils, and erosion and runoff from these soils are modeled. The model accounts for hydrolysis, volatilization, and sorption, as well as settlement, resuspension, growth and decay of solids, and activated aerobic biodegradation (that is, a higher rate based on the amount of biomass present) in the liquid phase, and hydrolysis and anaerobic biodegradation in the sediment.

Aerated Tank. The aerated tank is used for the treatment of wastewaters. Only tanks the size of a drum or larger are modeled. Each aerated tank has a maximum lifetime of 20 years; therefore, the operating lifetime assumes a tank replacement every 20 years.

The aerated tanks are assumed not to fail or leak liquids to soil or surface runoff. As a result, the only release pathway for an aerated tank is volatile emissions to air. Constituent loss within the tank is simulated through hydrolysis and aerobic biodegradation.

Landfill. The design of the landfill assumes a series of vertical cells of equal volume that are filled sequentially, with each cell being filled in one year. The landfill model is based on the assumption that the constituent mass in the landfill cells may be linearly partitioned into aqueous, vapor, and solid phases. Releases from the landfill can occur over the active lifetime of the landfill (30 years) and continue until virtually all of the constituent mass is released, or, for immobile constituents, releases can continue for a specified number of years.

The landfill modeled in the 3MRA system assumes minimal controls and is constructed below grade. In particular, the unit has no liner, and the cover at closure is a layer of natural soil. The design of the landfill allows volatilization and particle emissions, as well as infiltration, which leaches constituents from the waste. The belowgrade design prevents runoff and erosion. In addition, anaerobic biodegradation and hydrolysis processes can degrade constituents within the landfill.

Waste Pile. The waste pile manages wastes in a storage pile on the ground (above grade). The wastes are removed and the pile site closed at the end of its active life (assumed to be 30 years). Constituents are released only during the operating lifetime of the pile. Waste pile height and area are set and held constant at each site based on the volume of waste stored. The waste in the pile is assumed to be completely removed annually and replaced with new waste.

The waste pile is assumed to be uncovered, so that constituents can be released through infiltration and leaching, volatilization, particle entrainment by wind, and erosion and runoff. In addition, constituents can be degraded by hydrolysis and aerobic degradation at the surface of the pile and by hydrolysis and anaerobic degradation within the pile. Although the waste pile design does not incorporate management controls, the pile is assumed to be located within a local watershed in such a way that there is no run-on of uncontaminated soil onto the pile.

For the waste pile, after runoff and erosion have occurred for some period of time, downslope land areas will be contaminated and their soil concentrations can approach the residual constituent concentrations in the waste pile itself. Thus, after extensive runoff and erosion from a waste pile, the entire downslope surface area can be considered a source and becomes an extended source area in the model construct. Consequently, a holistic modeling approach was taken with the waste pile to incorporate it into the watershed of which it is a part.

Land Application Unit. The LAU allows for the placement of wastes in an open field for degradation, treatment, or disposal. Some industrial wastes are applied to land for purposes of soil amendment, thus constituting a reuse of the waste. The waste is applied to the surface soil periodically and then tilled into the top layer of the soil during each of the assumed 40 years of operation. Releases from the LAU can occur over the active lifetime of the LAU and beyond, and continue until virtually all of the constituent mass is released or, for immobile constituents, for a specified number of years. Other than tilling into the soil and a crop cover, no management controls are present to limit releases from the LAU.

Constituents are released from the LAU by leaching to the unsaturated zone, volatilization and particulate emissions to the air, runoff of dissolved constituents, and erosion and runoff of particles. Constituent losses include hydrolysis and aerobic biodegradation. Also, LAUs are on the land surface and are an integral part of their respective watersheds. Consequently, they receive run-on and erosion from upslope land areas and affect downslope land areas through runoff and erosion.

For the LAU, after runoff and erosion have occurred for some time, downslope land areas will be contaminated, and their soil concentrations can approach the residual constituent concentrations in the LAU (or conceivably even exceed them, long after operation ceases). Thus, after extensive runoff and erosion from the LAU, the entire downslope surface area can be considered a source and becomes an extended source area in the model construct. Consequently, a holistic modeling approach was taken with LAU to incorporate it into the watershed of which it is a part.

2.3.3 Transport Media, Fate Processes, and Intermedia Contaminant Fluxes

The 3MRA modeling system has five main environmental transport modules: the Air Module, the Watershed Module, the Surface Water Module, the Vadose Zone Module, and the Aquifer Module. Four of these modules (Air, Surface Water, Vadose Zone, and Aquifer) are based on existing well-established, peer-reviewed regulatory models. These legacy models provide both state-of-the-art environmental transport and fate modeling and well-established acceptability through various peer-review cycles and applications that have undergone stringent scrutiny. They have been incorporated into the 3MRA modeling system through the use of pre- and postprocessors that integrate the specific input and output requirements of these legacy models into the 3MRA modeling system. Within the modules, all functionality of the original model is maintained, including degradation processes, transformation processes, and release processes. Each of the transport modules is summarized below.

Air Module. The Air Module is based on the Industrial Source Complex Short-Term Model, Version 3 (ISCST3). ISCST3 uses a steady-state Gaussian plume modeling approach, which assumes that the plume of emissions follows a straight-line path in the direction of the mean wind flow, and the contaminant concentrations in the horizontal and the vertical directions (both orthogonal to the mean wind direction) follow a normal distribution. The model provides estimates of contaminant air concentration, dry deposition rates (particles only), and wet deposition rates (particles and vapors) for user-specified averaging periods (i.e., annually). It also has the capacity to model area sources or point sources. A point source is usually considered a source with a small area, such as a stack or vent. An area source is a source that covers some defined area that is large enough to have an impact on the dispersion across the source. The 3MRA modeling system sources are all area sources. There is also a regulatory definition of area source that refers to the quantity of emissions from a particular source. That definition does not apply to this discussion.

In the Air Module, ISCST3 is used to model the transport and diffusion of contaminants in the form of volatilized gases or fugitive dust emitted from area sources. The air concentrations are used to estimate bio-uptake from plants, and human exposures due to direct

3MRA Modeling System Transport Media, Fate Processes, and Intermedia Contaminant Fluxes

Transport Media

- Atmosphere
- Watershed
- Subsurface (vadose zone and aquifer)
- Surface water

Fate Processes

- Chemical/biological transformation (and associated products)
- Linear partitioning (water/air, water/soil, air/plant, water/biota)
- Nonlinear partitioning (metals in vadose zone)
- Chemical reactions/speciation (mercury in surface waters)

Intermedia Contaminant Fluxes

- Air → Watershed/farm habitat soil (wet/dry deposition, vapor diffusion)
- Air → Surface water (wet/dry deposition, vapor diffusion)
- Watershed soil → Surface water (erosion, runoff)
- Surface water → Sediment (sedimentation)
- Vadose zone → Ground water (infiltration)
- Watershed soil → Air (volatilization)
- Ground water → Surface water

inhalation. The predicted deposition rates are used to determine contaminant loadings to watershed soils, terrestrial habitats, farms, and surface waters.

ISCST3 is used as legacy code in the 3MRA modeling system. That is, the model was left intact and the necessary interfacing to the modeling system is handled using pre- and postprocessors. Together, the EPA air quality model (ISCST3) and the pre- and postprocessing code that integrates ISCST3 into the 3MRA modeling system are referred to as the Air Module. The pre- and postprocessing code also provides additional functionality to support other 3MRA modeling system requirements. Additional detail on the Air Module can be found in Section 6 of this document.

Watershed Module. Contaminant mass can be released from a WMU in the form of volatile and particulate emissions. These emissions can then be transported and deposited onto the soils of nearby land areas as wet or dry deposition (estimated by the Air Module). Once deposited, a contaminant is then subject to fate and transport processes, such as runoff, erosion, and degradation. Contaminants in the soil of the AOI are available either for direct exposure to human or ecological receptors or for indirect exposure through uptake in a food web. The Watershed Module accounts for these fate and transport processes across the AOI.

The loss mechanisms for contaminants deposited onto soils are volatilization, leaching, and biological and/or contaminant degradation. The fate and transport mechanisms for contaminants that are deposited onto soils include runoff and erosion into adjacent waterbodies. Because the surface transport processes are hydrologically related, the land areas surrounding the WMU are disaggregated into watershed subbasins. A watershed subbasin can vary in size from a portion of a hillside to much larger areas encompassing regional stream or river networks. In all cases, a watershed subbasin is treated as a single, homogeneous area with respect to soil characteristics, runoff and erosion characteristics, and contaminant concentrations in soil. No spatial disaggregation below the watershed subbasin level is made; that is, no spatial contaminant concentration gradients are estimated within a given watershed subbasin. Additional detail on the Watershed Module can be found in Section 7 of this document.

Surface Water Module. The Surface Water Module has the ability to model streams, lakes, ponds, and wetlands at a site. Constituent mass released from a WMU can enter a nearby surface waterbody network through runoff and erosion directly from the WMU, atmospheric deposition to the water surface, runoff and erosion from adjoining watershed subbasins, and interception of contaminated ground water. The chemical is then subject to transport and transformation processes occurring within the waterbody network, resulting in variable chemical concentrations in the water column and underlying sediments. These chemical 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 consists of a core model, Exposure Analysis Modeling System II (EXAMS II) (Burns, 1997; Burns et al., 1982), and the pre- and postprocessors for the model. The Surface Water Module estimates annual average total and dissolved chemical concentrations in the water column and sediments in stream reaches, ponds, and lakes. Transport and 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 include hydrolysis and biodegradation as 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.

EXAMS II is used as legacy code in the 3MRA modeling system. That is, the model is left intact and the necessary interfacing to the framework is handled using pre- and postprocessors. Together, the EXAMS II model and the pre- and postprocessing code that integrates EXAMS II into the 3MRA modeling system are referred to as the Surface Water Module. Additional detail on the Surface Water Module can be found in Section 8 of this document.

Subsurface (Vadose Zone and Aquifer) Modules. The Vadose Zone and Aquifer Modules consist of components from the EPA Composite Model for Leachate Migration with Transformation Products (EPACMTP) (U.S. EPA, 1996a,b,c) and pre- and postprocessors to provide compatibility with the 3MRA modeling system. The Subsurface Modules account for the fate and transport of constituents released from WMUs into the underlying unsaturated or vadose zone (soil) and saturated zone (surficial aquifer). The Subsurface Modules can consider the formation and transport of transformation products, the impact of ground water mounding on ground water velocity, finite source and continuous source scenarios, and metal transport.

The Vadose Zone Module consists of a one-dimensional (1-D) model that simulates infiltration and dissolved chemical transport through the unsaturated zone. The Vadose Zone Module accounts for sorption and attenuation of a chemical moving through the soils under the WMU. The Aquifer Module consists of a 3-D model that simulates transport through the saturated zone. The Aquifer Module consists of a 3-D ground water flow submodel and a 3-D contaminant transport submodel. The flow submodel accounts for the effects of leakage from a land disposal unit and regional recharge on the magnitude and direction of ground water flow. The contaminant transport submodel accounts for 3-D advection and dispersion and linear or nonlinear equilibrium sorption.

The Vadose Zone Module receives infiltration and solute mass fluxes from the source modules. The migration of chemicals in the vadose zone is terminated at the water table where the chemical 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, when present, in the AOI.

Both the Vadose Zone and Aquifer Modules can be described as legacy code in the 3MRA modeling system. The modules were left intact and the necessary interfacing to the framework is handled using pre- and postprocessors. The pre- and postprocessing code also provides additional functionality to support other 3MRA modeling system requirements. Additional detail on the Subsurface Modules can be found in Section 9 of this document.

2.3.4 Food Chain/Food Web Components

The 3MRA modeling system has three food web components: the Farm Food Chain Module, the Terrestrial Food Web Module, and the Aquatic Food Web Module. The processes

in each component include the uptake by plants and animals of chemicals released from the sources and transported through the environmental media. The Farm Food Chain Module provides estimates of chemical concentrations in homegrown produce and crops, beef, and milk produced on a farm. The Terrestrial and Aquatic Food Web Modules provide estimates of chemical concentrations in plants and animals that are used to evaluate the hazards to ecological receptors. The Aquatic Food Web Module also provides estimates of chemical concentrations in fish that may be eaten by recreational fishers.

Farm Food Chain Module. The Farm Food Chain Module calculates the concentration of a chemical 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 modeling construct for the Farm Food Chain Module is based on recent and ongoing research conducted by EPA ORD and presented in *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (U.S. EPA, 2000).

The Farm Food Chain Module is designed to predict the accumulation of a chemical in the edible parts of a plant from uptake of chemicals in soil and through transpiration and direct deposition of the chemical onto the plant surface. Concentrations are predicted for four 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 (e.g., those with protective covering, such as corn), protected fruits (i.e., those in which the outer skins or rinds are not eaten, such as melons or bananas), and root vegetables (e.g., potatoes). In addition, the chemical concentrations in beef and milk are estimated from the biotransfer of chemical in feed (i.e., forage, grain, and silage), soil, and drinking water to beef and dairy cattle through ingestion.

The Farm Food Chain Module predicts the concentration of chemicals in produce grown by home gardeners and 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 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, feed concentrations for 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.

Food Chain/Food Web Fluxes

- Air → Vegetation (particulate deposition; vapor diffusion)
- Farm/habitat/garden soil → Vegetation (root uptake, translocation, deposition)
- Vegetation, soil, surface water, ground water → Animals (uptake)
- Surface water, sediment → Aquatic organisms (uptake)

Because the behavior of each chemical is affected by its physical-chemical properties, the module takes into account whether the chemical is organic, metal, mercury, dioxin-like, or special. For most organic chemicals, the module calculates chemical-specific values for the biotransfer factors used in the various equations, including air-to-plant biotransfer factor, root concentration factor, and soil-to-plant biotransfer factor. For metals, dioxin-like chemicals, and special chemicals, the module generally uses empirical values from the literature for the various biotransfer factors, when available. If empirical values are not available for dioxin-like compounds and special chemicals, the biotransfer factors are calculated in the same way as for organics. Additional detail on the Farm Food Chain Module can be found in Section 10 of this document.

Terrestrial Food Web Module. 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 20 cm). The spatial averages are defined by the home ranges and habitats that are delineated within the AOI 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 Terrestrial Food Web 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, the Terrestrial Food Web 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, the 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.

As with the Farm Food Chain Module, the Terrestrial Food Web Module modeling construct is based on recent and ongoing research conducted by EPA ORD and presented in *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (U.S. EPA, 2000). The model can distinguish among different types of chemicals, using empirically derived algorithms for the various uptake factors for some chemicals and biouptake data from field or greenhouse studies for other chemicals. The Terrestrial Food Web Module accounts for uptake via root-to-plant translocation, air-to-plant transfer for volatile and semivolatile chemicals, and particle-bound deposition to edible plant surfaces.

To estimate the concentrations in other categories of terrestrial prey items (e.g., earthworms, small birds), the Terrestrial Food Web Module relies on soil-to-organism bioconcentration factors identified from empirical studies and/or generated using regression methods developed by the Oak Ridge National Laboratory (see, for example, Sample et al.,

1998a,b). Additional detail on the Terrestrial Food Web Module can be found in Section 11 of this document.

Aquatic Food Web Module. The Aquatic Food Web Module calculates chemical concentrations in aquatic organisms that are consumed by humans (e.g., game fish), and in ecological receptors (e.g., emergent aquatic plants). 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 in both coldwater and warmwater aquatic habitats.

The underlying framework for the Aquatic Food Web Module is the development of representative freshwater habitats for warmwater and coldwater systems. Four basic types of freshwater systems were included for the two temperature categories: streams/ivers, permanently flooded wetlands, ponds, and lakes. Simple food webs were constructed for each of the eight freshwater habitats (four coldwater and four warmwater) that specify: (1) the predator-prey interactions, (2) the physical and biological characteristics of the species that are assigned to each habitat (e.g., size, lipid content), and (3) the dietary preferences for fish in trophic levels 3 (TL3) and 4 (TL4). For each freshwater habitat, the feeding guilds (i.e., groups of species that use environmental resources, such as food, in a similar way) for various types and sizes of fish were used to construct a simple food web and to map dietary preferences for organisms in each habitat (U.S. EPA, 1999a). The food web structure and species assignments are critical in determining concentrations of hydrophobic contaminants in aquatic organisms. Additional detail on the Aquatic Food Web Module can be found in Section 12 of this document.

To estimate the concentrations in aquatic prey items, the Aquatic Food Web Module relies on bioconcentration factors identified from empirical studies and/or generated using regression methods developed by the Oak Ridge National Laboratory (see, for example, Sample et al., 1998a,b).

2.3.5 Human Exposure and Risk

Within the 3MRA modeling system, human exposure and risk are estimated using two modules: one for exposure and one for risk. The Human Exposure Module provides an annual average dose (i.e., in mg/kg-d) and focuses on receptor types, exposure pathways, and routes. The Human Risk Module calculates risk or hazard and determines the number of people associated with these risk levels.

The conceptual approach used in developing the human exposure assessment and risk calculations within the 3MRA modeling system accounts for the major sources of variability in human exposures and risk. In particular, the approach considers variability through (1) a suite of human receptors that reflect different behaviors that lead to exposure; (2) a suite of age cohorts that reflect variability in exposure factors, such as body weight and consumption or intake rates across ages, as well as some behavior patterns such as showering; (3) the use of distributions for most exposure factors to account for the variability within a receptor/cohort category (e.g., adult resident, farmer child aged 12 to 18); (4) the location of receptors that reflect the spatial variability in contaminant concentration across an AOI, as well as the existence or nonexistence of some pathways, such as ground water being used as drinking water; (5) the variability in

contaminant concentration in various pathways over time; and (6) the variability in the number of people exposed at various locations within an AOI. This site-based approach is used on multiple sites in a national assessment to address the variability both within an AOI for an individual site and across multiple sites.

Human Exposure Module. The Human Exposure Module calculates the applied dose (milligram of contaminant per kilogram of body weight) to human receptors from media and food concentrations calculated by other modules in the 3MRA modeling system. The applied dose is used for calculating carcinogenic risk for ingestion and inhalation exposure pathways and for calculating HQs for ingestion pathways. For inhalation pathways for noncarcinogens, the air concentration to which a receptor is exposed (expressed in milligrams of contaminant per cubic meter of air) is used. These calculations are performed for each receptor, cohort, exposure pathway, and year within each AOI.

Human Receptors. Human receptor types considered in the 3MRA modeling system are intended to cover the likely human receptor types evaluated at the national level. The 3MRA modeling system can model five different receptor types: residents, gardeners, beef farmers, dairy farmers, and fishers. Receptor types are used to differentiate behavior that leads to different profiles of exposure. For example, the exposure pathways evaluated for a resident include ingestion of soil and ground water and inhalation of airborne vapors and particulates. For home gardeners and farmers, contaminated foodstuffs are considered in addition to the pathways for the resident. Census and land use data are used to identify receptor types and populations that are potentially exposed within an AOI.

Age Cohorts. Each receptor type is divided into five age cohorts: infants, children aged 1 to 5 years, children aged 6 to 11 years, children aged 12 to 19 years, and adults. The only exposure pathway evaluated for the infant is the breast milk pathway, which is derived from the mother's exposure. The other age cohorts provide a way of estimating applied dose to different age groupings that exhibit different distributions of intake rates and body weights. For the 3MRA modeling system, statistical distributions were developed for these exposure factors for each age cohort using data available in the *Exposure Factors Handbook* (U.S. EPA 1997). The 3MRA modeling system samples from these distributions using a Monte Carlo approach.

Human Exposure Pathways. The approach used in human exposure assessment is to predict the type, timing, and magnitude of exposures that receptors may experience as a result of

3MRA Modeling System Human Receptors, Exposure Routes, and Risk Measures

Human Receptors*

- Resident
- Home gardener
- Dairy farmer
- Beef farmer
- Fisher**

* For each human receptor type, includes 5 age cohorts

** All other receptor types can also be fishers.

Age Cohorts

- Infants
- Child aged 1 to 5 years
- Child aged 6 to 11 years
- Child aged 12 to 19 years
- Adult (over 19 years)

Exposure Pathways

- Ingestion (plant, meat, milk, fish, water, soil, breast milk)
- Inhalation (gases, particulates)

Human Risk Measures

- Cancer (risk probability)
- Noncancer (hazard quotient)
- Population weighted risk distribution

contact with the contaminants of potential concern. An exposure pathway describes the course that a contaminant takes from a source to an exposed individual. Exposures are evaluated for all potentially complete exposure pathways. An exposure pathway is complete when there is a route by which a human receptor takes up a constituent that was released from the source of concern. For example, if ground water is predicted to be contaminated, and there are no private wells located in the contaminated plume or the receptors across the AOI are connected to a municipal water supply that is not contaminated, the drinking water pathway (private ground water wells) and the shower inhalation pathway would not be complete.

Exposure routes include uptake mechanisms such as ingestion, dermal contact, and inhalation. When modeling human exposure, the exposure routes that are included in the Human Exposure Module include

- Ingestion of soil,
- Ingestion of contaminated ground water (private ground water wells only),
- Inhalation of contaminated shower air (private ground water wells only),
- Inhalation of volatile emissions,
- Inhalation of particulate emissions,
- Ingestion of homegrown produce (gardeners, farmers) and beef and milk produced on farms (farmers only),
- Ingestion of fish caught by recreational fishers, and
- Exposure of an infant through ingestion of breast milk from an exposed mother.

These routes define the exposure media to be modeled in the risk analysis (i.e., ground water, soil, air, vegetables, beef, milk, and fish). EPA considered the inclusion of the dermal route of exposure but decided that health benchmarks for dermal toxicity are not sufficiently developed at this time for use in analyses that could support regulatory decisions.

The exposure pathways and routes that can be evaluated for each receptor type are shown in Table 2-5. Residents can be exposed to contaminants in the air (inhalation) and in soil (incidental ingestion) and are assumed to be exposed to potentially contaminated ground water (inhalation and ingestion) if the house is not connected to a public water supply. Home gardeners are residents who also grow some portion of their fruits and vegetables. Farmers have the same exposure pathways as home gardeners with the additional exposure to either contaminated beef or milk (depending on the type of farms present at a site). Recreational fishers are any of the above receptors with the added pathway of ingestion of contaminated fish from local streams or lakes. Thus, some fraction of residents, home gardeners, and farmers are also fishers.

Table 2-5. Human Exposure Pathways by Receptor Type

Pathway	Resident	Resident Fisher	Home Gardener	Home Gardener Fisher	Beef Farmer	Beef Farmer Fisher	Dairy Farmer	Dairy Farmer Fisher
Air inhalation	✓	✓	✓	✓	✓	✓	✓	✓
Shower air inhalation	✓	✓	✓	✓	✓	✓	✓	✓
Soil ingestion	✓	✓	✓	✓	✓	✓	✓	✓
Water ingestion	✓	✓	✓	✓	✓	✓	✓	✓
Crop ingestion			✓	✓	✓	✓	✓	✓
Beef ingestion					✓	✓		
Milk ingestion							✓	✓
Fish ingestion		✓		✓		✓		✓

The Human Exposure Module aggregates exposures across exposure pathways and routes, when appropriate (e.g., daily doses of beef contaminated by uptake from forage, silage, grain, soil, and drinking water), and provides estimates of total exposure for the eight routes listed above.

Within the 3MRA modeling system, the evaluation of human exposure is accounted for by a contaminant's distribution across a site, a contaminant's concentration profile with time, and also the variability and uncertainty in exposure factors for each receptor type. The exposure for each receptor type is estimated at each receptor location within the study area to capture spatial variability, and for every year over the modeling time frame to capture temporal variability. Additional detail on the Human Exposure Module can be found in Section 13 of this document.

Human Risk Module. The Human Risk Module calculates the population-weighted risk or hazard for each receptor location, receptor type, age cohort, pathway, and exposure period. Hazard or risk distributions are developed across the site by doing these calculations at each receptor location, providing a measure of the spatial variability at a site. These same distributions are developed for each exposure period in the modeling time frame providing a measure of temporal variability. At each location, the number of people for each receptor type/cohort is matched with the risk or hazard estimates, providing a population weighting for each receptor location.

Once the risk or hazard calculations are complete, the model generates the risk distribution across a site for each exposure period in the modeling time frame. Given the resulting pathway-specific, receptor-type/cohort-specific, and location-specific risks, HQs, or margins of exposure (MOEs) (for the breast milk pathway), a time series of population-weighted risk data is generated for each. This can be thought of as a set of cumulative frequency histograms. 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 2-9 shows an illustration of this concept of a cumulative frequency histogram

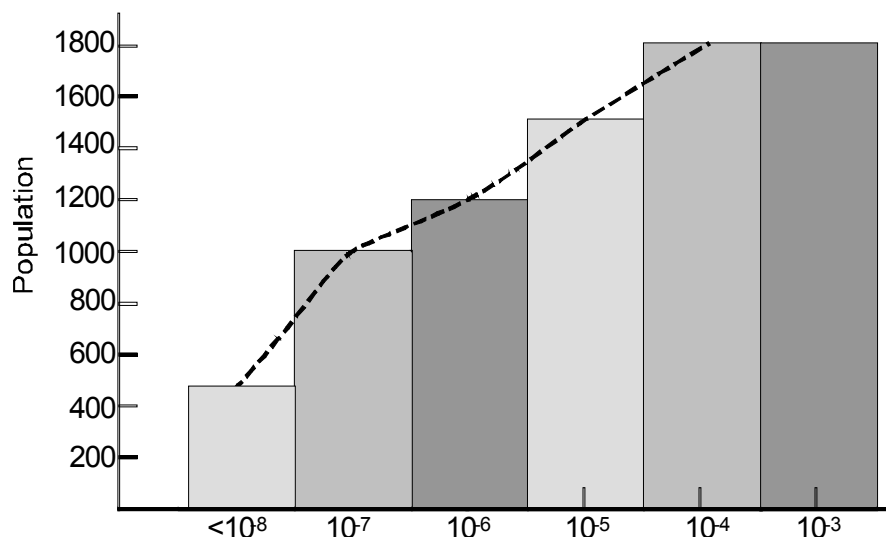


Figure 2-9. Example cumulative population risk histogram for the inhalation from ambient air pathway, single time period, single receptor.

of risk for one pathway, one receptor type, and one time period at one site. These types of histogram can be used to assess the variability of risk to the receptors across the AOI. The risk for this illustration ranges from below 10^{-8} for about 25 percent of the receptors within the AOI to 10^{-4} for about 15 percent of receptors within the AOI. Because the data sets are available for each pathway and each receptor type, a similar assessment can be made by looking at the contribution of each pathway to the total risk for a receptor type. When the time series for each data set is examined, the variability in risk from year to year can be assessed.

Given the resulting time series of pathway-specific and receptor-type/cohort-specific risk and/or HQ, the years during which the total risk or HQ across all receptors within the AOI is a maximum is determined. The exposure period with the highest total risk is termed the critical exposure period.

The distributions for the critical exposure period are the outputs for each site. For any given site, there is a distribution for each pathway independently, for all ingestion pathways together, for all inhalation pathways together, for the ground water-only pathways, and, where appropriate, for all ingestion and inhalation pathways together for each receptor type/cohort, all cohorts within a receptor type, and all receptor types together at various distances from the source and across the entire AOI. Additional detail on the Human Risk Module can be found in Section 14 of this document.

2.3.6 Ecological Receptors, Exposure Pathways, and Risk Measures

Ecological exposure and risk are estimated using two modules: one for exposure and one for risk. The Ecological Exposure Module focuses on receptors, habitats, and exposure pathways. The Ecological Risk Module estimates HQs for representative species.

Ecological Exposure Module. 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). However, just as in the Human Exposure Module, some exposures are expressed as media concentrations and are passed directly to the Ecological Risk Module to account for the way in which toxicity data are used. These dose estimates are then used as inputs to the Ecological Risk Module. The Ecological Exposure Module calculates the applied dose for each receptor placed within a terrestrial or freshwater aquatic habitat. Exposure is a function of (1) the habitat to which the receptor is assigned, (2) the spatial boundaries of the species' home range, (3) the food items (plants and prey) that are available in a particular home range, (4) the dietary preferences for food items that are available, and (5) the 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 home range is the area within a habitat that is needed for each receptor.

The conceptual approach for the ecological exposure assessment within the 3MRA modeling system accounts for the major sources of variability in ecological exposures. In particular, the approach considers variability through (1) the development of representative habitats; (2) selection of receptors based on ecological region; (3) the recognition of opportunistic feeding and foraging behavior using probabilistic methods; (4) the creation of a dietary scheme specific to region, habitat, and receptor; and (5) the application of appropriate graphical tools to capture spatial variability in exposure. The underlying framework for the Ecological Exposure Module is based on a representative habitat scheme to increase the resolution of general terrestrial and freshwater systems.

Depending on the type of habitat and contaminant-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. For example, an omnivorous vertebrate that inhabits a freshwater stream corridor habitat may ingest fish, small terrestrial vertebrates found in the stream corridor, terrestrial and aquatic plants, surface water, and soil. The dietary preferences are independent of the contaminant type; therefore, contaminant concentrations in some food items may be near zero for contaminants that do not bioaccumulate. The dietary preferences for each receptor are supported by an extensive exposure factors database containing information on, for example, dietary habits and natural history for more than 50 representative species of interest. The module includes an innovative approach to characterizing the diet: a probabilistic algorithm that cycles through the database on minimum and maximum prey preferences to simulate dietary variability.

Representative habitats currently delineated in the 3MRA modeling system include

Terrestrial Habitats Waterbody Margin Habitats

- Grasslands
- Shrub/scrub
- Forest
- Crop fields and pastures
- Residential
- Rivers/streams
- Ponds
- Lakes

Wetland Margin Habitats

- Permanently or intermittently flooded grassland
- Permanently or intermittently flooded shrub/scrub
- Permanently or intermittently flooded forest

The Ecological Exposure Module focuses on two areas:

- Representative ecological receptors, and
- Potential and relevant exposure pathways.

Representative Ecological Receptors. The ecological receptors considered in the 3MRA modeling system include the following:

- Terrestrial wildlife using habitats at or near WMUs; this wildlife can be directly exposed to waste or indirectly exposed by consuming plants, soil, or prey items that bioaccumulate constituents released from the WMU.
- Aquatic plants and other biota; these may be exposed to contaminants that are transported from a WMU to nearby aquatic habitats.
- Vascular plants and other terrestrial biota; these may be exposed to contaminants that are transported from the WMU to nearby terrestrial habitats (e.g., surficial soils).

Representative ecological receptors for the following groups of taxa were used to populate habitats:

Terrestrial Habitats **Wetland Margin Habitats**

- Terrestrial plants
- Soil biota
- Reptiles
- Birds
- Mammals

- Wetland plants
- Hydric soil-associated invertebrates
- Aquatic invertebrates

Waterbody Margin Habitats

- Aquatic plants
- Aquatic invertebrates
- Benthos
- Fish
- Amphibians
- Birds
- Mammals

- Fish
- Amphibians
- Reptiles
- Birds
- Mammals

Because all potentially affected species cannot be assessed in a national-level assessment, potentially affected plants and wildlife were organized into guilds of taxonomically and functionally related organisms (e.g., herbivorous birds, insectivorous birds, carnivorous mammals). Receptors were selected to represent each guild based on taxonomic relatedness, function in the ecosystem, and availability of wildlife exposure factors and toxicity data. For example, the American robin may be selected to represent insectivorous birds at a WMU because (1) it is a bird, (2) it eats insects and worms, (3) it is one of many thrushes observed at or near the WMU, and (4) wildlife exposure factors have been established (U.S. EPA, 1993).

Receptors were assigned to habitats within the AOI based on site-based and regional data. Representative ecological receptors were assigned to appropriate habitats based on documented foraging and feeding behavior and habitat usage.

Ecological Exposure Pathways. Table 2-6 lists the media and exposure routes that are evaluated by the Ecological Exposure Module. Direct contact with contaminants by terrestrial wildlife was not included in the model because dense undercoats or down effectively prevents contaminants from reaching the skin of wildlife species and significantly reduces the total surface area of exposed skin (Peterle, 1991; U.S. ACE, 1996). Also, results of exposure studies indicate that exposures due to dermal absorption are insignificant compared exposures due to ingestion for terrestrial wildlife (Peterle, 1991). Similarly, inhalation of volatile organic chemicals was not included in the model because concentrations of volatile chemicals released

Table 2-6. Ecological Exposure Routes Evaluated by Receptor Type

Receptor	Direct Contact			Ingestion		
	Surface Water	Sediment	Soil	Surface Water	Soil	Food
Plants						
Aquatic	✓	✓				
Terrestrial			✓			
Invertebrates						
Aquatic	✓	✓			✓	✓
Terrestrial			✓		✓	✓
Wildlife						
Fish	✓					
Amphibians	✓					
Reptiles				✓	✓	✓
Birds				✓	✓	✓
Mammals				✓	✓	✓

from soil to air are drastically reduced, even near the soil surface (U.S. ACE, 1996), and inhalation toxicity data for laboratory rats and mice show that volatile organic chemical concentrations in soils would have to be great to induce noncarcinogenic effects in wildlife (U.S. ACE, 1996). In addition, availability of inhalation benchmarks for ecological receptors is limited. Additional detail on the Ecological Exposure Module can be found in Section 15 of this document.

Ecological Risk Module. The Ecological Risk Module calculates HQs for a suite of ecological receptors assigned to habitats delineated at a site. 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 the Ecological Risk Module is largely determined by both the home ranges and the habitats delineated at each site. The habitats are intended to represent habitats across the United States that may be found at or near WMUs and that support wildlife receptors.

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. For example, contaminant concentrations to which the aquatic community is exposed are represented by a habitat-wide average that may include multiple stream reaches. The temporal resolution is based on annual average applied doses (for comparison with ecological benchmarks [EBs]) and media concentrations (for comparison with chemical stressor concentration limits [CSCLs]).

The 3MRA modeling system calculates HQs for all receptors assigned to the study site. The HQs are used in developing cumulative distributions of HQs. Each of the HQs calculated by the Ecological Risk Module has a series of attributes associated with it that allows ecological risks to be interpreted in a number of ways. For instance, distance from the source (i.e., 1 km, 1 to 2 km, or across the entire site) is important in understanding the spatial character of potential

ecological risks. Other 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), and
- Trophic level (i.e., producers, TL1, TL2, TL3 top predators).

The maximum HQ across the site is also reported along with its ecological risk attributes.

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 calculates HQs based on the EB or CSCL and the chemical exposure information, and provides summaries of ecological risk information from the simulation to determine when critical years with maximum HQs are experienced. Outputs are provided for all attributes associated with each receptor. Additional detail on the Ecological Risk Module can be found in Section 16 of this document.

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