SURFACE IMPOUNDMENT STUDY

TECHNICAL PLAN FOR HUMAN HEALTH AND ECOLOGICAL RISK ASSESSMENT

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DISCLAIMER

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1.0 Executive Summary

1.1 Background

1.1.1 Legislative Mandate for the Surface Impoundment Study and Consent Decree

The 1996 Land Disposal Program Flexibility Act (LDPFA) amended section 3004(g) of the Resource Conservation and Recovery Act (RCRA) to exempt decharacterized wastes from provisions of the RCRA land disposal restrictions. Decharacterized nonhazardous wastes are RCRA hazardous wastes whose hazardous characteristics of ignitability, corrosivity, reactivity, or toxicity have been removed through dilution or other treatment prior to being managed in land-based waste management units. The LDPFA exemption allows decharacterized wastes to be either (1) placed in surface impoundments that are part of wastewater treatment systems whose ultimate discharge is regulated under the Clean Water Act (CWA), or (2) disposed of in Class 1 nonhazardous injection wells regulated under the Safe Drinking Water Act (SDWA). Congress also mandated in the 1996 LDPFA that a 5-year study be conducted to evaluate any human health or environmental risks posed by the exempted wastes that are managed in these ways and to evaluate the extent to which existing state regulations address any such risks.

The Office of Solid Waste (OSW) in the U.S. Environmental Protection Agency (EPA, or the Agency) is conducting this study to assess those exempted wastes placed in surface impoundments and regulated under the Clean Water Act. (EPA's Office of Water is separately preparing a study to evaluate any risks through disposal of the exempted wastes in Class 1 nonhazardous injection wells.) In addition, the Surface Impoundment (SI) Study scope was expanded from decharacterized wastewater only to include all nonhazardous industrial wastewaters managed in surface impoundments whether or not they were once characteristic hazardous wastes to satisfy a requirement of Civ. No. 89-0598, *Environmental Defense Fund vs. Browner*. The expanded scope thus covers two regulatory status categories based on RCRA: impoundments with decharacterized wastes and impoundments with other nonhazardous industrial wastes that have never exhibited any of the characteristics of corrosivity, ignitability, reactivity, or toxicity.

1.1.2 Major Objectives of the Surface Impoundment Study

After reviewing the legislative history of the LDPFA, in 1997 OSW defined the principal study question as "Determine, with an acceptable degree of certainty, what risks to human health and the environment are posed by industrial wastewaters managed in surface impoundments." Together with a randomized two-stage sample design and a separate field sampling effort intended to "ground-truth" the data on existence of specific chemicals and their quantities, this technical plan provides the analytic approach for answering the principal study question.

To answer the study question, EPA will (1) develop descriptive statistics of nonhazardous wastes managed in surface impoundments, the geographic distribution of these surface impoundments, and their proximity to human populations and sensitive ecosystems; and (2) develop a screening-level risk profile (for human and ecological receptors) that presents risk ranges associated with different constituents, unit types, and facility types. These two steps will satisfy the legislative and consent decree requirements to conduct a study of human and ecological risks associated with surface impoundments. In addition, the Agency may conduct a more detailed risk analysis based on multimedia modeling for constituents, units, and pathways of potential concern either during the time frame of this study or subsequent to this study.

1.1.3 Study Design and Components

The Surface Impoundment Study is designed to be based to the extent possible on data collected from a representative sample of the study population. This section briefly describes the definition of facilities, impoundments, and constituents within the scope of the study; the selection of a representative sampling of facilities to survey and assess; other data sources that will be used in addition to the survey results; and the analytic procedure for assessing these data and drawing conclusions about potential risks presented by industrial wastewaters managed in surface impoundments.

1.1.3.1 <u>Definition of "In-scope" Facilities and "In-scope" Surface Impoundments</u>. A facility is within the scope of this study if it meets the following criteria:

- It is a direct discharger (i.e., has a National Pollutant Discharge Elimination System [NPDES] permit), a zero discharger (generally, designed to infiltrate or evaporate wastewater), or an indirect discharger (discharges wastewater to a publicly owned treatment works).

- It conducts activities within the manufacturing sector (Standard Industrial Classification [SIC] codes 20-39), selected transportation subsectors (SIC codes 4212 - Local Trucking Without Storage, and 4581 - Airports, Flying Fields, and Airport Terminal Services), the waste management service sector (SIC codes 4953 - Refuse Systems and 4952 - Sewerage Systems, but excluding publicly owned treatment works), or selected wholesale trade subsectors (SIC codes 5085 - Industrial Supplies, 5093 - Scrap and Waste Materials, and 5171 - petroleum bulk terminals).

- It has one or more "in-scope" surface impoundments. A surface impoundment is within the scope of the study if it has been used to manage certain nonhazardous wastes since June 1990.

1.1.3.2 <u>Definition of "In-scope" Wastes (Based on Type of Constituents and pH)</u>. Nonhazardous wastes are within the scope of the study if they either contain at least one of 256 constituents of potential concern or have a typical pH that falls just outside the range of hazardous wastes. The pH criterion is included because one of the common "hazardous characteristics" that is removed when wastewaters are treated is the corrosivity characteristic,

defined as the condition when a representative sample of a waste has a pH below 2 or above 12.5. EPA is interested in knowing the extent to which wastewaters in surface impoundments are managed in the pH range just outside the hazardous characteristic range. EPA developed the list of 256 constituents to include constituents that are of interest from a policy standpoint and constituents required to be studied based on the *EDF vs Browner* consent decree. Appendix A lists the constituents within the scope of this study.

1.1.4 Selection of Representative Sample for Data Collection

In February 1999, EPA conducted a "screener" survey of over 2,000 facilities to identify facilities and surface impoundments that are potentially within the scope of the survey. Selecting from among the facilities that reported having in-scope impoundments and wastes, EPA developed a representative sample of 215 facilities to participate in a more detailed survey. EPA developed this representative sample of facilities for the study by selecting a stratified random sample of the direct and zero dischargers and a purposive sample of the indirect dischargers (since there were relatively few indirect dischargers that reportedly used surface impoundments).

The 215 selected facilities received a second detailed survey in November 1999, the Survey of Surface Impoundments, with responses due in February and March 2000. This survey requests detailed data on impoundment design, operation, and closure; the constituents that are present in impoundments and emissions; and data on the subsurface hydrogeology and activities of nearby humans. Both the long survey and the list of facilities that received it (excluding facilities whose information is being handled as confidential business information) can be viewed at http://www.epa.gov/epaoswer/hazwaste/ldr/icr/ldr-impd.htm.

Figure 1-1 shows the estimated distribution of study-eligible facilities used to select the sample population of 215 facilities completing the detailed survey.

1.1.5 Current Knowledge of Study Population

Based on the responses to the 1999 screener survey, EPA estimates that the number of nonhazardous waste surface impoundments in the United States that meet the criteria for inclusion in the Surface Impoundment Study is 19,000 impoundments, located at 8,500 facilities. Major industries represented include the food processing, paper, chemical, petroleum, and stone/clay/glass/concrete industries. An estimated 1,000 facilities, predominantly in the paper, chemical, and petroleum refining sectors, have at least one impoundment with decharacterized wastewaters.

Figure 1-2 shows the universe of surface impoundment facilities having in-scope impoundments by industry category.

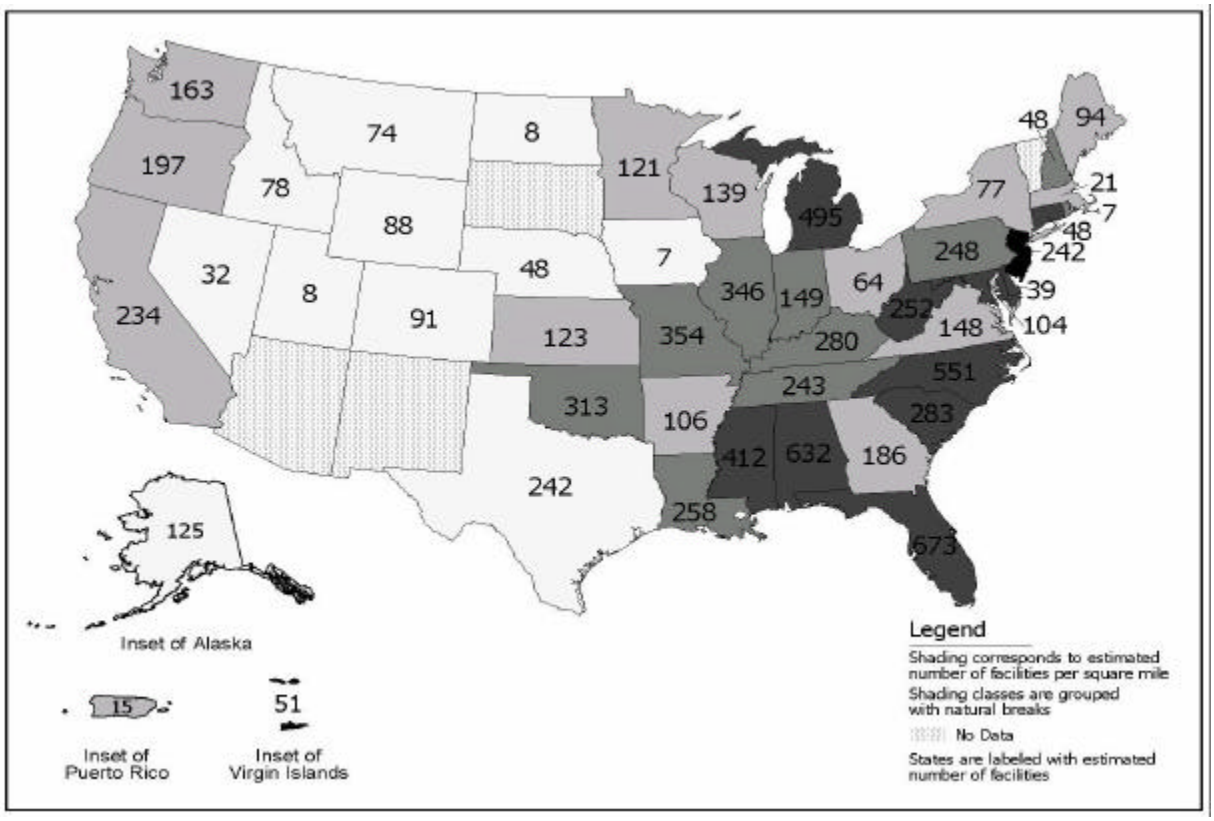
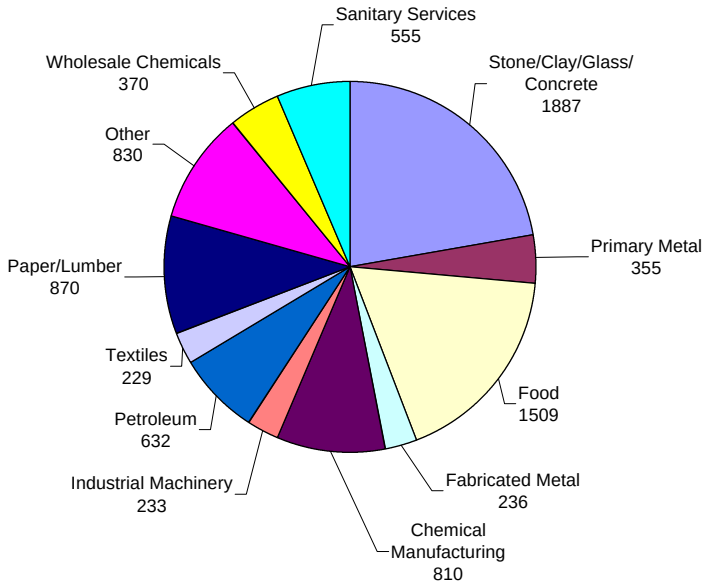


Figure 1-1. Estimated distribution of study-eligible facilities with surface impoundments



Note: Values shown are national estimates of the number of "study-eligible" facilities (facilities using surface impoundments that meet criteria for being in the study).

Figure 1-2. Universe of surface impoundment facilities with in-scope impoundments by industry category.

1.1.6 Additional Data Sources for Study

In addition to the survey results, EPA will also use data from EPA Region and state files (for those facilities that are permitted under RCRA and under EPA authorities); publicly available data sources including census tract data to help evaluate the potential for population exposures; and geographic information system (GIS) data to assist in describing Regional and site-specific geological and ecological conditions. EPA will also collect and analyze wastewater and sludge samples at 15 to 20 facilities selected from among the 215 facilities being surveyed. This is a relatively major sampling effort that will provide important information to supplement that submitted under the survey and will also serve as a quality assurance step. In addition, EPA will include six facilities that were the subject of a 1997-1998 pilot study. Thus, in all, there are 221 facilities under review in this study.

1.1.7 Science Advisory Board Comments

The Agency has submitted the overall design and methodology for the Surface Impoundment Study to EPA's Science Advisory Board (SAB). SAB commented that they found "considerable technical merit in the proposed study structure . . ." (U.S. EPA, 1998c). The SAB also commented that it would be extremely resource-intensive to undertake comprehensive site characterization for multiple units and constituents, and that therefore EPA should use a screening approach to prioritize its efforts.

1.1.8 Purposes of Technical Plan

The major purposes of this technical plan are to provide the analytic blueprint for assessing potential risks associated with the surface impoundment universe (using the data from the surveys and other sources) and to obtain peer review comment on the approaches and methodologies described.

1.2 Summary of Technical Plan for the Analysis

EPA will conduct the technical risk analysis in two stages, with the basic objective of screening all the reported surface impoundment units and constituents during Phase I and conducting more detailed multimedia modeling on some units and constituents in Phase II. Phase I will be the screening and prioritization stage, during which the large number of surface impoundments and constituents anticipated to be reported under the survey will be examined, screened, and prioritized using clear and straightforward science decision rules. During Phase I, EPA will screen out from further analysis those constituents or units that pose negligible risks and will prioritize for additional analysis the remaining units and constituents. Those units and constituents that merit additional analysis of potential risks will proceed to Phase II. In addition, some ambiguous cases will proceed to Phase II to ensure that the Agency is not overlooking areas of potential risk. During Phase II, EPA will use the multimedia model developed for the Hazardous Waste Identification Rule (HWIR), updated for the Surface Impoundment Study, to conduct fate and transport modeling and assess potential risks associated with these units and constituents. (Development of this model is near completion and the model is currently undergoing independent verification to support its use in this and other analyses.) The risk

results for the Phase II stage of the analysis will be used to revise the appropriate portions of the overall risk profile generated during Phase I.

EPA anticipates that the screening-level risk profile of the universe of surface impoundments generated during Phase I and the risk analyses conducted on higher priority units, constituents, and pathways during Phase II will be completed by March 2001 and will be included in the final study that satisfies the statutory and consent decree requirements described above. The Phase I risk profile, because it is a screening-level assessment and based on protective assumptions, will not be a precise representation of risks. As work progresses on Phase II multimedia analyses, the new risk estimates that are based on more realistic exposure assumptions will replace the corresponding Phase I risk estimates, and EPA anticipates that the overall risk profile will generally decrease. (One exception will be for constituents with a high potential to bioaccumulate or persist, for which the Phase II multimedia modeling may show potential risks not identified during Phase I.) The Agency also anticipates that the relative risks will remain approximately the same in the two phases (e.g., comparing different industry categories, constituents, or unit types.) This two-stage analysis is designed to optimize EPA's ability to identify areas of potential concern within a limited period of time.

1.2.1 Phase I. Screening and Prioritization of Constituents, Units, and Pathways of Potential Concern

1.2.1.1 Background. Given the large number of constituents (256 chemicals), in-scope impoundments (anticipated to be approximately 600 surface impoundments at 221 reporting facilities), EPA must conduct a screening in order to prioritize those units, constituents, and pathways of most concern. This point was reinforced by the comments of EPA's Science Advisory Board that it would be extremely resource-intensive to undertake comprehensive site characterization for multiple units and constituents and that EPA would need to prioritize areas for review. In addition, the Agency anticipates that a significant number of units may contain very low levels of constituents and not require lengthy and costly fate and transport modeling. Therefore, two major purposes of Phase I of the analysis are to screen the reported constituents, units, and pathways to identify those of negligible concern that will not require fate and transport modeling and to prioritize those that proceed for further analysis.

At appropriate points throughout the screening and prioritization process, EPA will verify the presence of expected constituents by comparing with constituents that are identified in NPDES and RCRA permits (where applicable), and by cross checking within particular industry categories. If a constituent has not been reported that one might reasonably have expected would be reported, one of several actions could occur: the facility might be considered a candidate for sampling conducted by EPA; the facility might receive followup queries concerning the nature of the waste; and/or EPA might infer the presence of the constituent for modeling purposes.

EPA considers that a sound screening process is a fundamental and integral part of the analysis and is proposing to base the screening on clear science decisions rules related to threshold concentrations of potential concern.

1.2.1.2 <u>Development and Use of Science Decision Rules</u>. EPA proposes to sequentially apply a series of decision rules in determining whether to retain a reported constituent at a reported surface impoundment for further analysis in Phase II.

1.2.1.3 <u>Phase IA: Initial Screening</u>

Basic Approach: Use of Screening Factors. The first step will be for EPA to compare the reported concentration data (in surface impoundment water, sludge, and emissions) collected from the facility survey with threshold concentrations that are protective of human health (residential exposures) and protective of selected representative ecological receptors. The threshold concentrations, or "screening factors," will be developed to provide a suitable margin of protection that, in most cases, will encompass the potential for indirect exposures and background exposures, as discussed below. Surface impoundment units reporting concentrations below the screening factors will be screened out from any further analysis for that particular constituent or pathway. However, the screening level risk that is calculated will be included in the overall risk profile for the surface impoundment universe.

Appendix A provides a table of the health-based benchmarks selected to use in this study for the constituents within the scope of this study; and Section 2.2 the methodology used to calculate screening factors from these benchmarks. This methodology includes the use, at this stage, of highly protective exposure factors, such as direct ingestion of surface impoundment wastewaters and direct inhalation of emissions.

Section 2.3 describes the screening process for ecological risks in detail, including the selection of existing benchmarks for species representative of major taxonomic groupings and protective exposure assumptions. In selecting benchmarks, the preferred toxicological responses will be those related to reproductive fitness and the stability of populations. In addition, EPA will highlight for special evaluation any facilities that are proximate to sensitive habitats such as managed wildlife preserves.

At this stage, EPA's objective is to ensure a suitable margin of protection to human health and the environment in the screening decisions because of the final nature of the screening action in removing a particular constituent, unit, or pathway from any further analysis, with the consequence that there will be no further consideration of the contributions to indirect and cumulative exposures. EPA considers that, for many constituents, screening based on direct ingestion of the surface impoundment influent and direct inhalation of the emissions is, by its nature, very protective. That is, if fate and transport modeling were to be conducted, the potential risks would invariably be lower. EPA may also provide an additional margin of protection to recognize the potential for indirect exposures and for exposures to background levels (i.e., sources other than those within the scope of the survey). In addition, special consideration will be given to constituents with relatively high potential to bioaccumulate or persist in the environment (see discussion below).

Special-Case Constituents. There are a number of constituents with a relatively high potential to be persistent or bioaccumulative that require special consideration. These constituents may represent human health or ecological risks, yet not be identified as constituents

with potential risks through the Phase I screening process. To ensure that these types of constituents are identified, each constituent will be ranked on the basis of persistence (P), bioaccumulation (B), and toxicity (T) to human and ecological receptors, using the procedures and criteria developed for the Revised Waste Management Prioritization Tool (WMPT) (U.S. EPA, 1998e). "Special-case" constituents will be those identified as having high-ranking PBT scores and will be reported along with the relative-risk distributions developed under Phase I. These special-case constituents will proceed to the Phase II multimedia risk analysis.

Risk Criteria. The risk criteria—the levels above which the risk to an individual are considered significant—are as follows:

- For carcinogens: excess cancer risk = 10^{-5}
- For noncarcinogens: hazard index (HI) =1.

These criteria apply to a specific constituent-unit-pathway combination as well as to summations of risks for a constituent, an impoundment, or a facility. Summations of HIs will be considered only if to the same target organ. By separating risks according to target organ, the resulting HI can be summed across the ingestion and inhalation exposure pathways for each of the potentially affected target organs.

Margin of Protection. For purposes of its initial screening, EPA will apply an additional margin of protection of 10^{-1}. This is intended to allow reasonable certainty that constituents and units screened out from further consideration present a negligible risk. Among the considerations leading to the use of a margin of protection are that EPA is not assessing multimedia risks through indirect pathways in Phase I or background levels of exposures that are not within the scope of this study. Note, however, that special-case constituents with high potential to bioaccumulate or persist in the environment will automatically proceed to Phase II analysis.

Representing Risk Ranges and Cumulative Risks. The calculated screening risks for each constituent for a specific impoundment and facility will be combined to generate three cumulative risk estimates: constituent risk, impoundment risk, and facility risk. The risk estimates generated during Phase I for specific constituents, impoundments, and facilities will be accumulated into risk ranges or "bins" to portray potential risk distributions for the surface impoundment universe and various subsets (such as zero dischargers, particular industries, or particular constituents). The human health risk bins currently under consideration include:

- **Excess Cancer Risk (6 bins):** $< 10^{-8}$, $\geq 10^{-8}$ and $< 10^{-7}$, $\geq 10^{-7}$ and $< 10^{-6}$, $\geq 10^{-6}$ and $< 10^{-5}$, $\geq 10^{-5}$ and $< 10^{-4}$, $\geq 10^{-4}$.

- **Noncancer HI (6 bins, by target organ):** < 0.01, ≥ 0.01 and < 0.1, ≥ 0.1 and < 1, ≥ 1 and < 10, ≥ 10 and < 100, ≥ 100).

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

Section 2.2.1 describes the process of aggregating risks for purposes of presenting an initial risk profile after completion of Phase I.

The execution of the screening process (as a practical matter) occurs in a tiered approach, beginning at the facility level and proceeding down through individual units and constituents. The net effect is that constituent, unit, and pathway combinations that are of negligible concern do not proceed to Phase II. For a unit to reach Phase II analysis, it must manage wastes with at least one constituent exceeding the decision criteria; for a facility to reach Phase II analysis, it must manage wastes with at least one constituent exceeding the decision criteria.

The constituents and units of negligible concern will be included in the lowest risk bins at this stage and that risk description will carry forward for them. Even though they will not be analyzed further based on more realistic exposure assumptions, the risks associated with them are already projected to be negligible.

This "binning" approach is taken to serve the dual objectives of (1) screening out particular constituent/unit/pathway combinations of negligible concern from further analysis; and (2) developing an initial overall relative risk ranking of the surface impoundment universe.

Figure 1-3 provides a sample representation of risk ranges based on Phase IA screening results.

Phase IB Human Health Screening Models. EPA expects to use screening-level fate and transport models IWAIR and IWEM[1] (developed for use under the Industrial D guidance) to supplement the initial screening performed under Phase IA. In general these screening models will be appropriate where the major routes of exposure are expected to be direct ingestion of drinking water or direct inhalation (i.e. indirect pathways are not expected to contribute significantly). Also, IWAIR will be used in cases where volatile constituents are known to be present, but there are no air concentration data provided in the surveys. At this stage, EPA will use a limited amount of data from the surveys for the most sensitive parameters, including constituent concentrations, unit size, and close-in receptors. Because some constituents and units may be screened from further analysis, EPA is proposing to use some protective modeling approaches, such as assessing risks for close-in receptors. This stage of screening-level fate and transport modeling is expected to improve the precision of the risk estimates and likely will yield lower risk results than use of the screening factors in Phase IA. The relative-risk profile developed under Phase IA will be revised and updated based on the results of the Phase IB modeling.

[1] The Agency is reviewing the IWAIR and IWEM models to ensure they are updated based on major comments received during a recent peer review, such as the need to correctly incorporate biodegradation rates in IWAIR. This process is expected to be completed in time to use these models in the Surface Impoundment Study. Alternative models that may be used include SCREEN 3 or CHEMDAT 8 for inhalation pathway and EPACMTP for ingestion of drinking water.

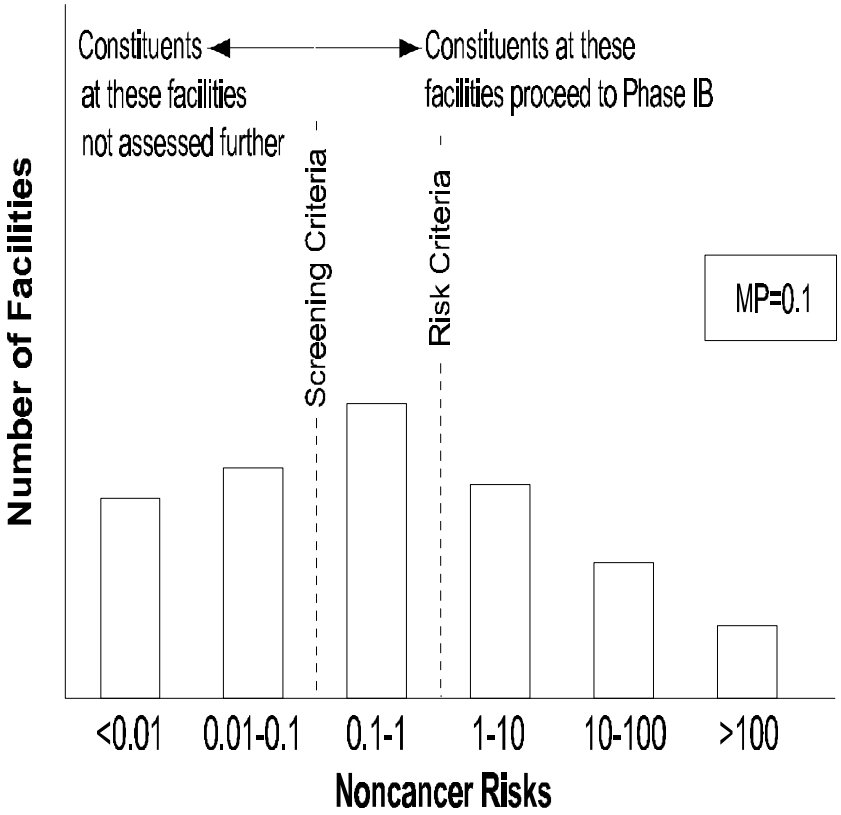


Figure 1-3. Sample representation of risk ranges based on Phase IA screening results.

Phase IC Prioritization. If the number of constituents, units, and facilities that could move into Phase II is large (e.g., more than 25 percent of the study sample), then EPA will prioritize them for further analysis based on the relative risk rankings that were developed during Phases IA and IB. Alternatively, if the number of constituents, units, and facilities that move to Phase II is small and the resulting Phase II effort is within allocated resources, then the prioritization scheme will not be necessary.

Prioritization will occur by assigning overall scores of 1 (highest priority), 2, or 3 based on the degree to which a constituent/unit or facility exceeds the risk criteria for human and ecological risks. For example, an HI of 100 would receive a higher score (1) than an HI of 10 (score = 2). The ranking will also integrate the human health and ecological scores into one score, placing greater emphasis on human health considerations but also addressing high-priority ecological concerns. A qualitative review of Phase I relative risk distributions may also lead the Agency to focus on particular industries, unit types, or constituents of concern. The result of Phase IC will be to identify high-priority constituents, units, and facilities for comprehensive multimedia risk modeling during Phase II.

Anticipated Outcome of Phase I. The outcome of Phase I will be development of an initial risk profile, which represents a relative ranking of potential risks associated with different constituents, unit types, or facilities within the surface impoundment universe. Because this will

be a screening-level risk profile based on protective exposure assumptions, subsequent analysis will develop greater precision for these initial risk estimates. Another outcome of Phase I will be the identification of a subset of surface impoundment units, constituents, and pathways that will proceed for further risk analysis during Phase II.

Units and constituents screened out during Phase I will be presented as having negligible risks in the overall risk profile in the final Surface Impoundment Study. The units and constituents to be studied further, as well as those screened out from further analysis, will be profiled according to significant patterns (if any) such as industry type, unit characteristic, and constituent type.

1.2.2 Phase II Modeling Approaches for Constituents and Units of Potential Concern

1.2.2.1 <u>Background</u>. There will be some units and constituents identified during Phase I that meet the criteria for proceeding to the Phase II analysis and merit further analysis to characterize with greater precision any potential risks to health and the environment. The magnitude of the Phase II effort is unknown at this time, and, depending on the number of units and constituents that require further analysis, EPA intends to undertake one of two approaches. If, as anticipated, a fairly limited number of units and constituents proceed to Phase II, EPA will conduct multimedia fate and transport modeling of potential human and ecological risks using the HWIR multimedia model, as modified for the Surface Impoundment Study and using, to the extent possible, the site-specific hydrogeologic data, watershed parameters, and receptor data provided in the surveys and available through other data sources such as GIS files. This is a fairly intensive modeling approach that will be possible only for a relatively limited number of cases. Alternatively, in the event that a large number of sites meet the criteria for proceeding to Phase II, EPA will develop a range of appropriate hydrogeologic and watershed "scenarios" (approximately 20 to 30 representative scenarios) to simplify the process of data file development and modeling for a large number of sites. This will greatly streamline the use of the HWIR model while maintaining the advantages of this powerful tool to describe multimedia fate and transport. The Agency is also considering extending the "representative scenario" approach to include representative ranges of populations exposed.

Phase II results will be used to revise the risk profile for the surface impoundment universe based on more realistic exposure assumptions and multimedia fate and transport modeling.

1.2.2.2 <u>Choice of Models to Use during Phase II</u>. EPA's preferred approach for the multimedia modeling during Phase II will be to use its multimedia, multipathway, multireceptor risk analysis (3MRA) model being developed to support the HWIR rulemaking and other analytic efforts. An alternative approach considered was to use the MMSOILS model, as currently updated. Major considerations leading to the recommendation that 3MRA be used were the ability to use many of the same data files for default parameters that had been developed to support the HWIR effort; the automatic integration of the various modules for different media thereby minimizing the quality assurance/quality control (QA/QC) necessary for manual integration of modules; and (3) the feasibility of using the system both in screening-level multimedia analyses and comprehensive multimedia analyses. The MMSOILS model met many

of these criteria; however, the integration of the modules for various media is not fully automated and the manual integration is expected to be too time-consuming to consider for this analysis.

1.2.2.3 <u>Alternative Approaches for Data File Development</u>. At this point it is not possible to foresee the number of constituents and units that will require modeling during Phase II after completion of the screening and prioritization that occurs during Phase I. Depending on the number, the Agency proposes to manage the effort in one of two ways that differ primarily in the level of site-specific data required to be developed and entered for each unit.

- **Screening-level multimedia analysis for a large number of units and constituents:** EPA will use the information reported in the surveys to choose the closest matching from among a series of representative scenarios of hydrogeologic and watershed conditions. The representative scenarios will be defined using the HWIR database, and EPA will ensure that the scenarios span the appropriate range of conditions reported in the Surface Impoundment Survey. EPA will review data reported in the surveys to select the best representative scenario, including number and proximity of waterbodies, hydrogeologic information, soil types, and receptor types and ranges. In the modeling, EPA will directly use a significant amount of site-specific data from the surveys, such as the location of actual close-in receptors and direction of groundwater flow, information on constituent concentrations, and information of sensitive ecological habitats.

- **Comprehensive multimedia analysis for a small number of units and constituents:** EPA will develop input parameters for the 3MRA model using as much site-specific data as possible from the surveys, Regional and state files, and publicly available databases. A comprehensive data file will be developed for each site, which will be modeled to account, with the greatest possible precision, for any potential risks associated with that site.

Under either alternative, EPA will use the 3MRA model in a deterministic mode for as many iterations as possible within the allocated time and resources. The basic approach will be to model at least one “high-end” and central tendency analysis for each pathway, based on the closest real receptors (“high-end”) and central tendency receptors as reported in the surveys or identified from other data sources.

1.2.2.4 <u>Risk Profile Generated</u>. EPA anticipates that the risk estimates generated during Phase II will provide a comprehensive National profile of potential risks posed by the universe of surface impoundments for several reasons:

- The sample of 215 facilities is a statistically representative sample of the universe

- The potential risks modeled for major pathways at each surface impoundment are based on real concentration and exposure data reported by facilities and Regions

- The high-end and central tendency scenarios–based on these real receptors–provide a realistic span of potential risks.

This risk profile generated during Phase II will also serve to identify any unit types, constituents, or facilities (industries) that may require additional followup analysis.

1.2.3 Anticipated Outcome of Analysis

The Agency will prepare a study by March 2001 that characterizes the potential risks associated with the surface impoundment universe for 256 constituents.[2] This will include a discussion of any constituents, unit types, or facility categories for which additional analysis is recommended subsequent to the study. The study will provide a profile of the surface impoundment universe by unit type, industry type, and constituent; provide a descriptive profile of the subset of the universe that is of negligible concern and requires no further risk analysis; and provide a relative-risk profile for the entire universe of surface impoundments for these 256 constituents. The study is expected to also include risk analyses based on multimedia modeling for a limited number of high-priority constituents, units, and facilities.

1.3 Peer Review Process and Comments Solicited

EPA is providing this technical plan to several peer reviewers with expertise in human and ecological risk analyses, fate and transport modeling, and screening and statistical procedures for identifying potential risks from managing industrial wastewaters in surface impoundments. The Agency is seeking comments on the technical merits of the overall approach and is specifically soliciting comments in the following areas:

- **Derivation of human health screening factors:** EPA is seeking comment on whether the methodology for calculating screening factors is a suitable methodology and whether there are other data sources that are readily available that would provide credible benchmarks for the limited number of cases for which we do not have benchmarks.

- **Derivation of ecological screening factors:** EPA is seeking comment on whether the list of representative species is suitable for achieving a screening level assessment that will highlight possible ecological risks associated with surface impoundments and whether there are any serious gaps in the consideration of potential ecological risks that can be addressed by readily available data and benchmarks not identified here.

- **Level of protectiveness:** EPA has designed the screening process to ensure that constituents and units proceeding to subsequent stages of the analysis merit

[2] There are a few constituents in the list of 256 in-scope constituents that currently lack human health benchmarks. EPA is attempting to identify suitable benchmarks to allow their inclusion in this screening analysis. If benchmarks are not available, then EPA will include these constituents in the overall description of the survey results but not conduct any risk analyses on them.

further analysis and that those that do not proceed to subsequent stages have negligible risks (or alternatively, have very well-characterized risks and do not require further analysis). The intent is that the early stages of the analysis will include protective assumptions and that there will be a negligible possibility of overlooking potential risks. The Agency is seeking comment on whether the proposed screening approach achieves these objectives.

Approach for dealing with lack of information on chemical composition of wastewater in the impoundments or emissions: The technical plan proposes a number of approaches for dealing with situations where facilities do not report concentration or emissions data for constituents that are present in impoundments. These include approaches for the use of data from other impoundments at the same facility, the use of data from other facilities in the same industrial category, the use of sampling data acquired by EPA from facilities in the same industrial category and modeling or backcalculating to infer concentrations. EPA is soliciting comment on these various approaches for estimating concentration data that are not reported.

Approach for representing cumulative risks: EPA has designed an approach for representing cumulative risks for each constituent, unit, and facility reported under this survey. (An assessment of background risks, i.e., due to sources other than in-scope surface impoundments, is beyond the scope of this survey and analysis.) The Agency is seeking comment on the methodology for accumulating and representing risks within the scope of this survey.

Modeling approaches: EPA is seeking comment on the overall approach and methodology for conducting screening-level modeling during Phase I and multimedia modeling during Phase II. For example, at this point EPA is uncertain how many units and constituents will merit multimedia modeling. As time and resources allow, EPA will undertake comprehensive multimedia modeling for each site. Alternatively, if a large number of sites merit modeling, EPA may use predefined representative scenarios for hydrogeologic conditions and watersheds (while still using as much site-based data as possible.) EPA seeks comments on these alternatives as well as the other modeling strategies outlined in this Technical Plan.

1.4 Organization of the Technical Plan

The remainder of this Technical Plan is organized as follows:

Section 2 describes the Phase IA and IB human health and Phase I ecological risk screening process, and the Phase IC method of prioritizing results of Phase I.

Section 3 describes the Phase II multimedia, multipathway modeling approach to estimate risks to human and ecological receptors.

- References are included in Section 4.

Supporting documentation is included in the following appendixes:

- Appendix A, Comprehensive List of Toxicity Benchmarks for Human Health Risk Assessment
- Appendix B, Statistical Analysis Weights and Variance Estimation for the Surface Impoundment Study Screening Survey
- Appendix C, Examples of Toxicity Benchmarks for Ecological Risk Assessment
- Appendix D, 3MRA Simulation Modules: Assumptions, Limitations, Inputs, and Outputs

2.0 Phase I Screening Assessment

2.1 Introduction

Experience to date suggests that comprehensive risk analysis, based on multimedia fate and transport modeling, is both time consuming and costly and should be used where screening analyses point to the need for sophisticated modeling. The Agency expects that a number of responses to the detailed questionnaires sent to 215 facilities will describe very low levels of some constituents in some impoundments. Two major purposes of this stage of the analysis are to screen (i.e., reduce the number of) constituents, impoundments, and facilities that require fate and transport modeling and to prioritize those remaining for subsequent analysis. The screening and prioritization will be based on clear science decision rules related to threshold concentrations of potential concern and low likelihood of exposures. These decision rules will allow EPA to screen out those constituents, impoundments, and facilities presenting negligible potential risks and to focus on analyzing those that may present higher potential risks.

EPA proposes to apply a series of decision rules sequentially in determining the constituents, impoundments, and facilities that will be evaluated further in Phase II, as shown in Figure 2-1. Both human health and ecological risk decision rules will be applied.

Human health risk screening consists of two phases:

- Phase IA compares reported constituent concentrations in surface impoundments to concentrations protective of human health.

- Phase IB estimates human health risk levels based on modeled exposure concentrations. Phase IB risk screening will be done for all constituents not eliminated from further evaluation based on Phase IA.

Ecological risk screening consists of one phase that parallels the human health Phase IA screening:

- Phase I compares reported constituent concentrations to concentrations protective of ecological receptors.

Risk screening identifies those constituents, impoundments, and facilities that have risks that are greater than the identified risk criteria and therefore require further analysis. Risk screening may still result in a large number of constituents, impoundments, and facilities for Phase II analysis. Therefore, Phase IC decision rules will be applied:

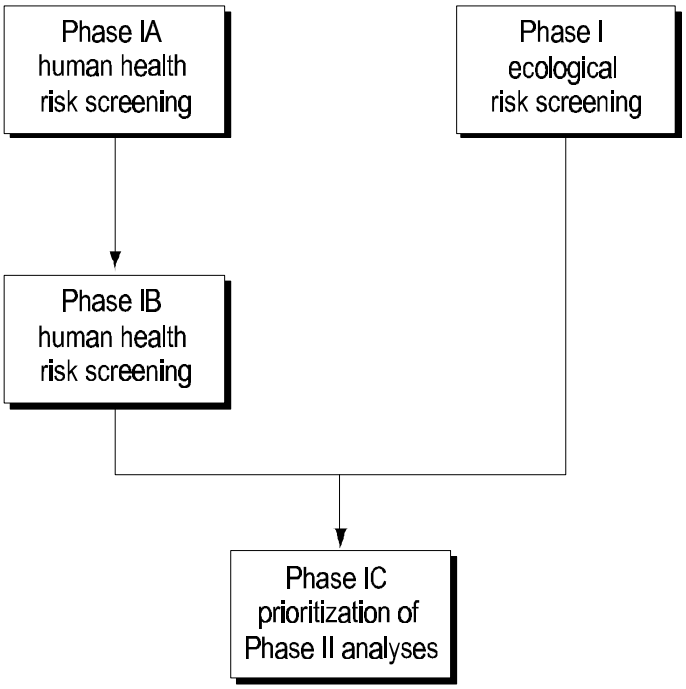


Figure 2-1. Overview of Phase I decision rules.

- Phase IC ranks the human health and ecological screening risks to prioritize constituent impoundments and facilities for Phase II analysis.

Key features of the human health risk screening approach are as follows:

- There are two stages in human health risk screening.
- The first stage will compare the arithmetic mean of reported concentration data (water, sediment, and air) collected from the facility survey to backcalculated health screening factors protective of residential exposure.
- The second stage will include more realistic evaluations of air and groundwater risks by evaluating fate and transport processes in the environment. The EPA screening models Industrial Waste Air Model (IWAIR) and Industrial Waste Evaluation Model (IWEM) (U.S. EPA, 1998a, b; 1999a, b) will be used to calculate risks.

The ecological risk screening approach can be characterized by the following key features:

- The screening will compare the arithmetic mean of reported concentration data (water and sediment) collected from the facility survey to screening factors.

- Screening factors will be existing threshold concentrations for adverse ecological effects such as the Ambient Water Quality Criteria for the protection of aquatic life.

- Screening factors for a limited set of representative species and representative habitats will be established using peer-reviewed data from HWIR (i.e., wildlife exposure factors, biological uptake factors, toxicity benchmarks) supplemented by toxicity data gathered for constituents not evaluated in HWIR (U.S. EPA, 1999n).

2.2 Phase I Human Health Risk Screening

The Phase I human health risk screening consists of a series of two decision rules, Phase IA and IB, applied to evaluate whether a constituent, impoundment, or facility can be excluded from further evaluation or must continue to Phase II. The Phase IA decision rule will calculate risk estimates for groundwater ingestion, soil ingestion, and air inhalation based on reported impoundment concentrations. The Phase IB decision rule will calculate risk estimates for groundwater ingestion and air inhalation based on air and groundwater screening model exposure concentration estimates. The risk estimates will be compared to risk criteria to determine if the constituent, impoundment, or facility can be excluded from further evaluation. Phase IB will be invoked for two conditions: (1) constituents that volatilize but for which there are no air concentration data provided in the responses to the survey questionnaire, and (2) constituents that were not excluded based on the Phase IA risk screening.

2.2.1 Phase IA Human Health Initial Risk Screening

The Phase IA risk screening is described in four sections:

- Design goals and overview
- Development of screening factors
- Procedure for risk screening
- Results of risk screening.

2.2.1.1 <u>Phase IA Human Health Design Goals and Overview</u>. The goal of the Phase IA initial screening assessment is to identify constituents, impoundments, and facilities that have negligible risks and do not need further assessment in the SI Study. The Phase IA approach will calculate screening risks to an individual receptor based on concentrations of constituents in and emissions from surface impoundments reported in the survey questionnaire and risk screening factors. The human health risk screening factors will be based on toxicity benchmarks for direct ingestion of drinking water, direct air inhalation, and direct soil ingestion (for the in-place closure scenario). These screening risks will be protective because they are based on the highly protective assumptions that a resident will drink the impoundment water, inhale the air at the impoundment, and eat the sludge. To account for indirect exposures and cumulative exposures from multiple constituents or impoundments, the Agency may choose

to use a margin of protection (MP) in determining whether a constituent, impoundment, or facility should be excluded from further evaluation. If risks are less than the selected risk criteria times the MP, then they will be considered negligible risks and no longer considered in subsequent phases.

The screening risks for each constituent, impoundment, and facility will also be accumulated to provide initial risk distributions. Risk distributions will provide the basis for prioritizing for Phase II (see Section 2.4). These risk distributions, while protective, will also provide the initial risk profiles that describe the national scale surface impoundment population. That is, although we expect the risk estimates to decrease as more site-specific data collection and multimedia exposure modeling are performed in subsequent phases, the overall distribution should be similar. For instance, if a certain industry has Phase I screening risks that are high relative to other industries, then the relative risk level will likely remain in Phase II. One major exception may be constituents that tend to persist and bioaccumulate. The relative risks for these constituents may be very different in Phase II because indirect (rather than direct) exposure pathways are driving the risks. These risk distributions will be refined with each subsequent phase.

2.2.1.2 <u>Development of Phase IA Human Health Screening Factors</u>. The Phase IA screening risk will be calculated as the ratio of the reported concentrations to the screening factors multiplied by the risk criteria, as follows:

$$Screening\ Risk = \frac{Reported\ Concentration}{Risk\ Screening\ Factor}\ x\ Risk\ Criteria\ .$$

It should be noted that the screening risk calculation is mathematically equivalent to a standard forward calculation of risk, whereby the exposure concentration is converted to a dose and multiplied by the cancer slope factor (if carcinogenic) or divided by the reference dose (if noncarcinogenic). The risk calculation process is also equivalent to the standard approach for evaluating airborne chemical exposures wherein exposure concentrations are divided by the reference concentration (if noncarcinogenic). The above calculation is easier to use for this SI Study screening phase. Also, development of the risk screening factor as a threshold concentration provides a simple comparison method that EPA, regulated parties, and the public can use to examine the survey data and screening results.

To develop a human health risk screening factor for each constituent, EPA will

- Identify human receptors
- Identify exposure pathways
- Define toxicity benchmarks
- Identify the risk criteria
- Calculate screening factors.

Human Receptor Types. The human health-based risk screening factors will be based on residential exposure. The exposure factors used to characterize the residents will be based on the receptor, toxicological endpoint, and exposure pathways evaluated as follows:

- For carcinogenic risks, a time-weighted child/adult resident
- For noncarcinogenic risks, a child resident for the soil and groundwater ingestion pathways and an adult resident for the air inhalation pathway.

A time-weighted resident is considered for carcinogenic risks because of concerns that a child with a small body weight typically has higher levels of exposure for the same levels of intake as an adult. Inclusion of multiple age groups more accurately reflects potential residential exposures and is supported by data provided in EPA guidance for different age groups (*Exposure Factors Handbook*, U.S. EPA, 1997a). A child resident is considered for noncarcinogenic risks for the soil and groundwater ingestion pathways to ensure a protective level of exposure, since a child with a small body weight typically has higher levels of exposure for the same levels of intake as an adult. An adult resident is considered for noncarcinogenic risks for the air inhalation pathway only because development of the toxicological benchmark for the inhalation pathway, the reference concentration (RfC), is based on the assumption that an exposed individual would be comparable to an adult resident (i.e., have a default inhalation rate of 20 m^3 per day and a body weight of 70 kg). EPA considers the RfC protective of child and adult receptors. Although this approach to evaluating inhalation risks may result in some level of uncertainty in the risk estimates, EPA considers this acceptable for screening purposes.

Human Exposure Pathways. Risk screening factors will be developed for the following exposure pathways:

- Ingestion of impoundment water (as a protective estimate of groundwater ingestion)
- Ingestion of sludge/soil (as a protective estimate of postclosure in place)
- Inhalation of volatile emissions from an impoundment (as a protective estimate of inhalation).

Inhalation of particulate emissions from sludge (postclosure in place) will not be considered because this pathway typically represents negligible risks.

Figure 2-2 presents the Phase I risk conceptual model and potential exposure pathways for human receptors.

Toxicity Benchmarks. Human health risk screening factors will be based on toxicity benchmarks (i.e., cancer slope factors, reference doses, and reference concentrations) in the Integrated Risk Information System (IRIS) and Health Effects Assessment Summary Tables (HEAST) (U.S. EPA, 1999c; U.S. EPA, 1997c). If benchmarks are not available in IRIS or HEAST, then other EPA or alternative (e.g., ATSDR) health benchmarks will be considered. If

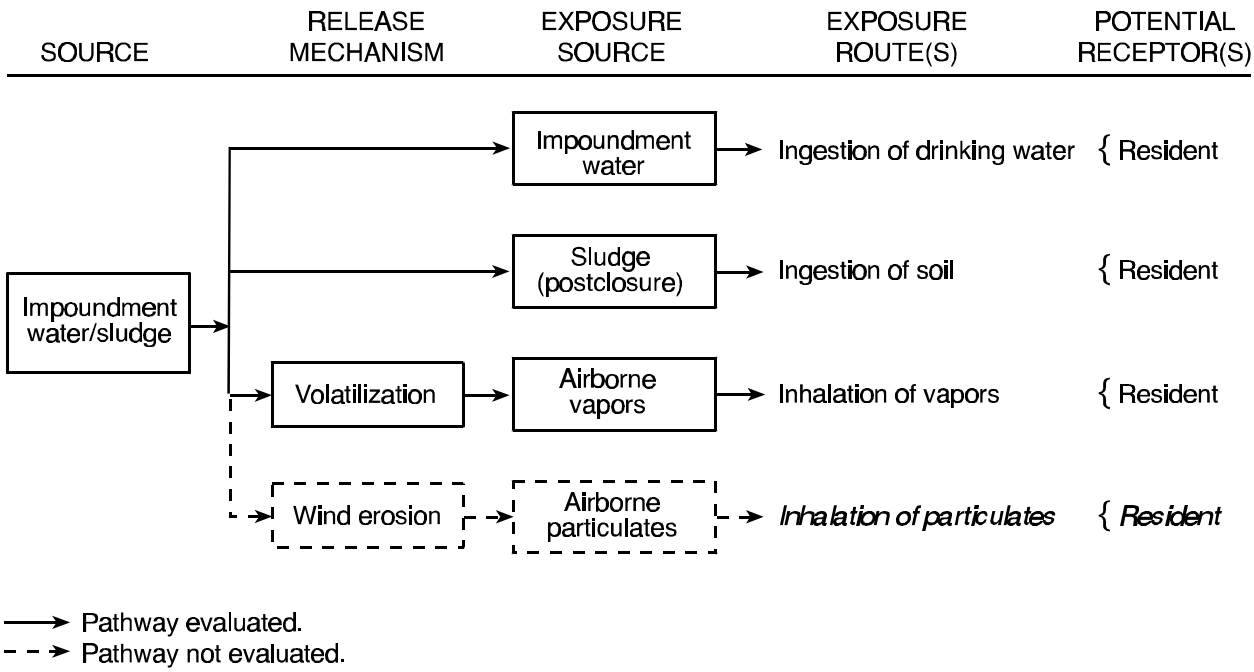


Figure 2-2. Phase I human health risk conceptual model and potential exposure pathways.

no health benchmarks are available, a regulatory standard (e.g., maximum contaminant level [MCL]) may be used to develop the risk screening factor. If benchmarks or regulatory standards are not available, then the Agency proposes using the provisional approach developed for HWIR to develop interim human health benchmarks for screening purposes. This process may also incorporate use of risk-based criteria, such as the preliminary remediation goal for residential exposure to lead in soil, to ensure that all toxicants of concern are addressed.

Risk Criteria. The risk criteria, the levels above which the risk to an individual are considered significant, are as follows:

- For carcinogens, excess cancer risk = 10^{-5}
- For noncarcinogens, hazard index (HI) = 1.

These criteria apply to a specific constituent-impoundment-pathway combination as well as to summations of risks for a constituent, an impoundment, and a facility. Summations of HIs will be considered only if to the same target organ. By separating risks according to target organ, the resulting HIs can be summed across the ingestion and inhalation exposure pathways for each of the potentially affected target organs.

Calculation of Human Health Screening Factors. The carcinogenic and noncarcinogenic risk screening factors will be developed using the equations shown in Table 2-1. The equations for the three pathways are based on EPA guidance (U.S. EPA, 1989).

Table 2-1. Equations for Development of Human Health Screening Factors

Carcinogenic	Noncarcinogenic
Inhalation	***Inhalation***
$$CRSF_{air} = \frac{RC_c \cdot AT \cdot 365}{SF \cdot EF \cdot \left(\sum_{i=1}^{5} \frac{INR_i \cdot ED_i}{BW_i} \right)}$$	$$NCRSF_{air} = RC_n \cdot RfC$$
where $CRSF_{air}$ = carcinogenic risk screening factor for air (mg/m^3) RC_c = risk criteria for carcinogens AT = averaging time (yr) = 70 SF = slope factor (kg-d/mg) EF = exposure frequency (d/yr) i = index on age group (e.g., <1 yr, 1-5 yr, 6-11 yr, 12-18 yr, adult) INR_i = inhalation rate of air for age group i (m^3/d) BW_i = body weight for age group i (kg) ED_i = exposure duration for age group i (yr)	where $NCRSF_{air}$ = noncarcinogenic risk screening factor for air (mg/m^3) RC_n = risk criteria for noncarcinogens RfC = reference concentration (mg/m^3)
Ingestion of Water	***Ingestion of Water***
$$CRSF_{water} = \frac{RC_c \cdot AT \cdot 365}{SF \cdot EF \cdot \left(\sum_{i=1}^{5} \frac{IRW_i \cdot ED_i}{BW_i} \right)}$$	$$NCRSF_{water} = \frac{RC_n \cdot BW_c \cdot RfD \cdot 365}{EF \cdot IRW_c}$$
where $CRSF_{water}$ = carcinogenic risk screening factor for water (mg/L) RC_c = risk criteria for carcinogens AT = averaging time (yr) = 70 EF = exposure frequency (d/yr) SF = slope factor (kg-d/mg) i = index on age group (e.g., <1 yr, 1-5 yr, 6-11 yr, 12-18 yr, adult) IRW_i = ingestion rate of water for age group i (L/d) BW_i = body weight for age group i (kg) ED_i = exposure duration for age group i (yr)	where $NCRSF_{water}$ = noncarcinogenic risk screening factor for water (mg/L) RC_n = risk criteria for noncarcinogens RfD = reference dose (mg/kg-d) BW_c = body weight for child (kg) EF = exposure frequency (d/yr) IRW_c = ingestion rate of water for child, ages 1-5 yrs (L/d)

(continued)

Table 2-1. (continued)

Carcinogenic	Noncarcinogenic
Ingestion of Soil	***Ingestion of Soil***
$$CRSF_{soil} = \frac{RC_c \cdot AT \cdot 365}{SF \cdot EF \cdot 10^{-6} \cdot \left(\sum_{i=1}^{5} \frac{IRS_i \cdot ED_i}{BW_i} \right)}$$	$$NCRSF_{soil} = \frac{RC \cdot RfD \cdot BW_c \cdot 365}{EF \cdot IRS_c \cdot 10^{-5}}$$
where	where
$CRSF_{soil}$ = carcinogenic risk screening factor for soil (mg/kg) RC_c = risk criteria for carcinogens AT = averaging time (yr) = 70 EF = exposure frequency (d/yr) SF = slope factor (kg-d/mg) i = index on age group (e.g., <1 yr, 1-5 yr, 6-11 yr, 12-18 yr, adult) IRS_i = ingestion rate of soil for age group i (mg/d) BW_i = body weight for age group i (kg) ED_i = exposure duration for age group i (yr)	$NCRSF_{soil}$ = noncarcinogenic risk screening factor for soil (mg/kg) RC_n = risk criteria for noncarcinogens RfD = reference dose (mg/kg-d) BW_c = body weight for child (kg) EF = exposure frequency (d/yr) IRS_c = ingestion rate of soil for child, ages 1-5 yr (mg/d)

The values of the exposure parameters used in the equations are provided in Table 2-2. All data are from the *Exposure Factors Handbook* (U.S. EPA, 1997b). The means for inhalation rate, water intake rate, and body weight are consistent with the data means identified or calculated in HWIR's Human Exposure Factors (U.S. EPA, 1999q). All human exposure factors were developed for the following subpopulations:

- Adult resident
- Children ages 12 to 19 years
- Children ages 6 to 11 years
- Children ages 1 to 5 years
- Children ages <1 year (infants).

For noncarcinogenic risks for the soil and groundwater ingestion pathways, the age group that produces the lowest screening factor (i.e., has the highest ratio of ingestion rate to body weight) will be used. For the soil ingestion pathway and the groundwater ingestion pathway, this is the 1- to 5-yr-old age group.

The age ranges for children are consistent with the age groups for which most data are provided in the *Exposure Factors Handbook*. With the exception of exposure duration and soil

Table 2-2. Exposure Parameter Values

Receptor	Inhalation Rate (m^3/d)	Ingestion Rate of Water (L/d)	Ingestion Rate of Soil (mg/d)	Exposure Frequency (d/yr)	Exposure Duration (yr)	Body Weight (kg)
Child < 1	4.5	0.30	ND	350	1	9.1
Child 1-5	7.55	0.70	200	350	5	15.5
Child 6-11	11.75	0.79	50	350	6	30.8
Child 12-18	14.0	0.96	50	350	7	58.4
Adult Resident	13.3	1.38	50	350	11	71.4

ingestion rates for children, exposure factors were selected to represent typical or central tendency values, not high-end values.

An overall exposure duration of 30 years was selected as a high-end value for residents. This was then allocated to the various age ranges desired, based on the number of years in each age bracket. The exposure frequency is the number of days per year that a receptor is exposed. A value of 350 days per year was selected for all residents, based on an exposure of 7 days per week, with the receptor being elsewhere on vacation for 2 weeks per year (U.S. EPA, 1997b).

Based on data provided in the *Exposure Factors Handbook* (Layton, 1993), the inhalation rates for each age group were first averaged for males and females for each age group if they were not presented as combined male and female. The combined male/female mean inhalation rates for each child age group were then averaged to get the desired age groups (e.g., combined values for ages 1 to 2 and 3 to 5 were averaged to get value for ages 1 to 5). For adults (19 to 65+ years), the recommended mean values for males and females (15.2 and 11.3 m^3/d, respectively) were averaged.

For soil ingestion rates, the *Exposure Factors Handbook* only distinguishes between children under 6 and all other ages, so the ingestion rates were assigned accordingly. EPA recommends 100 mg/d as the best estimate of mean soil ingestion for children under the age of 6; however, EPA also notes that this value may underestimate soil intake rates because children were studied for short periods of time and the prevalence of pica behavior is not known. Therefore, EPA recommends 200 mg/d as a conservative mean for soil intake in children under 6 years of age. No soil ingestion data are available for infants (children <1 year old).

Based on data provided in the *Exposure Factors Handbook* (Ershow and Cantor, 1989), the mean drinking water intake rates were calculated from weighted (by sample size) averages of means for each age group.

For body weights, the *Exposure Factors Handbook* contained mean body weights for 1-year age intervals for male and female children; these values were averaged (weighted by

sample size) across the ranges used here. For mean adult body weight, the weighted average (based on sample size) of the values presented in the *Exposure Factors Handbook* for males and females ages 18 to 74 were used.

If a carcinogenic or noncarcinogenic risk screening factor cannot be developed for a chemical based on an EPA or alternative health benchmark, a risk screening factor that is equivalent to the regulatory standard (e.g., maximum contaminant level or MCL) may be used. If a regulatory standard is unavailable, then an interim toxicity benchmark will be developed and used. The Agency considers that, for a screening level analysis, it is appropriate to use draft provisional benchmarks for constituents lacking established health benchmarks.

Cumulative Effects. The cumulative effects for air, groundwater, and soil exposure to the same resident will be evaluated, although the exposures may occur at different times. This is a protective assumption to ensure that risks are not underestimated.

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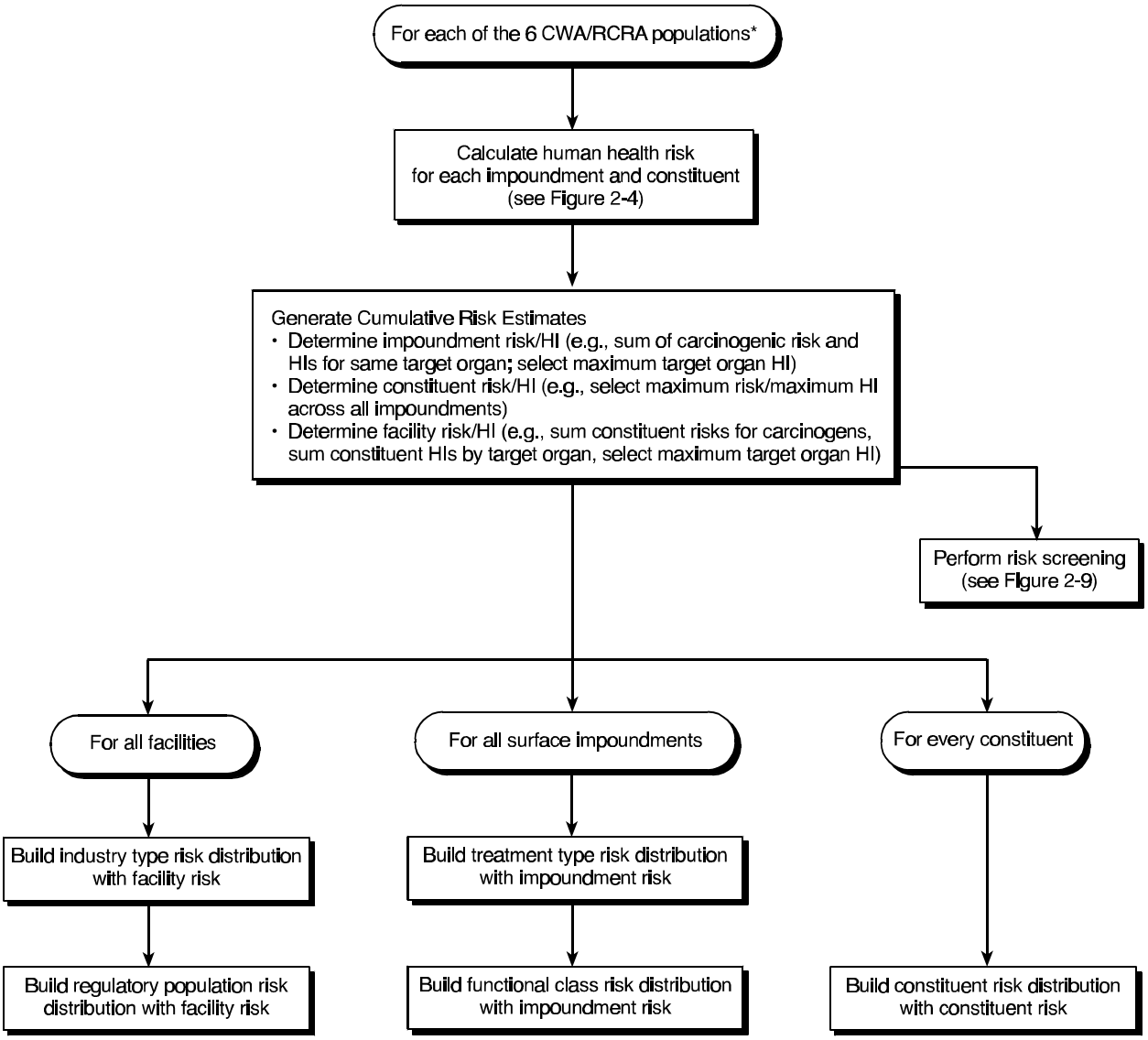
2.2.1.3 <u>Procedure for Phase IA Human Health Risk Screening</u>. The overall human health screening process is shown in Figure 2-3. The human health risk screening calculation will be performed for each constituent in each surface impoundment for each of the 221 sample facilities. At this point, the screening risk estimates will be constituent-specific risks or HIs that have been summed across exposure pathways. Cumulative risks will then be calculated for each impoundment and each facility and for each constituent (summed over all impoundments at the facility) . The cumulative risk estimates will be used to build initial risk distributions for the surface impoundments within the scope of the study. The units within the study scope are defined in Section 1. These fall within six categories (“populations”) depending upon their regulatory status under the Clean Water Act and RCRA. Risk distributions will be generated for impoundment functional type, impoundment treatment type, industry type, and constituent. The risk distributions will be used to exclude constituents, impoundment types, or facilities from further analysis. Further, the risk distributions will provide the basis for prioritizing evaluations conducted in Phase II (see Phase IC discussion in Section 2.4).

The four main elements to the Phase IA human health screening process are

- Human health risk calculation
- Cumulative risk calculation
- Risk distribution development
- Risk screening.

Human Health Risk Calculation. The risk calculation process is shown in Figure 2-4. The groundwater ingestion pathway will always be evaluated; surface impoundment wastewater concentrations will be used in Phase IA as conservative estimates of potential groundwater exposure levels. The air inhalation pathway will be evaluated for a constituent in Phase IA if the constituent is a volatile organic chemical (VOC) and airborne chemical concentration or emissions data are provided by the survey. The soil ingestion pathway will be evaluated for a constituent if sludge accumulates in the impoundment. Once the air, water, and sludge



Notes:
*Direct discharger - decharacterized
Direct discharger - nondecharacterized
Indirect discharger - decharacterized
Indirect discharger - nondecharacterized
Zero discharger - decharacterized
Zero discharger - nondecharacterized

Figure 2-3. Flow diagram for Phase IA human health risk screening.

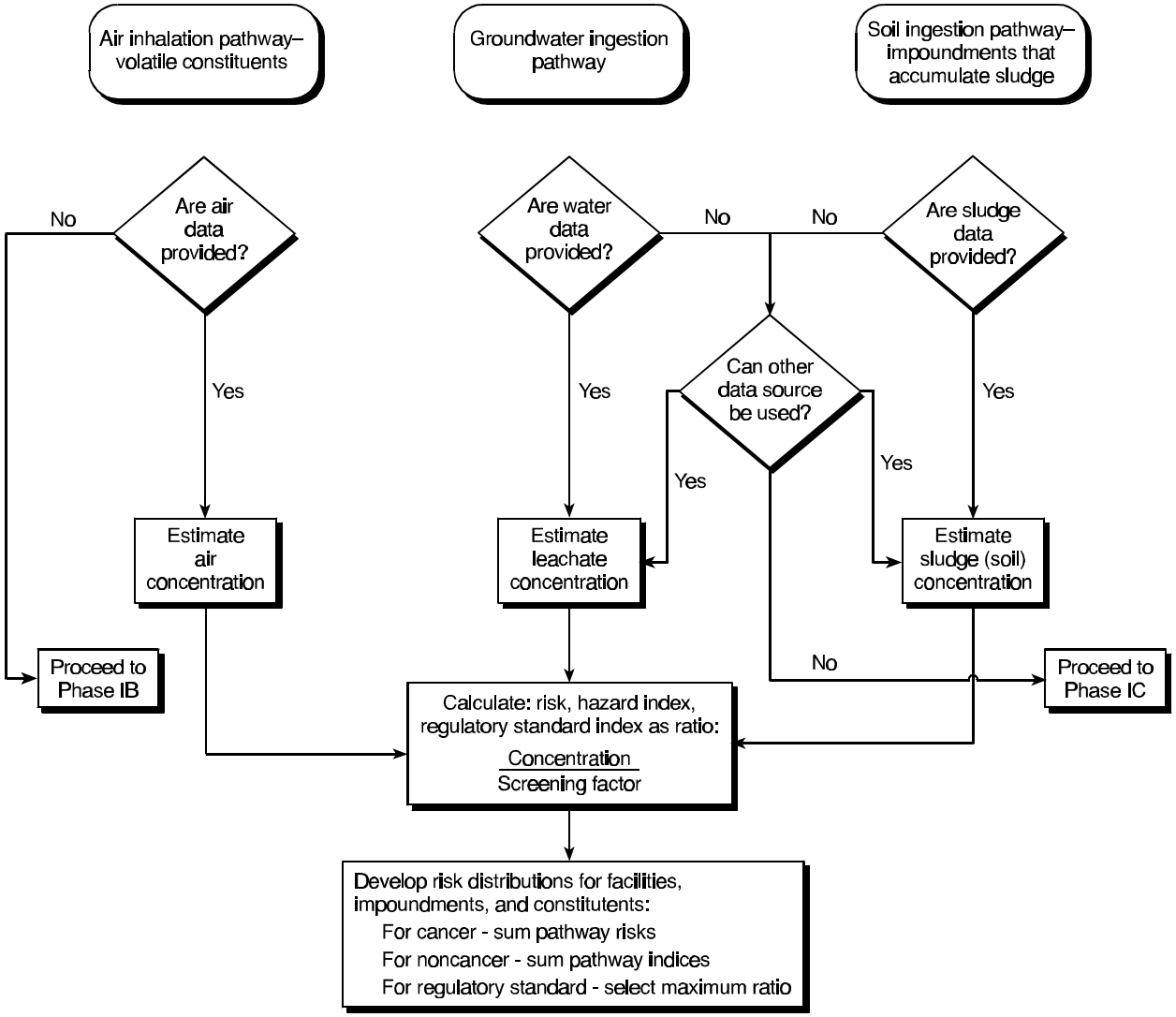


Figure 2-4. Decision tree for calculating Phase IA human health risk estimates.

concentrations are determined from the survey results, the risks will be calculated by dividing the concentration by the appropriate screening factor and then multiplying by the risk criteria. If the screening factor is based on a regulatory standard, then the ratio of concentration to the screening factor will be calculated. Finally, the constituent risk and HI will be calculated by summing the risks and hazard quotients (HQs) for all pathways for that particular constituent. If the screening for the constituent has used a regulatory standard, then the maximum ratio of all pathways for that constituent will be selected.

Concentration data from the facility survey questionnaire will provide exposure concentrations for the Phase IA risk estimates. Figures 2-5 through 2-8 describe how the air, water, and sludge concentrations will be used or calculated from the facility survey data. The decision trees outline the order of preference for using concentration data. The specific survey questions that will provide the data are noted in the decision trees. A special condition exists for calculating air inhalation risks from survey data. If the survey questionnaire does not provide an air concentration or emission rate for a VOC constituent but does provide water concentrations, then the air emissions and concentration will be estimated using screening models and will be performed in Phase IB (see Section 2.2.2).

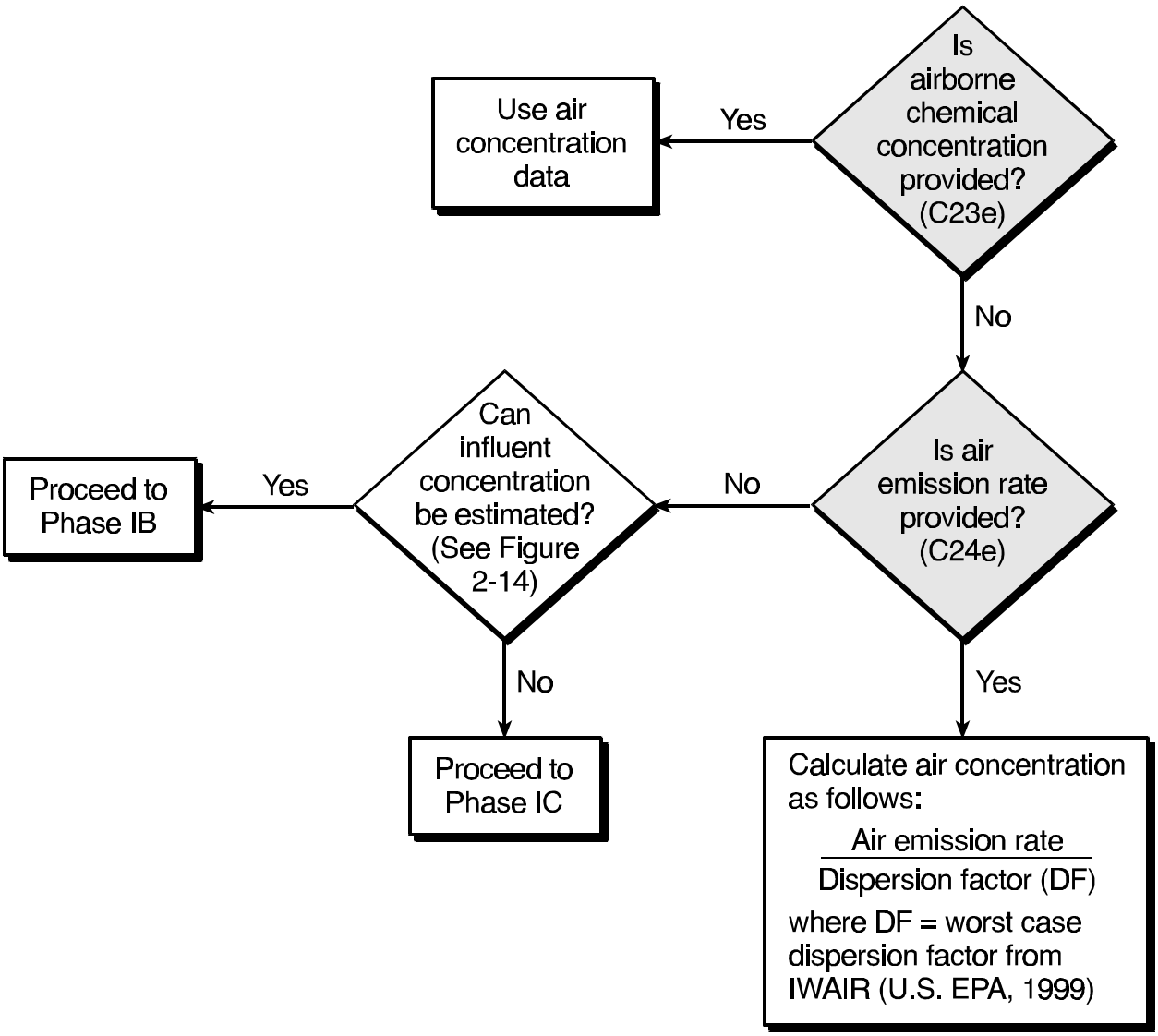
In cases when the air, wastewater, or sludge concentration is not provided in the survey questionnaire, a concentration will be estimated. An air concentration will be estimated from the survey-reported emission rate using the worst case dispersion factor from IWAIR (see Section 2.2.2 and Figure 2-5). A sludge concentration will be estimated from the leachate concentration assuming equilibrium partitioning to sludge (see Figure 2-8). If the survey questionnaire does not provide water concentration data for a particular impoundment, data from other impoundments will be used to estimate the water concentration (see Figure 2-7).

Average concentrations of constituents in impoundments have been requested as part of the survey questionnaire. The average concentration is considered to be a reasonable level of exposure to use in evaluating long-term chronic exposures because an individual is unlikely to be exposed to the maximum concentration of a constituent for 30 years. Thus, average concentrations are likely to represent long-term exposures. This approach is considered protective for this screening health risk analysis because risks are based on highly protective exposure assumptions, such as assuming that an individual would directly consume water from the surface impoundments.

Cumulative Risk Calculation. The calculated screening risks for each constituent for a specific impoundment and facility will be combined to generate three cumulative risk estimates: impoundment risk, constituent risk, and facility risk. The cumulative risks will be used in the risk screening and risk distributions, as follows.

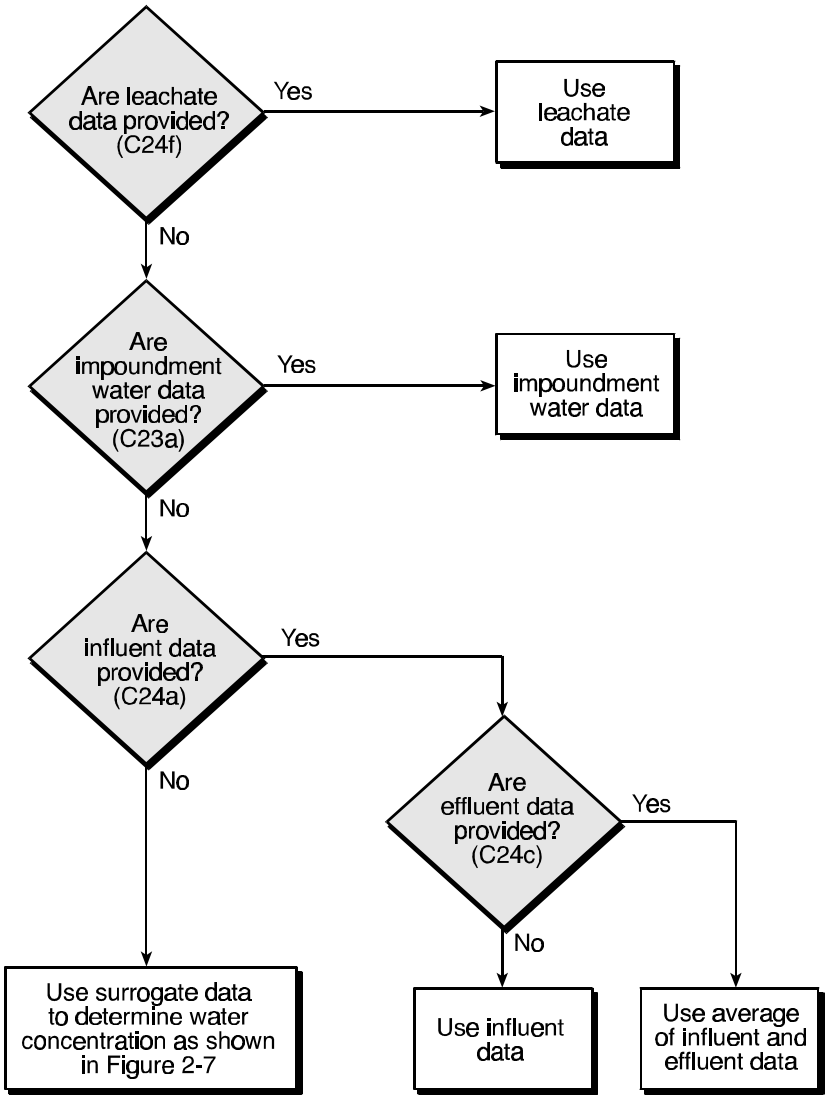
HQ - Hazard quotient is the ratio of estimated exposure (dose or concentration) and the appropriate toxicity value (reference dose or reference concentration) for a single exposure pathway and chemical.

HI - Hazard index is the summation of HQs across pathways and across chemicals affecting the same target organ.



Key:
Shaded boxes indicate information needed from survey questionnaire.
Survey question number appears in parentheses.

Figure 2-5. Decision tree for determining Phase IA air concentrations.



Key:
Shaded boxes indicate information needed from survey questionnaire.
Survey question number appears in parentheses.

Figure 2-6. Decision tree for determining Phase IA water concentration.

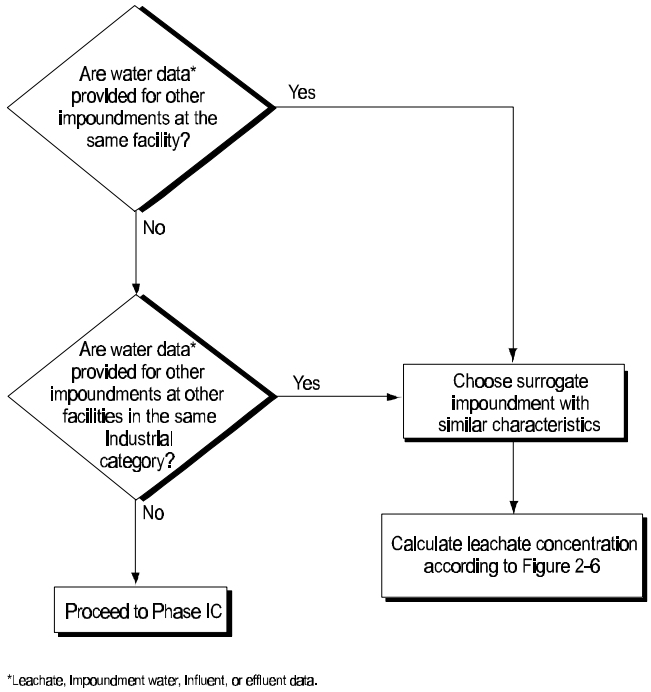


Figure 2-7. Steps to calculate impoundment water concentration if no survey data available.

The impoundment risk (i.e., risk for a particular impoundment for a particular facility)

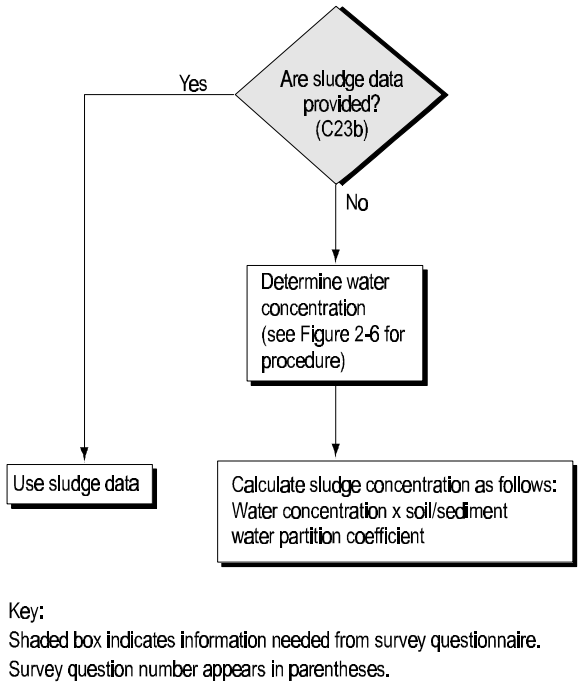


Figure 2-8. Decision tree for determining sludge concentration.

will be determined as follows:

- For carcinogenic risks, sum risks from all carcinogenic constituents.
- For noncarcinogenic risks, sum the HIs for all constituents potentially affecting the same target organ; then select the maximum HI from the target organ HIs.
- To represent constituents with risks based on regulatory standards, select the maximum ratio.

The constituent risk (i.e., risk for a particular constituent for a particular facility) will be determined as follows:

- For carcinogenic risks, select the maximum risk for the constituent across all impoundments for the particular facility.
- For noncarcinogenic risks, select the maximum HI for the constituent across all impoundments for the particular facility.
- To represent constituents with risks based on regulatory standards, select the maximum ratio across all impoundments for the particular facility.

Facility risks will be calculated as follows:

- For carcinogenic risks, sum the constituent risks.
- For noncarcinogenic risks, sum the HIs from all constituents potentially affecting the same target organ; then select the maximum HI from the target organ HIs.
- To represent chemicals with risks based on regulatory standards, select the maximum ratio from all constituents.

Note that this approach takes into account that an individual receptor's exposure factors will only be counted once for the entire facility (e.g., 1.4 L ingested per day or 11 m^3 inhaled per day).

Risk Distribution Development. Cumulative frequency histograms of the risks/HIs will be developed from the impoundment, constituent, and facility cumulative risks. A risk cumulative histogram will be defined by a set of six class intervals or "bins." The carcinogenic risk ranges defining those bins are: 0 to 10^{-8}, 10^{-8} to 10^{-7}, 10^{-7} to 10^{-6}, 10^{-6} to 10^{-5}, 10^{-5} to 10^{-4}, and 10^{-4}. An HI cumulative histogram will be defined by six bins: 0 to 0.01, 0.01 to 0.1, 0.1 to 1.0, 1.0 to 10, 10 to 100, and greater than 100.

Impoundment risks will be used to develop the impoundment type risk and treatment type risk distributions. For a given impoundment, the impoundment risk will be compared to the risk bins and the appropriate bin identified. A unitary value (1), representing the impoundment, will then be placed in the appropriate bin in the risk distribution. If the impoundment is in a statistically sampled population, the unitary value will be multiplied by the facility sample weight (see Appendix B for a discussion of the facility sample weights before being added to the bin.

Constituent risks will be used to develop the chemical-specific risk distribution. Facility risks will be used to develop the industry-type-specific risk distributions and the regulatory population-specific risk distributions. The development of these risk distributions follows the procedure described above for the impoundment risk distribution.

EXAMPLE: Adding an impoundment risk to a treatment type risk distribution.

An impoundment for a particular facility (ID 6123) is a biological treatment unit and has a cumulative impoundment cancer risk of 2×10^{-5} and a cumulative impoundment HI of 0.06. The facility is in the CWA direct discharger population. The risks will be added to the biological treatment type risk distributions. There will be two risk distributions, one for cancer risk and one for HI. For the cancer risk distribution, the cancer risk falls in the 10^{-5} to 10^{-4} risk bin. Because the CWA direct discharger population is a statistically sampled population, the unitary value is multiplied by the sample weight for that facility (weight = 38.7). This value is added to the risk bin. For the noncancer risk distribution, the HI falls in the 0.01 to 0.1 bin. The value of 38.7 is added to the 0.01 to 0.1 bin.

Risk Screening. The Phase IA risk screening will use the three cumulative risk distributions to identify

- Constituents, impoundments, and facilities that have risks below a decision criterion and therefore are considered to have negligible risks and are not assessed in any further phases.

- Constituents, impoundments, and facilities that have risks above a decision criterion and that will be assessed in Phase IB.

The risk screening procedure is outlined in the decision tree shown in Figure 2-9. A three-tiered approach is taken because each descending tier provides less information on the overall facility risk characterization but more detail on what constituents or impoundments can be excluded from further evaluation. The facility risk accounts for cumulative effects of multiple impoundments and constituents. Therefore, it is used as the first tier. However, the first tier indicates only if a facility must be assessed further or not; it does not indicate whether specific impoundments or constituents can be excluded. The second tier screens using the cumulative impoundment risk. This tier, however, can only address cumulative effects for multiple constituents at a single impoundment; it does not indicate whether specific constituents can be excluded. However, this second tier provides the subcategory of impoundments for a facility that

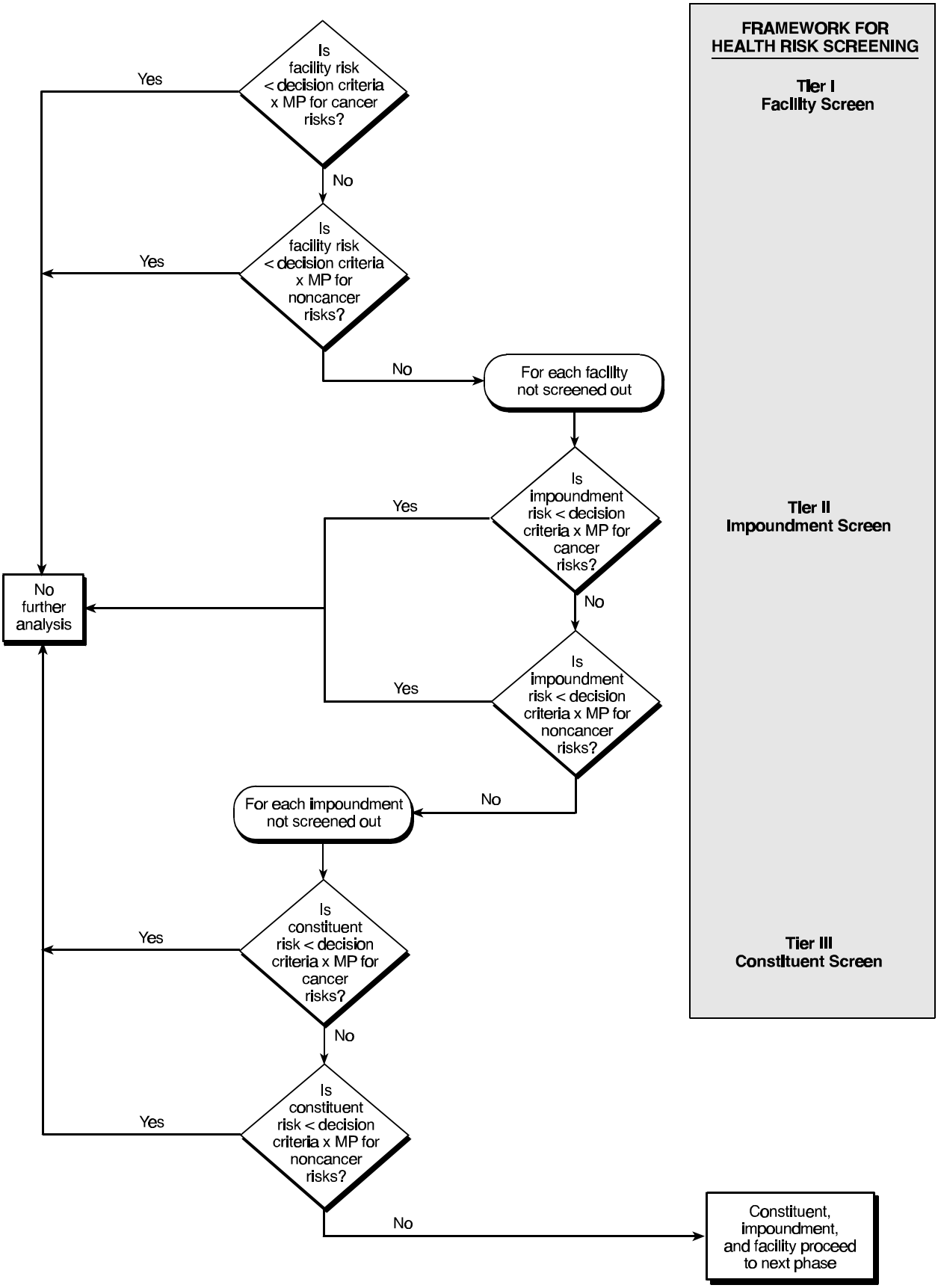


Figure 2-9. Decision tree for performing Phase I human health risk screening.

must proceed to Phase IB. The third tier identifies the constituents for the Tier 2 impoundments that must proceed to Phase IB.

The screening procedure first screens facilities by comparing the facility cumulative risk to the risk decision criteria, which may be adjusted by a margin of protection of 0.1 (risk decision criteria × MP = "screening criteria"). If the facility has a risk above the screening criteria, then the impoundment cumulative risk for each impoundment for that facility is compared to the screening criteria. If the impoundment has a risk above the screening criteria, then the constituent cumulative risk for that facility is compared to the screening criteria. If the constituent has a risk above the screening criteria, then the constituent passes to Phase IB for further screening. The constituent will be further evaluated **only** for those impoundments at the facility that have risks above the screening criteria. The risk screening will be performed for both cancer and noncancer risks.

EXAMPLE. Calculating the cumulative risks and risk screening for a facility.

The example facility has the risk estimates shown in Table 2-3. The first table presents the risk estimates for each chemical in each of the four impoundments.

The second table shows the cumulative facility, impoundment, and constituent risks. The impoundment risk is the sum of the chemical risks for the impoundment; the impoundment HI is the maximum HI of the two target organ HIs. For instance, for Impoundment A, the carcinogenic risk of 3.7×10^{-4} is the sum of Chemicals 1 and 4. The HI of 0.5 is the HI for Target Organ B.

The constituent risks and HIs are the maximum of risks and HI for all four impoundments. For instance, Chemical 1 is detected in Impoundments A, B, and D. Impoundment A has the maximum risk of 3.7×10^{-4} (from Impoundment A).

The facility risk of 3.7×10^{-4} is the summation of all carcinogenic constituent risks (Chemicals 1, 4, and 6). The facility HI of 11.05 is the summation of constituent HIs for target organ A. Specifically, this is Chemical 2 from Impoundment A and Chemical 5 from Impoundment B.

The third table shows the risk screening results for the facility. One impoundment and three chemicals are screened from further assessment at this facility. Three chemicals at three impoundments move on for further assessment in Phase IB.

This example illustrates that the decision criteria incorporate a margin of protection in determining which units and constituents proceed to Phase IB and II; however, the calculated risks with no MP are added to the risk distribution (see further discussion below).

Table 2-3. Example Screening Risks for a Facility

			HI	
Impoundment	**Chemical**	**Risk**	**Target Organ A**	**Target Organ B**
Impoundment A	Chemical 1	3.7E-04		
	Chemical 2		0.05	
	Chemical 3			0.3
	Chemical 4	1.1E-08		
Impoundment B	Chemical 1	2.0E-05		
	Chemical 3			0.007
	Chemical 4	8.0E-08		
	Chemical 5		11.00	
Impoundment C	Chemical 2		0.0004	
	Chemical 3			0.8
	Chemical 5		0.003	
Impoundment D	Chemical 1	5.0E-12		
	Chemical 6	3.0E-08		
Cumulative Risk		Risk	HI	
Impoundment Risk				
	Impoundment A	3.7E-04	0.3	
	Impoundment B	2.0E-05	11.00	
	Impoundment C	-	0.80	
	Impoundment D	3.0E-08	-	
Constituent Risk				
	Chemical 1	3.7E-04		
	Chemical 2		0.05	
	Chemical 3		0.8	
	Chemical 4	8.0E-08		
	Chemical 5		11	
	Chemical 6	3.0E-08		
Facility Risk		3.7E-04	11.05	

Risk Screening Results:		
Tier 1	**Facility**	risk and HI > decision criteria*
Tier 2	**Impoundment A**	risk and HI > decision criteria*
	Impoundment B	risk and HI > decision criteria*
	Impoundment C	HI > decision criteria*
	Impoundment D	risk < decision criteria*
Tier 3	**Chemical 1**	risk > decision criteria*
	Chemical 2	HI < decision criteria*
	Chemical 3	HI > decision criteria*
	Chemical 4	risk < decision criteria*
	Chemical 5	HI > decision criteria*
	Chemical 6	risk < decision criteria*
Conclusion:	Impoundment A: Chemicals 1 and 3 to be assessed in next phase	
	Impoundment B: Chemicals 1 and 5 to be assessed in next phase	
	Impoundment C: Chemical 3 to be assessed in next phase	
	Impoundment D: No further assessment of chemicals 1 and 6; no further assessment at this facility	

*Decision criteria: 10^{-5} for cancer risk; 0.1 for noncancer risk.

Decision Criteria. As described above, the Agency will use risk criteria of 10^{-5} for carcinogenic risk and HI = 1 for noncarcinogenic risk throughout the analysis. The decision to remove a particular constituent, unit, or facility from any further analysis is final (i.e., no further analysis is warranted). Therefore, EPA may apply a margin of protection of 0.1 in Phase I to determine whether Phase IB and II modeling is necessary. EPA may consider applying alternative MPs depending on the screening results presented in the risk distributions.

EPA considers that, for many constituents, screening based on direct ingestion of the surface impoundment influent and direct inhalation of the emissions is by its nature very protective; that is, if fate and transport modeling were to be conducted, the potential risks would invariably be lower. The intent of a margin of protection is to address potential concerns for indirect exposures. In addition, special consideration will be given to constituents known to bioaccumulate in setting priorities during Phase IC.

2.2.1.4 <u>Results of Phase IA Human Health Risk Screening</u>. The risk characterization resulting from the Phase IA analyses will consist of two primary outputs:

- Phase IA risk distributions
- Screening of constituents, impoundments, and facilities.

Risk Distributions. The Phase IA screening risks for each constituent, impoundment, and facility will provide initial risk distribution profiles that describe the national scale surface impoundment population. The risk distributions will be provided for the categories that are of concern to the SI Study:

- Six regulatory status categories of interest
- Three functional classes (storage, treatment, and disposal)
- Types of treatment (e.g., biological, settling)
- Types of industry (by SIC code)
- Types of constituents.

By providing risk distributions for these categories, EPA can determine what types of industries or impoundments have the highest potential risks and merit additional analysis.

The distribution of the sample population of facilities is shown in Tables 2-4 and 2-5 by regulatory category and industry type. The direct discharger and zero discharger types are statistically sampled populations and have the largest number of facilities. The indirect discharger population is smaller and consists of preselected and purposively selected facilities. Risk distributions will be provided for the CWA discharger type and RCRA nonhazardous waste type.

The facility distribution by industry type (see Table 2-4) shows that certain industries were given higher priority in the SI Study; these industries (e.g., SIC group 26, 28, 29, 32, and 33) are sampled at a higher rate. Development of risk distributions by industrial type may be grouped by high- or low-priority industry groups, and, because the CWA discharger types are

Table 2-4. Facility Distribution by Regulatory Category

Type of CWA Facility	Type of RCRA Nonhazardous Waste	Number of Facilities
Direct discharger	Decharacterized	79
	Nondecharacterized [a]	82
Zero discharger	Decharacterized	6
	Nondecharacterized [a]	34
Indirect discharger	Decharacterized	2
	Nondecharacterized [a]	12
	TOTAL	**215**

[a]Could include some missing responses.

three distinct populations, risk distributions by industry type will be developed separately for each CWA discharger type.

EXAMPLE: An example distribution by industry type is provided in Figure 2-10. Risk distributions are shown for three different industry types for cancer risks. The figure indicates that industry type B has the highest percentage of its facilities with cancer risks less than the screening decision criteria of 10^{-6}. In contrast, industry type C has a large percentage of its facilities with risks greater than the risk decision criteria.

The distributions of the sample population of facilities by functional class, treatment type, and constituent will be defined by the survey questionnaire responses.

These risk distributions will be refined with each subsequent phase (see Phase IB Risk Characterization Outputs for approach). The risk distributions will also provide the basis for the prioritization for evaluations to be conducted in Phase II (see Section 2.4).

Risk Screening. The Phase IA risk screening approach identifies

- Constituents, impoundments, and facilities that have risks below the screening criteria and therefore are considered to have negligible risks and are not assessed in any further phases.

- Constituents for specific impoundments and facilities that have risks above the screening criteria and will proceed to Phase IB risk screening.

Table 2-5. Facility Distribution by Industry Type

SIC Major Group	SIC Code	Description	Number of Industry Facilities
20	-	Food and Kindred Products	19
22	-	Textile Mill Products	5
24	-	Lumber and Wood Products, Except Furniture	7
26	-	Paper and Allied Products	31
28	-	Chemicals and Allied Products	38
29	-	Petroleum Refining and Related Industries	25
30	-	Rubber and Miscellaneous Plastics Products	9
32	-	Stone, Clay, Glass, and Concrete Products	20
33	-	Primary Metal Industries	24
34	-	Fabricated Metal Products, Except Machinery and Transportation Equipment	5
35	-	Industrial and Commercial Machinery and Computer Equipment	3
36	-	Electronic and Other Electrical Equipment and Components, Except Computer Equipment	5
37	-	Transportation Equipment	5
49	4952 (Except POTWs)	Sewerage Systems	1
	4953	Refuse Systems	3
50	5085	Industrial Supplies	1
51	5171	Petroleum Bulk Stations and Terminals	7
97	-	National Security and International Affairs	2
		TOTAL	**210**[a]

[a]Total does not include five CBI facilities

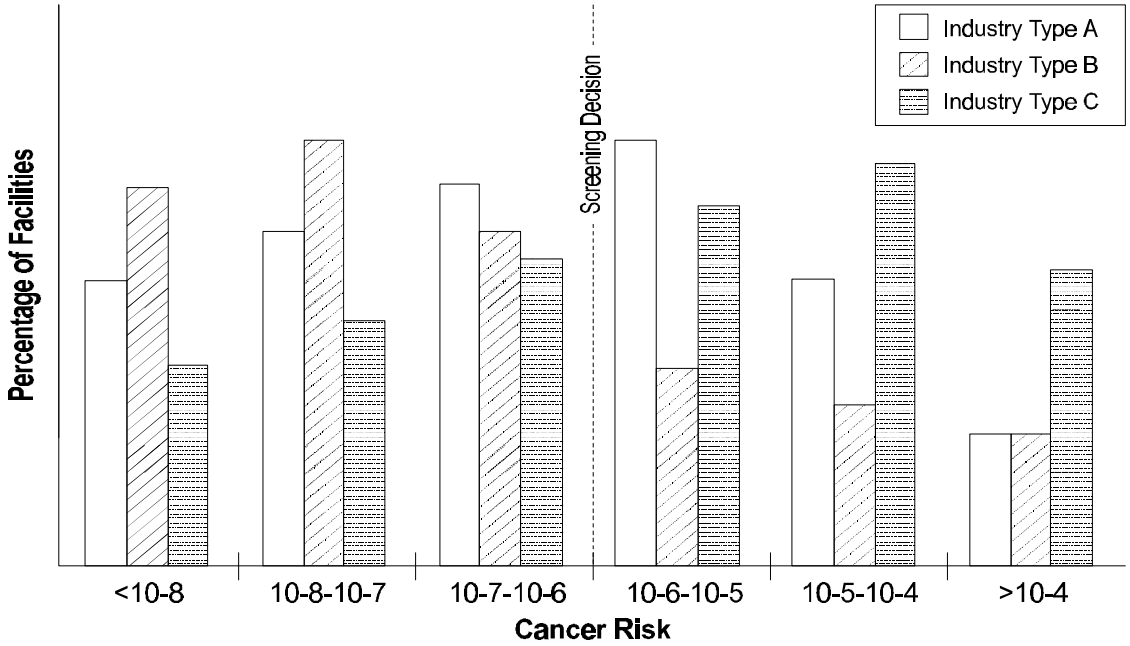


Figure 2-10. Example risk distributions for three industry types.

The results of the risk screening are best presented using the risk distributions based on the constituent, impoundment, and facility risks. These are unweighted distributions because the purpose is to present the number of facilities that must be assessed further. (In comparison, the risk distributions in Figure 2-10 show percentage of facilities because we want to characterize the national population.)

EXAMPLE. An example of the screening results is shown in Figure 2-11. The facility risk distribution for noncancer risks clearly delineates the facilities that will be assessed further in Phase IB and those that are considered to have negligible risks and will not be further evaluated. The screening criteria separate the two categories. The impoundment risk distribution is also divided into two categories based on the screening criteria. The impoundments proceeding to Phase IB are only associated with the facilities that must be assessed further. Some of the impoundments for a facility that must go to Phase IB are not further analyzed; these impoundments fall to the left of the criteria. The third distribution is on a constituent basis and shows the constituents that will be assessed in Phase IB. This constituent distribution applies to the subset of impoundments and facilities that have proceeded to Phase IB. Note that a margin of protection will be considered at each screening decision.

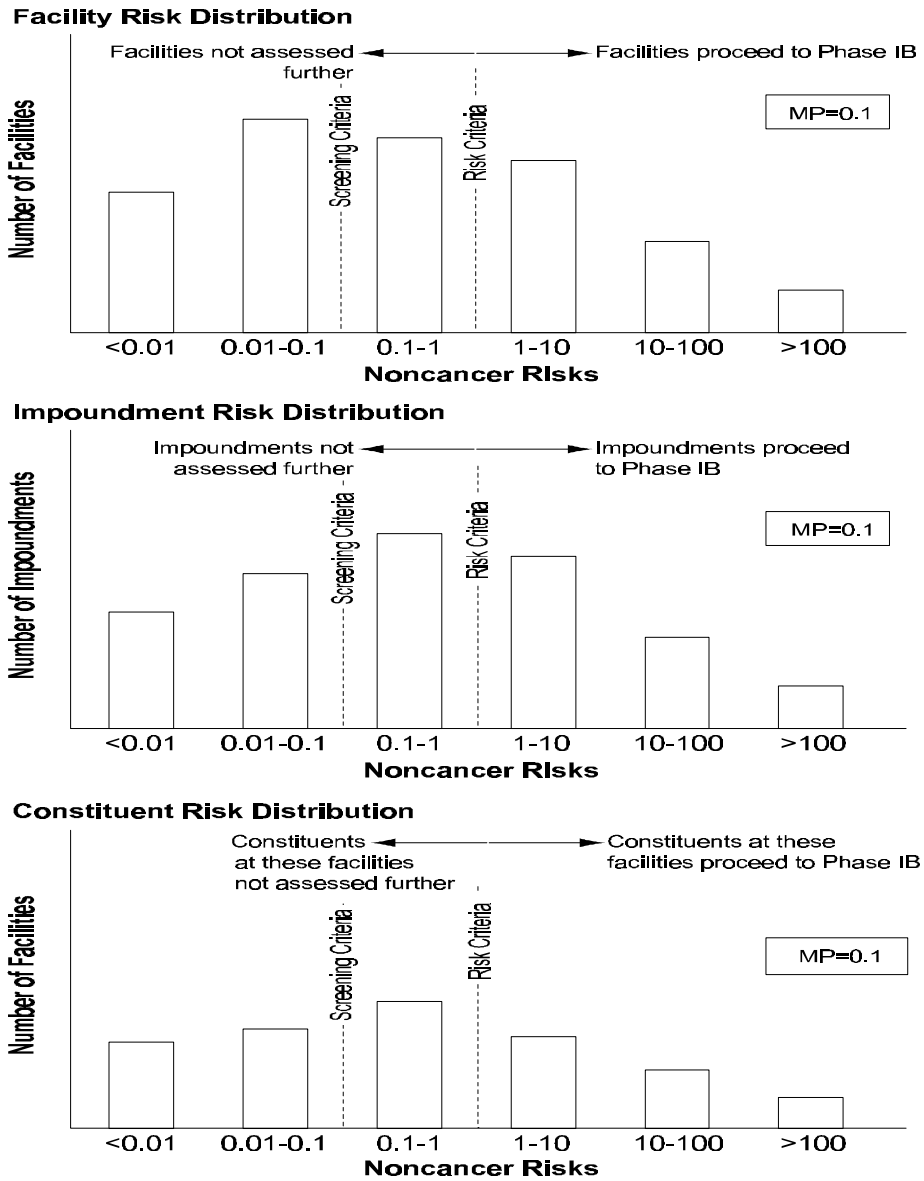


Figure 2-11. Example risk screening results.

2.2.2 Phase IB Human Health Screening

The Phase IB risk screening is described in four sections:

- Design goals and overview
- Screening models
- Procedure for risk screening
- Results of risk screening.

2.2.2.1 <u>Phase IB Human Health Screening Design Goals and Overview</u>. EPA will use screening models to supplement the initial screening performed under Phase IA. Use of screening models provides additional characterization of exposure by evaluating the fate and transport of constituents from their release from the surface impoundment through the environmental media to the point of exposure. Therefore, the Phase IB screening will provide a more realistic tier in the phased approach.

The use of screening models will be necessary when there is uncertainty about eliminating a constituent from further evaluation. Two main categories of uncertainty will be addressed: (1) constituents that volatilize, but for which there are no air concentration data provided in the survey questionnaire, and (2) constituents that were not eliminated for the Phase IA screening. Phase IB modeling will be performed on all constituents identified by the Phase IA screening.

The Phase IB screening will address only the major routes of exposure that are expected to contribute significantly to potential risks (i.e., ingestion of drinking water and inhalation of air). This phase will use a limited amount of site-specific data from the survey questionnaire. However, because constituents from specific units may be screened from further analysis, the Phase IB modeling approach will use protective assumptions, such as assessing risks for close-in receptors.

EPA screening models IWAIR and IWEM, developed for use under the Industrial D guidance, will be used to calculate screening risk estimates. These risk estimates will replace or supplement the corresponding Phase IA screening risk estimates and therefore will refine and improve the overall Phase IA risk distributions.

2.2.2.2 <u>Phase IB Human Health Screening Models</u>. IWAIR and IWEM assess the risks from potential exposure of air and groundwater, respectively, due to constituents released from surface impoundments. The screening models, as described below, follow different approaches. However, both models will provide screening analyses that are useful in characterizing exposure and incorporate more site-specific data. Despite the difference in modeling approaches, the results from each of the Phase IB models constitute a defensible basis to provide screening-level estimaters of risk. Use of IWAIR and IWEM for Phase IB assumes that any software model errors that were identified by the previous peer review will have been addressed.

IWAIR. The IWAIR model will be used to calculate risks due to inhalation of airborne volatile constituents released from surface impoundments. IWAIR incorporates the CHEMDAT8 volatile emission model to calculate the constituent release (i.e., emission rate) from an impoundment, uses dispersion factors developed from Industrial Source Complex Short Term (ISCST3) modeling simulations to calculate an air concentration, uses exposure and risk calculations following EPA guidance (*Risk Assessment Guidance for Superfund*, U.S. EPA, 1989), and uses a chemical and toxicological database for 95 chemicals to calculate carcinogenic and noncarcinogenic chronic inhalation risks. CHEMDAT8 has undergone extensive review by both EPA and industry representatives and is publicly available. ISCST3 is another regulatory

standard model that has undergone substantial review and use by industry. The dispersion factor approach for risk screening purposes is recommended by EPA guidance (*Soil Screening Guidance*, U.S. EPA, 1996d, e). Dispersion factors for multiple source area sizes, receptor distances, and meteorological conditions are provided.

IWAIR uses the same exposure factors as Phase IA from the *Exposure Factors Handbook* (U.S. EPA, 1997b). An age-weighted resident is considered for carcinogenic chemicals. This approach is also generally consistent with the establishment of risk-based criteria such as ambient water quality criteria. An adult resident is considered for noncarcinogenic chemicals. Phase IA toxicological benchmarks will be used (in place of IWAIR toxicological benchmarks) to calculate screening risks with IWAIR. For SI Study constituents that are not included in the IWAIR chemical database, the physicochemical properties from CHEMDAT8 and Phase IA toxicity benchmarks will be added to IWAIR. IWAIR will then be used to calculate the constituent risks and HIs.

The IWAIR model is computationally fast and easy to use and requires minimal input data. The site-specific data required will be obtained from the survey and include: constituent waste concentration, impoundment depth, area, annual wastewater flow rate, and whether or not aeration occurs. Default or additional site-specific data can be provided for aeration parameters and wastewater parameters important for biodegradation. These are attributes required by the Phase IB screening because a large number of constituents and units may be assessed in Phase IB.

The IWAIR model is currently in the public comment period. Peer review comments have been favorable to the approach and the computer program. Use of the IWAIR model in the SI Study Phase IB calculations is outlined in Section 2.2.2.3.

IWEM. The IWEM Tier 1 model will be used to calculate the risks due to exposure to groundwater containing constituents released from surface impoundments. IWEM Tier 1 is a table containing leachate concentration threshold values for a specific chemical based on a dilution attenuation factor (DAF) and the toxicity reference levels for 190 constituents. The toxicity reference level is based on the toxicological benchmark or the MCL. The DAFs were generated by modeling the migration of waste constituents from an impoundment through the underlying soil to a monitoring point in the aquifer using the EPA Composite Module for Leachate Migration with Transformation Products (EPACMTP) in a national Monte Carlo probabilistic analysis. The DAFs are multiplied by the toxicity benchmark to provide the leachate concentration threshold value for each chemical.

Leachate concentration threshold values and DAFs are provided for three impoundment liner scenarios: no liner, single liner, and a composite liner. The no liner scenario represents an impoundment that is relying upon location-specific conditions such as low-permeability native soils beneath the unit or low annual precipitation rates to mitigate the release of contaminants to the groundwater. The single liner scenario represents a 3-foot-thick clay liner with a low hydraulic conductivity (10^{-7} cm/s) beneath the impoundment. The composite liner scenario consists of a 3-foot-thick clay liner beneath a 40-mil-thick high-density polyethylene (HDPE) flexible membrane liner.

IWEM Tier 1 is based on a health-protective Monte Carlo probabilistic analysis that accounts for the nationwide variability of groundwater modeling parameters. The Monte Carlo procedure randomly drew input parameter values from representative statistical distributions for each parameter. A set of input parameter values was developed and the model was run to compute the groundwater monitoring well concentration and the DAF. This process was repeated thousands of times until a distribution of thousands of output values (DAFs) was produced. The DAF values were ranked from high to low, and the 90th percentile DAF was determined. The 90th percentile DAF represents the amount of dilution and attenuation that would occur in at least 90 percent of the cases modeled. In other words, the DAF is protective in at least 90 percent of the modeled cases. The selection of 90th percentile DAF is based on

- The need to choose a level of protection that is protective and consistent with other EPA analyses, including the proposed Hazardous Waste Identification Rule (HWIR) of 1995 (U.S. EPA, 1995b) and hazardous waste listing evaluations (e.g., the Petroleum Refinery Waste Listing Determination, U.S. EPA, 1997d)

- The desire to have a large degree of confidence that the results are adequately protective of human health and the environment given the degree of uncertainty inherent in the data and the analyses.

The Monte Carlo approach used in EPACMTP has been applied in various EPA regulatory efforts, including the proposed 1995 HWIR and hazardous waste listing evaluations, such as those mentioned previously. As such, the Monte Carlo procedure and its applicability to national analyses has been extensively reviewed within EPA and by the Science Advisory Board and has been subject to public review and comment (U.S. EPA, 1999aa). The model is currently in the public comment period.

To maintain consistency with Phase IA in the risk calculation, only the DAFs from IWEM will be used. For each chemical, the DAF from each liner scenario will be multiplied by the carcinogenic or noncarcinogenic risk screening factor from Phase IA to develop a new SI Study-modified IWEM Tier 1 table containing the leachate concentration threshold values. This approach ensures that receptors are evaluated with the same exposure factors (e.g., amount ingested and inhaled) used in Phase IA.

There are a number of SI Study constituents that are not included in the IWEM Tier 1 table. For these constituents, a leachate concentration threshold value using a DAF from a surrogate chemical will be calculated. The leachate concentration threshold value will be calculated by using the IWEM procedure for estimating DAFs of chemicals for which EPACMTP was not simulated, as follows: the DAF will be determined by interpolating between the DAFs of chemicals whose hydrolysis rate and retardation factor are in the same range as the hydrolysis rate and retardation factor of the new chemical.

Use of the SI Study-modified IWEM Tier 1 table in the SI Study Phase IB calculations is outlined in Section 2.2.2.3.

2.2.2.3 <u>Procedure for Phase IB Risk Screening</u>. The overall human health screening process is shown in Figure 2-12. The overall process is the same as Phase IA:

- Risks will be calculated for each constituent, impoundment, facility, and regulatory population.
- Cumulative risks will be calculated.
- Risk distributions will be developed.
- Risk screening will be performed.

The analyses, however, will be performed only for a subset of constituents, impoundments, and facilities defined by the Phase IA screening results. Each element is outlined in more detail below. The primary difference between Phase IA and IB is the procedures used for calculating risks.

Human Health Risk Calculation. Phase IB risk estimates will be for the air inhalation and groundwater ingestion pathways only (see Figure 2-12). Phase IB does not include the soil ingestion pathway. Risks for the air exposure pathway will be estimated using IWAIR if the Phase IA risk estimate is greater than the screening criteria or if the constituent is a VOC, but air concentration or emission data were not provided in the survey response. Risks for the groundwater exposure pathway will be estimated using IWEM if the Phase IA risk estimate is greater than the screening criteria.

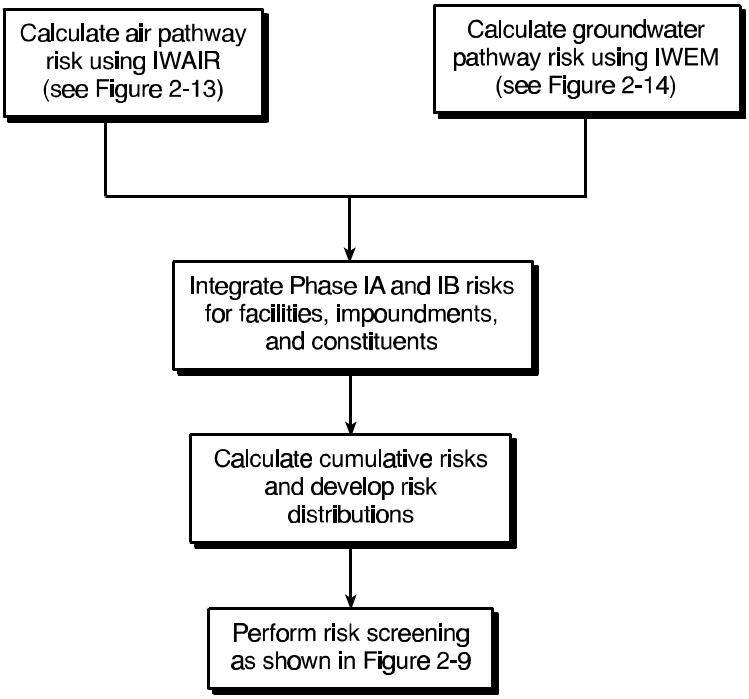


Figure 2-12. Decision tree for Phase IB human health risk screening.

The decision tree for calculating the Phase IB air exposure risks using IWAIR is presented in Figure 2-13. The types of site-specific data that will be used are outlined; the survey question that will provide the data is noted in the figure. The decision tree for defining the influent waste concentration from survey data is shown in Figure 2-14. IWAIR default data will likely be used for the aeration and waste characteristics data. Because IWAIR must represent wind conditions across the continental United States, IWAIR contains wind dispersion data based on 29 meteorological stations. Because the wind pattern may not be representative of the actual site conditions, a close-in receptor at 25 m will be assumed for the Phase IB screen. If a constituent is not currently in IWAIR, its physicochemical and toxicological data will be added to the IWAIR chemical database.

The decision tree for calculating the Phase IB groundwater exposure risks using the modified IWEM Tier 1 table is presented in Figure 2-15. The Phase IB groundwater risk calculation will consider the type of lining at each impoundment in determining the appropriate groundwater screening factor, called the leachate concentration threshold value (LCTV) in IWEM. The site-specific liner questions are outlined in Figure 2-15. The calculation of the leachate concentration is shown in Figure 2-6. The risk calculation mirrors the Phase IA calculation: calculate the ratio of the leachate concentration to the LCTV and multiply by the risk criteria.

Cumulative Risk Calculation. The calculated screening risks for each constituent for a specific impoundment and facility will be combined to generate three cumulative risk estimates: impoundment risk, constituent risk, and facility risk. The calculation of the cumulative risks is defined in Figure 2-3 and Section 2.2.1.3. It is important to note that the cumulative risks are a combination of the Phase IA and Phase IB calculated risks for each constituent, because the Phase IB risk estimate is considered a refinement of the initial Phase IA risk estimate.

Risk Distribution Development. The risk distribution approach is identical to that defined in Phase IA (see Section 2.2.1.3 for the development approach). Because the Phase IB cumulative risks are a combination of Phases IA and IB results, the risk distributions also represent the combined analysis of Phase IA and IB.

Risk Screening. The risk screening approach is also identical to that defined in Phase IA (see Section 2.2.1.3 for the development approach).

2.2.2.4 <u>Results of Phase IB Risk Screening</u>. The risk characterization resulting from the Phase IB analyses will consist of two primary outputs:

- Combined Phase IA and IB risk distributions
- Combined Phase IA and IB screening of constituents, impoundments, and facilities.

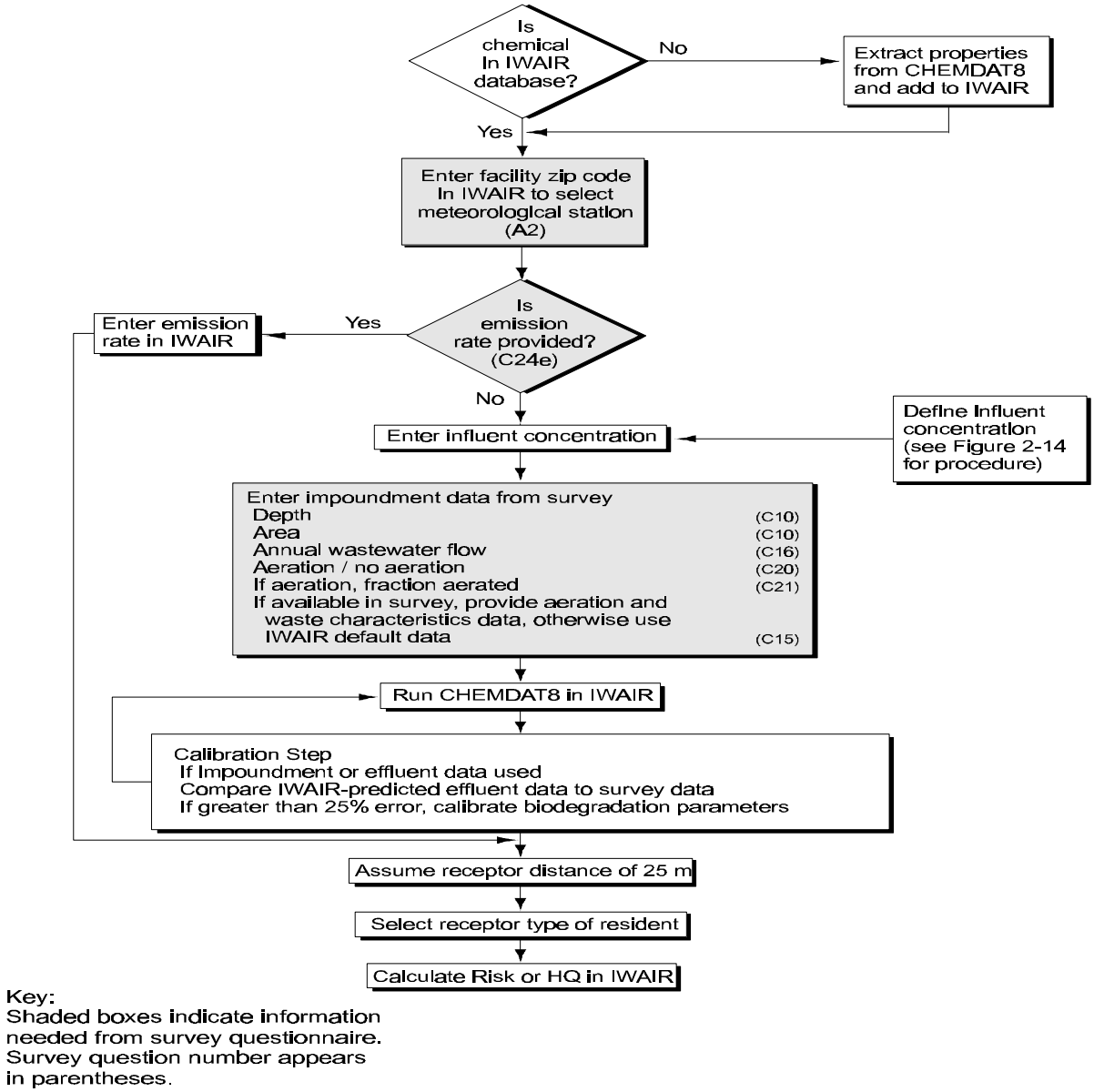
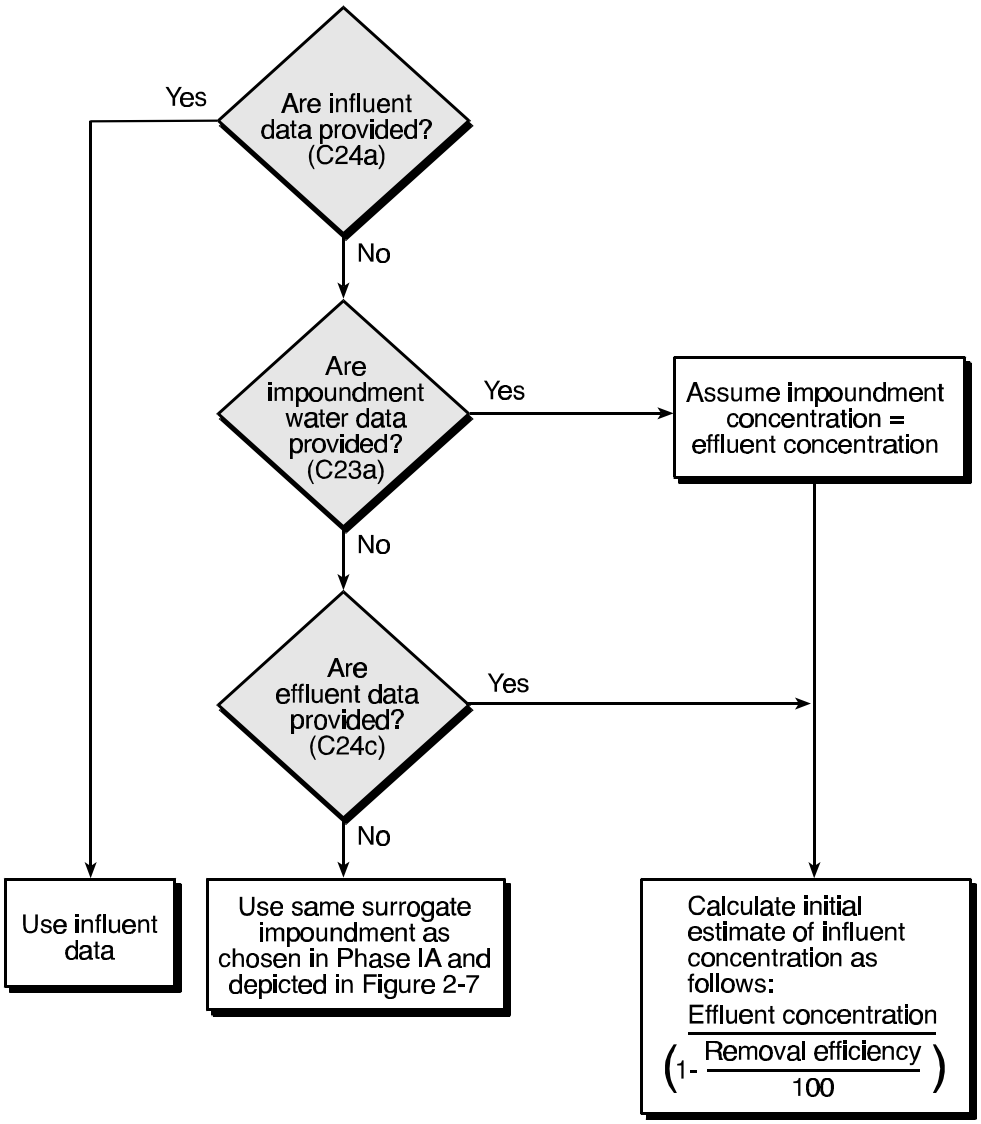
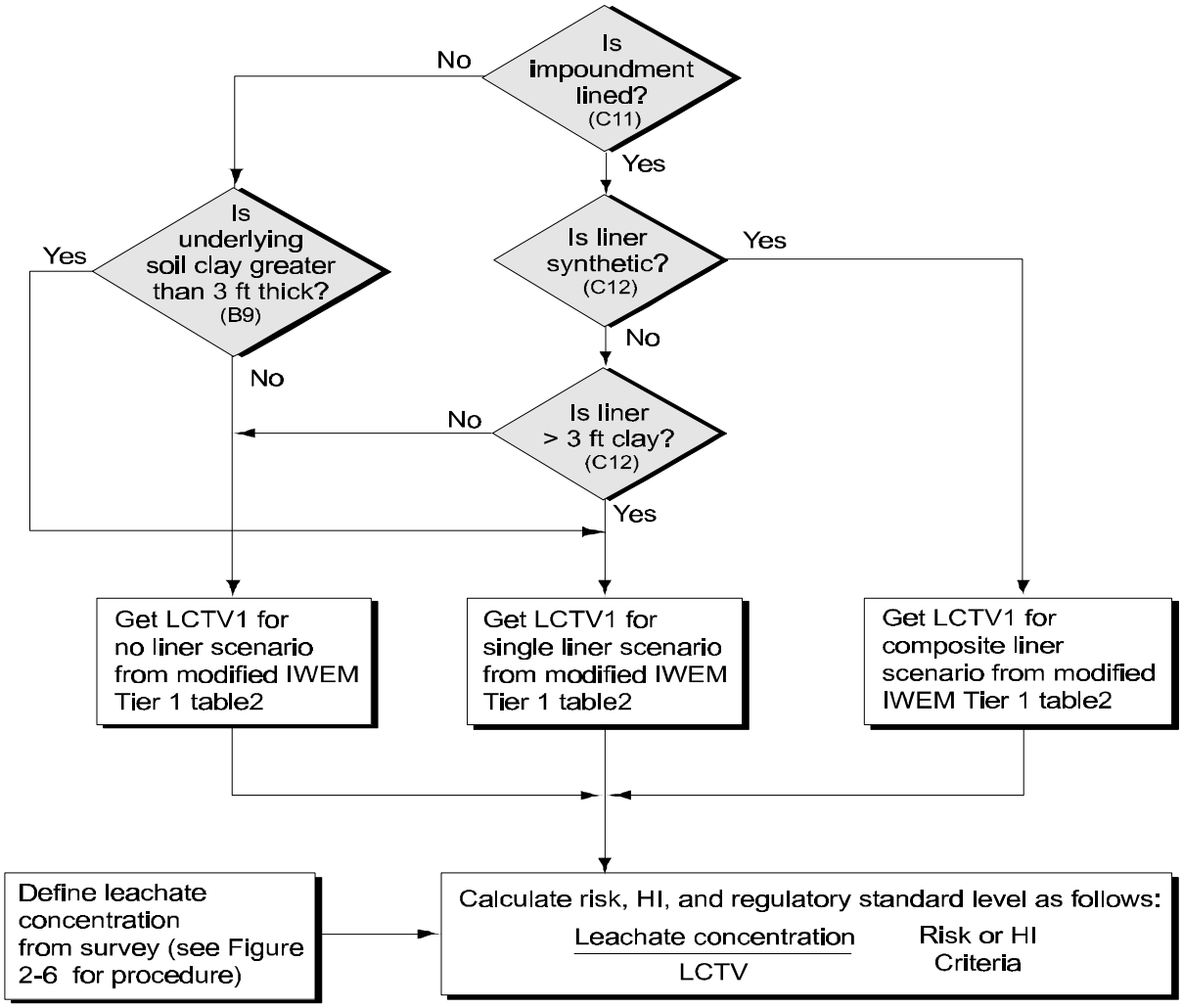


Figure 2-13. Decision tree for Phase IB air screening using IWAIR.



Key:
Shaded boxes indicate information needed from survey questionnaire.
Survey question number appears in parentheses.

Figure 2-14. Decision tree for calculating influent waste concentration for IWAIR.



Key:

1Leachate concentration threshold value.

2IWEM lookup table modified to include HWIR toxicity data and all SI study chemicals.

Shaded boxes indicate information needed from survey questionnaire.

Survey question number appears in parentheses.

Figure 2-15. Decision tree for Phase IB groundwater screening using IWEM.

Risk Distributions. The combined Phase IA and IB screening risks for each constituent, impoundment, and facility will provide initial screening-level risk distribution profiles for the national scale surface impoundment population. The risk distributions will be provided for the categories that are of concern to the SIS, as outlined in Section 2.2.1.4.

The refinement of the screening-level risk distribution from Phase IA to Phase IB is shown in Figure 2-16. The example risk distribution shown previously for Phase IA (see Figure 2-10) is now updated to include the Phase IB risk screening results. The new figure shows the modified risk distributions for the three industry types. It is expected that the Phase IB analyses, by including the attenuating factor of exposure modeling, will result in more accurate and generally lower risk estimates. Therefore, percentages below the screening criteria are expected to increase. The shaded portions of the percentages of facilities in each risk bin are the added Phase IB percentages. Above the screening criteria, the percentages are expected to decrease. For the most part, the facilities with risks above the screening criteria are from Phase IB analyses. Only risks from sludge ingestion, which is a Phase IA analysis only, would contribute to the facilities with risks above the screening criteria.

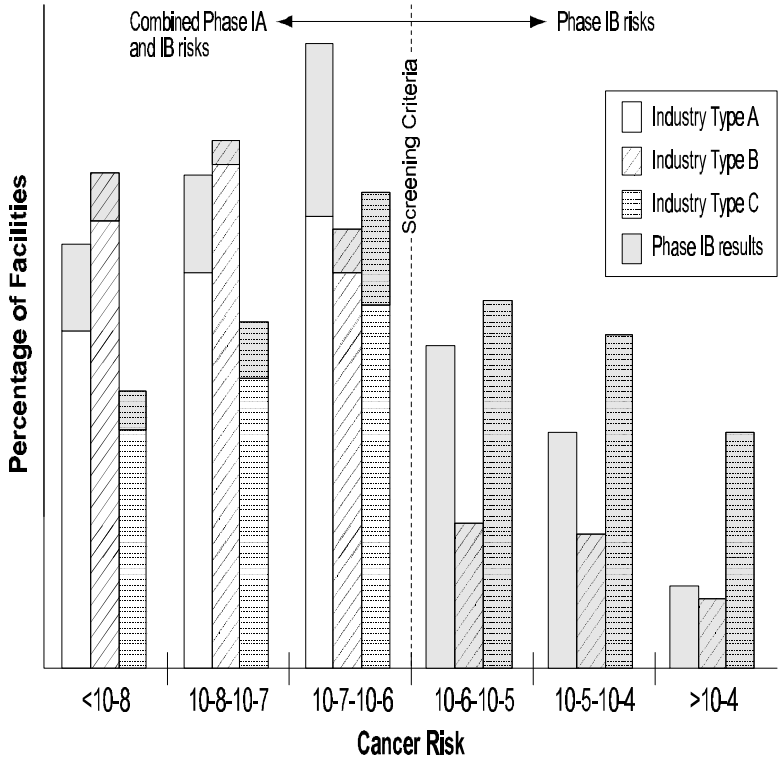


Figure 2-16. Example combined Phase IA and IB risk distributions for three industry types.

Risk Screening. The combined Phase IA and IB risk screening approach identifies

- Constituents, impoundments, and facilities that have risks below the screening criteria and therefore are considered to have negligible risks and are not assessed in any further phases

- Constituents for specific impoundments and facilities that have risks above the screening criteria and should proceed to Phase II analysis, depending on the factors described in the Phase IC initial prioritization.

In addition to the risk screening, constituents that are considered special cases will automatically proceed to Phase II. The definition and categorization of special cases is discussed in the next section.

2.2.3 Special Cases

Certain constituents may present human health or ecological risks yet not be identified as constituents with high risks in the screening process described above. These constituents are likely to be persistent or bioaccumulative. To ensure that these types of constituents are identified, each constituent will be ranked according to a special set of criteria. EPA developed the Revised Waste Minimization Prioritization Tool (U.S. EPA, 1998e), which scores constituents on the basis of their persistence (P) in the environment, bioaccumulation (B) potential, and toxicity (T) to humans and ecological receptors. Because the SI Study is concerned with the same issues, the procedures used in the WMPT will be used to score constituents (see Figure 2-17). The persistence (P) scoring is based on a steady-state, nonequilibrium multimedia partitioning model to estimate constituent half-life. The potential for bioaccumulation (B) is scored using either measured or estimated bioaccumulation factors (BAFs) or bioconcentration factors (BCFs). Human and ecological toxicity (T) of the constituents is also scored. For human health, the highest score for either the carcinogenic or noncarcinogenic health effects is selected. For ecological effects, the highest toxic effect to aquatic organisms is identified. Depending on the data available to assess constituent characteristics, P, B, and T scores are qualified to indicate which data from the established hierarchy (i.e., high, medium, or low data preferences) have been used in the scoring process. These factors are consolidated into an overall score for human health effects from each constituent by summing the P and B scores and summing this score with the highest T score for either noncarcinogenic or carcinogenic chemicals. A similar process is used to develop scores for ecologically important constituents, with aquatic toxicity data used to develop T scores for the ecologically important constituents. The final score is the higher of either the human or ecological scores.

The SIS will use the PBT scores developed by the WMPT after reviewing the toxicity data to determine whether the data used in both studies are consistent. If necessary, new scores will be developed for constituents with new toxicity data or for constituents not evaluated previously. Furthermore, since EPA intends to continue revising the WMPT in response to the public and EPA comments, changes in the WMPT procedures will also be addressed, if necessary. Thus, special case constituents will be identified as those with the highest PBT

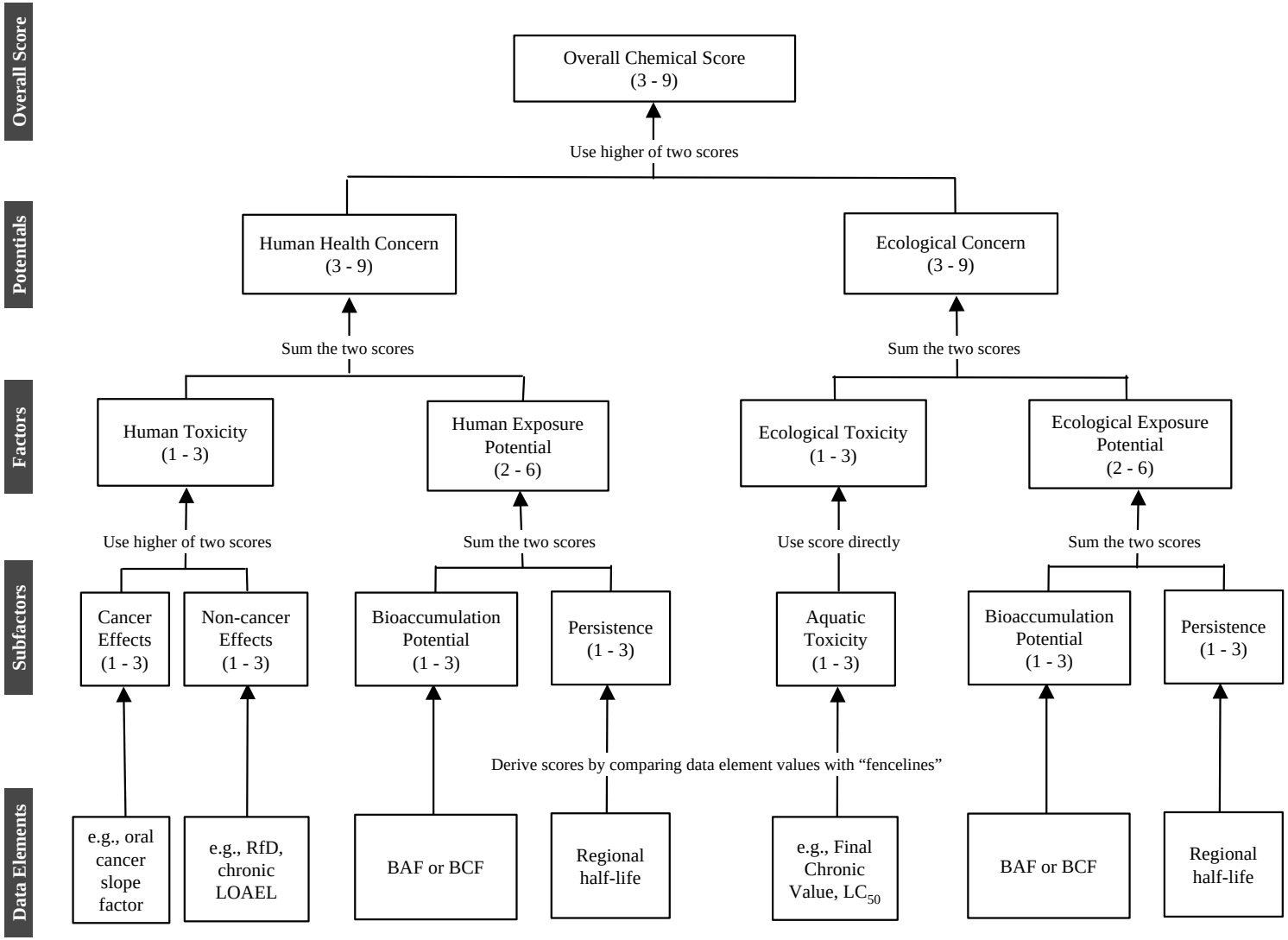


Figure 2-17. Overview of the revised WMPT scoring algorithm (U.S. EPA, 1998e).

ranking. The list of special case constituents will be reported with the risk distributions reported for the Phase I screening process.

2.3 Phase I: Ecological Screening Assessment

The Phase I ecological risk screening is somewhat different from the Phase I human health screening in that a single comparison between screening factors and constituent concentrations is conducted to determine whether a constituent, impoundment, or facility should be included for further evaluation in Phase II. Depending on the ecological receptor of concern, the Phase I analysis will either estimate risks from the ingestion of contaminated plants, prey, and media, or it will estimate risks associated primarily with direct contact with a contaminated medium such as sediment or soil. The ecological risk estimates will be compared to risk criteria to prioritize the list of constituents, impoundments, and facilities that may warrant further evaluation to determine the likelihood of adverse ecological effects. It is important to note that the ecological priority list will be used **in conjunction** with the Phase I human health screening results to delineate the universe for the Phase II analysis. The Phase I results from the ecological screening will be used to inform the selection of constituents, impoundments, and facilities that are most likely to pose significant risks to both human **and** ecological receptors.

2.3.1 Phase I Ecological Risk Screening

The Phase I ecological risk screening is described in five sections:

- Design goals and overview
- Management goals and assessment endpoints
- Development of screening factors
- Procedure for risk screening
- Results of risk screening/prioritization.

2.3.1.1 <u>Design Goals and Overview</u>. As suggested above, the primary goal of the Phase I ecological screening assessment is to establish a priority list of constituents, impoundments, and facilities based on the potential for adverse ecological effects. The secondary goal of this phase is to use the screening-level results to generate ecological risk profiles for the universe of surface impoundments included in the SI Study. These risk profiles provide a “snapshot” of the potential for environmental effects and will be used to identify constituents, impoundments, and facilities that have negligible ecological risks. The Phase I approach considers the potential for adverse effects to a suite of ecological receptors that may be attributed to terrestrial, freshwater, and wetland habitats including, for example, mammals, birds, and soil and benthic fauna. The habitats and receptors considered in this study are consistent with the national assessment strategy developed to support the Hazardous Waste Identification Rule (HWIR) proposed in November 1999. Because the HWIR risk assessment framework was intended to support national studies of waste management practices, the SI Study has adopted this framework as the basis for selecting receptors and habitats.

As with the Phase I screening approach for human health, the ecological screening analysis calculates risks to individual ecological receptors (e.g., red fox, aquatic biota) based on the ratio between ecological risk screening factors and the reported concentrations of constituents

in surface impoundments reported in the survey questionnaire. Consequently, ecological risk screening factors are given in units of concentration (e.g., mg/kg or mg/L). The ecological risk screening factors will include both standard ecological benchmarks such as the Ambient Water Quality Criteria (AWQC) as well as benchmarks developed for other EPA analyses such as HWIR. The use of screening factors is considered to be protective because the factors are:

- Derived using established EPA protocols for use in evaluating ecological risk (e.g., sediment quality criteria)
- Based on highly protective assumptions regarding the toxicological potency of a constituent (e.g., no adverse effects levels)
- Calculated assuming that all media and food items originate from a contaminated source.

In addition, the application of the screening factors assumes that ecological receptors are exposed directly to chemical concentrations in the sludge and wastewater found in the surface impoundment. For mammals, birds, and selected herpetofauna, these screening factors reflect ingestion of contaminated media, plants, and prey. For other receptor groups such as soil fauna, these screening factors are intended to reflect both the direct contact and ingestion routes of exposure. The results of the screening assessment for these representative species will be used to infer potential risks to taxonomically and ecologically similar receptors.

2.3.1.2 <u>Management Goals and Assessment Endpoints</u>. Perhaps the most important step in developing the assessment strategy (often referred to as the problem formulation phase) is the selection of assessment endpoints. The selection of assessment endpoints, defined as "explicit expressions of the actual environmental value that is to be protected" (U.S. EPA, 1998f) serves as a critical link between the ecological risk assessment (ERA) and the management goals. For the SI Study, the management goals may be summarized as follows: "prioritize the constituents, impoundments, and facilities based on the potential for adverse ecological effects, and describe the national distribution of ecological risks associated with the management of wastes in surface impoundments." Candidates for assessment endpoints often include threatened/endangered species, commercially or recreationally important species, functional attributes that support food sources or flood control, or aesthetic values, such as the existence of charismatic species like eagles (U.S. EPA, 1998f). However, it should be emphasized that two key elements are required to define an assessment endpoint: (1) a valued ecological entity (e.g., a species, a community) and (2) an attribute of that entity is important to protect (e.g., reproductive fitness).

Given the similarity in the management goals for HWIR, the assessment endpoints for the SI Study were chosen to be consistent with those selected for the proposed Hazardous Waste Identification Rule. As with the HWIR risk analysis, ecological exposures are presumed to occur at facilities that may be located anywhere within the contiguous United States. Consequently, a suite of assessment endpoints was chosen based on: (1) their significance to the ecosystem, (2) their ability to represent a variety of habitat types, (3) their position along a continuum of trophic levels, and (4) their susceptibility to chemical stressors managed in surface impoundments meeting certain regulatory criteria. In Table 2-6, the assessment endpoints (i.e., values to be protected) selected for the SI Study analysis are defined in terms of: (1) the

significance of an ecological entity, (2) the ecological receptor representing that entity, (3) the characteristic about the entity that is important to protect, and (4) the measures of effect used to predict risk. The intent of including multiple receptors is that, by protecting producers (i.e., plants) and consumers (i.e., predators) at different trophic levels, as well as certain structural components (e.g., benthic community), a degree of protection from chemical stressors may be inferred to the ecosystem as a whole. Consequently, the selection of the assessment endpoints for each receptor taxon is critical to the development of ecological screening factors.

In addition to using screening factors to infer risks to representative species populations and communities, it is also important to consider the potential effects on managed lands (e.g., National Wildlife Refuges), critical habitats (e.g., wetlands), and threatened and endangered species. Although metrics to evaluate the impacts on the ecological "health" of these entities are not available for use in screening analyses, the presence of valued habitats and species may require alternative risk modeling approaches to determine the likelihood of adverse effects. These assessment endpoints will not be evaluated in Phase I; however, the intrinsic value of managed lands and critical habitats will be considered in Phase IC and Phase II.

2.3.1.3 <u>Development of Ecological Screening Factors</u>. The development of ecological screening factors will involve four basic steps:

- Select representative species and receptor groups.
- Identify relevant exposure pathways.
- Select appropriate ecotoxicological studies:
  - studies used in population-inference
  - studies used in community-inference.
- Calculate ecological screening factors
  - screening factors for receptor populations
  - screening factors for receptor communities.

Examples of ecological screening factors and the studies selected to support their development are presented in Appendix C. Because these data will be used in both the Phase I and Phase II analysis, Appendix C uses the generic term of "toxicity benchmarks" to refer to screening factors as well as ecotoxicological study data. The following discussion describes the methods and data sources used in the development of screening factors shown in Appendix C.

Selection of Representative Species/Receptor Groups. The HWIR ecological risk assessment approach included a series of representative habitats for terrestrial (five), freshwater margins (three), and wetlands (three permanently flooded). These habitats were selected to capture the variability in ecological systems throughout the United States and to provide a

Table 2-6. Assessment Endpoints and Measures of Effects

Examples of Ecological Significance	Assessment Endpoint	Representative Receptors	Characteristic(s)	Measure of Effect
# Multiple trophic levels represented # Represent species with large foraging ranges # Represent species with longer life spans # Variety of dietary exposures represented	Viable mammalian wildlife populations	Deer mouse, meadow vole, red fox, e.g.	Reproductive and developmental success	Chronic or subchronic NOAEL(s) for developmental and reproductive effects
	Viable avian wildlife populations	Red-tailed hawk, northern bobwhite, e.g.	Reproductive and developmental success	Chronic or subchronic NOAEL(s) for developmental and reproductive effects
# Species represent unique habitat niches # Many species are particularly sensitive to exposure	Protection of amphibian and reptile populations ("herps") against acute effects	Frog, newt, snake, turtle, e.g.	Lethality and percent deformity	Acute LC_{50}s for developmental effects resulting from early life stage exposures
# Represents base food web in terrestrial systems # Habitat vital to decomposers and soil aerators # Crucial to nutrient cycling	Sustainable soil community structure and function	Nematodes, soils mites, springtails, annelids, arthropods, e.g.	Growth, survival, and reproductive success	95% of species below no effects concentration at 50th percentile confidence interval
# Primary producers # Act as food base for herbivores # Constitute essential habitat for virtually all receptor groups (e.g., nests)	Maintain terrestrial primary producers (plant community)	Soy beans, alfalfa, rye grass, e.g.	Growth, yield, germination	10th percentile from LOEC data distribution
# Important food source for animals that live in waterbody margins # Diverse aquatic life important to maintain biotic integrity	Sustainable aquatic community structure and function	Fish (salmonids), aquatic invertebrates (daphnids), e.g.	Growth, survival, reproductive success	National Ambient Water Quality Criteria for aquatic life (95% species protection)
# Provide habitat for reproductive lifestages (e.g., eggs, larval forms) # Act to process nutrients and decompose organic matter	Sustainable benthic community structure and function	Protozoa, flat worms, ostracods, e.g.	Growth, survival, reproductive success	10th percentile from LOEC data distribution
# Primary producers # Base food source in the aquatic system	Maintain primary aquatic producers (algal and plant community)	Algae and vascular aquatic plants, e.g.	Growth, mortality, biomass, root length	EC_{20} for algae; lowest LOEC for aquatic plants

meaningful "ecological context" for receptor selection. A detailed description of the criteria used to identify representative habitats is provided in the HWIR documentation, *Ecological Receptors and Habitats* (U.S. EPA, 1999n); however, it is important to recognize that the intent of a representative habitat scheme was to develop a site-based framework to perform spatially explicit risk analyses. In the Phase I screening analysis for the SI Study, the representative habitats will simply be used to support the inclusion of representative species and receptor groups.

Because one of the major goals of the Phase I assessment is to prioritize facilities, impoundments, and constituents for further analysis, a strategy was developed to: (1) organize receptors into feeding guilds of taxonomically similar organisms (e.g., herbivorous birds, carnivorous mammals), and (2) select a species to represent each guild. Habitat-receptor correlations, food webs, and available exposure factors will be used to identify "screening-indicator" species that could be expected to receive the highest exposure to constituents, thus ensuring a protective screening assessment. Common species generally will be preferred as indicator species because they are found in a variety of habitats and may be used to represent different guilds. Table 2-7 presents the crosswalk of some of the likely indicator species for various guilds and the representative habitats with which they are associated.

Identification of Relevant Exposure Pathways. Ecological exposure pathways for the Phase I screening analysis will be identified based on: (1) both active and postclosure scenarios for surface impoundments, and (2) likely routes of exposure for receptors assigned to simple food webs. Chemical constituents may volatilize from active surface impoundments and deposit onto adjacent soils, plants, or surface waters. In addition, constituents may leach into ground water and contaminate nearby surface waters and sediments. Following closure, a surface impoundment may be integrated with local habitats (assuming the contaminant concentration does not prevent vegetative growth) and serve as a long-term source of exposure to certain types of constituents (e.g., metals). As shown in Figure 2-18, receptors may be exposed to contaminated media and/or prey and plants in both terrestrial and aquatic systems. Consequently, the exposure pathways that will be represented in Phase I are:

- Direct contact with contaminated sludge/soil (e.g., plants, soil fauna)
- Ingestion of contaminated sludge/soil (e.g., mammals, birds)
- Ingestion of plants/prey on contaminated sludge/soil (e.g., mammals, birds)
- Direct contact with contaminated surface water (e.g., fish, amphibians)
- Direct contact with contaminated sludge (e.g., benthos)
- Ingestion of aquatic plants/prey in contaminated surface water (e.g., birds)
- Ingestion of contaminated surface water (e.g., mammals)

Exposure routes that will be not addressed in the Phase I ecological screening assessment include

- Dermal absorption from contaminated surface water or sludge (e.g., mammals)
- Inhalation of volatile constituents in air.

Table 2-7. Representative Habitats, Receptor Groups, and Representative Species

	Representative Habitats									
	Aquatic Habitats			Wetland Habitats			Terrestrial Habitats			
Representative Species	**Impoundment/Ponds**	**Streams/Rivers**	**Lakes**	**Permanently Flooded Grasslands**	**Permanently Flooded Shrubs/Scrub**	**Permanently Flooded Woodlands**	**Grasslands**	**Shrubs/Scrub**	**Forests**	**Crops/Pastures**
Plants										
Algae and emergent aquatic plants	!	!	!	!	!	!				
Terrestrial plants							!	!	!	!
Invertebrates										
Aquatic invertebrates	!	!	!							
Sediment-associated biota	!	!	!	!	!	!				
Soil invertebrates				!	!	!	!	!	!	!
Fish	!	!	!	!	!	!				
Amphibians										
Bullfrog	!	!	!	!	!	!				!
Gopher frog							!	!	!	
Reptiles[a]	!	!	!	!	!	!	!	!	!	!
Birds										
Herbivorous Birds[b]										
Song sparrow	!	!	!				!	!	!	!
Mallard	!	!	!	!	!	!				
Insectivorous Birds[c]										
American robin							!	!	!	!
Tree swallow				!						
American woodcock	!	!	!		!	!				
Carnivorous Birds[d]										
American kestrel	!	!	!	!	!	!			!	
Red-tailed hawk							!	!		!
Mammals										
Herbivorous Mammals										
Meadow vole	!	!	!	!	!		!	!		!
Pine vole									!	
Mule deer				!	!	!				
White-tailed deer	!	!	!				!	!	!	!
Insectivorous Mammals										
Short-tailed shrew							!			!
Deer mouse	!	!	!		!	!		!	!	
Carnivorous Mammals										
Raccoon	!	!	!	!	!	!				
Coyote	!	!	!				!	!	!	!

[a] Reptiles will not be assessed in Phase I due to the lack of applicable toxicity data.
[b] Birds and mammals whose diet is predominantly plants (i.e., vegetative, flowers, fruits, and/or seeds)
[c] Birds and mammals whose diet is predominantly invertebrates (e.g., insects, soil invertebrates, sediment-associated invertebrates).
[d] Birds and mammals whose diet is predominantly birds or mammals.

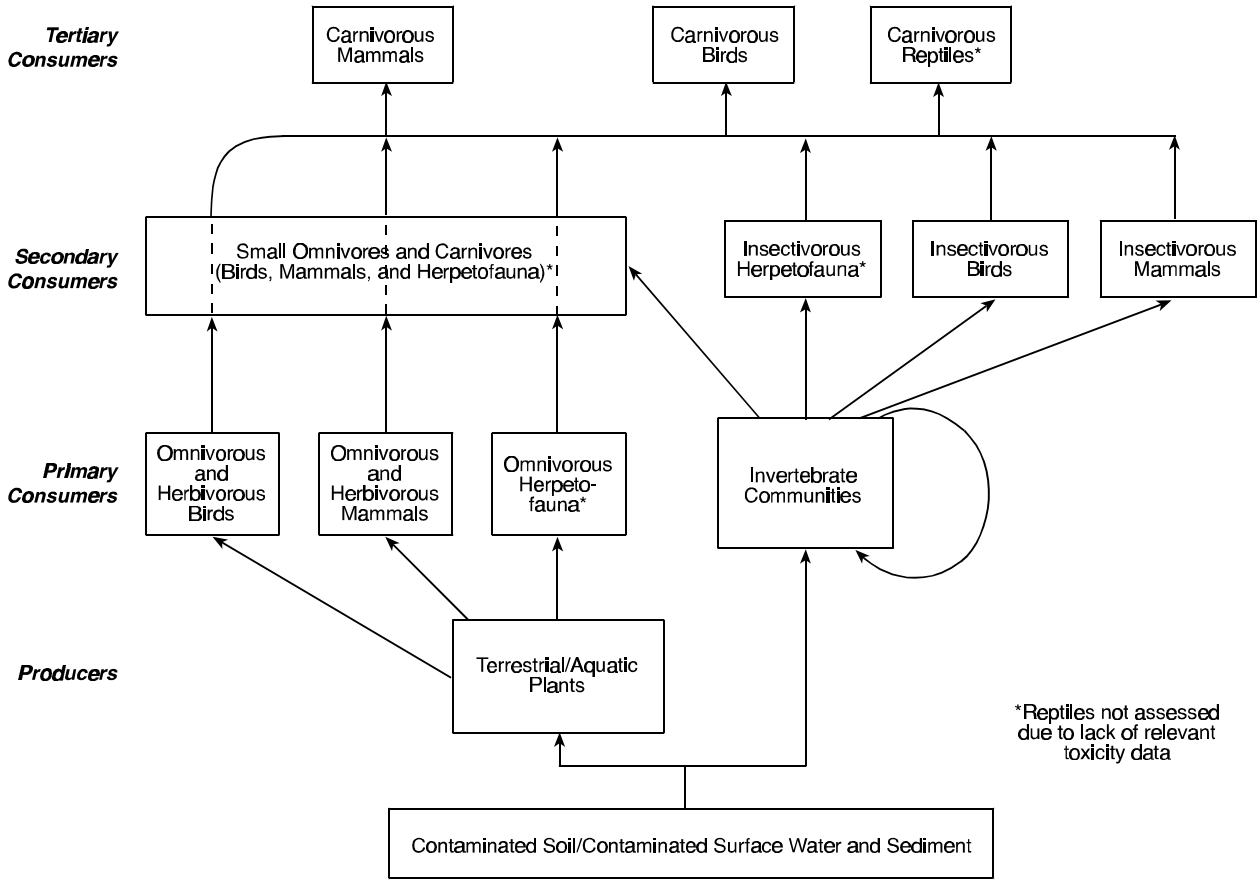


Figure 2-18. General food web model for aquatic and terrestrial systems.

Dermal absorption of constituents is considered to be an insignificant exposure pathway for potentially exposed wildlife receptors and will not be assessed because

- Dense undercoats or down effectively prevents chemicals from reaching the skin of wildlife species and significantly reduces the total surface area of exposed skin (Peterle, 1991; U.S. ACE, 1996)

- Results of exposure studies indicate that exposures due to dermal absorption are insignificant compared to ingestion for terrestrial receptors (Peterle, 1991).

Inhalation of volatile compounds will not be assessed for wildlife receptors because

- Concentrations of volatile chemicals released from soil to aboveground air are drastically reduced, even near the soil surface (U.S. ACE, 1996)

- Significant concentrations of VOCs would be required to induce noncarcinogenic effects in wildlife based on inhalation toxicity data for laboratory rats and mice (U.S. ACE, 1996).

Selection of Appropriate Ecotoxicological Studies—Population Inference. As suggested in Table 2-6, risks to four groups of receptors (mammals, birds, amphibians, and reptiles) will be estimated based on endpoints relevant to population sustainability. It is important to note that screening factors will not be developed based on population-level studies. Rather, we will use ecotoxicological data on selected physiological endpoints (e.g., developmental effects) to infer risks to wildlife populations.

For amphibians, the development of screening factors is severely limited by data availability. After a review of several compendia presenting amphibian ecotoxicity data (e.g., U.S. EPA, 1996g; Power et al., 1989) as well as primary literature sources, it was determined that there was a general lack of chronic or subchronic ecotoxicological studies. Consequently, studies on acute exposures during sensitive amphibian life stages will be selected to develop screening factors. The potential sensitivity of this receptor group warrants their inclusion even though chronic study data are not yet available. Amphibian studies considered appropriate for development of Phase I screening factors must include the following information:

- Test organism
- Toxicological endpoint
- Exposure duration
- Life stage at which exposure occurred (e.g., embryo, tadpole).

Appropriate toxicity data for amphibians will include reproductive effects, developmental effects, or lethality from studies conducted for an exposure duration of less than 8 days. Limiting the study duration to short exposures will allow use of a larger data set in deriving the screening factors.

For mammals, birds, and reptiles, only toxicity studies relevant to ingestion will be reviewed (e.g., gavage); studies where the chemical was administered via injection or implantation will not be reviewed. At a minimum, studies must report the following to be considered for use in developing the ecological screening factors:

- Test organism
- Toxicological endpoint
- Dose-response information
- Exposure duration
- Exposure route
- Sample size

Preferred Studies. Toxicity studies that reported reproductive impairment, developmental abnormalities, and mortality will be preferred to studies on other physiological endpoints because these endpoints are highly relevant to the assessment endpoints selected for the SI Study (e.g., population sustainability). In addition, the use of reproductive and developmental toxicity data has been recommended in guidance across several federal agencies (U.S. EPA, 1998f; Department of the Air Force, 1997; U.S. ACE, 1996). Studies that report no observed adverse effects levels (NOAELs) will be preferred to those that include only effects levels and low observed adverse effects levels (LOAELs). Several other important aspects of study selection are summarized below.

Duration of exposure - Duration is critical in assessing the potential for adverse effects to wildlife. However, since definitive guidance is not available on subchronic versus chronic exposures, we will define chronic exposures as greater than 50 percent of the life span of mammalian wildlife representative species. Little information exists concerning the life span of birds used in toxicity studies, and a standard study duration has not been established for avian toxicity tests. Therefore, exposures greater than 10 weeks will be considered chronic for birds; exposures less than 10 weeks will be considered subchronic (Sample et al., 1996).

Timing of exposure - The timing of exposure is critical in assessing the potential for adverse effects to wildlife. For example, early development is a particularly sensitive life stage due to the rapid growth and differentiation occurring within the embryo and juvenile. For many species, exposures of a few hours to a few days during gestation and early fetal development may produce severe adverse effects (Sample et al., 1996). Therefore, in the absence of chronic studies on developmental or reproductive effects (e.g., multigenerational studies), studies that report exposures during reproductive and/or developmental stages may be selected for use in developing ecological screening factors.

Endpoint of interest - Our review of toxicity data indicated that reproductive or developmental effects were frequently observed at doses that were lower than those causing mortality . Therefore, chronic mortality studies will only be used when reproductive or developmental data are not available. Physiological (e.g., enzyme activity), systemic, and behavioral responses will be less preferred because it is often difficult to relate these responses to quantifiable decreases in reproductive fitness or the persistence of wildlife populations. Tumorigenic and carcinogenic toxicity studies will not be considered ecologically relevant and

will not be used to develop toxicity benchmarks because debilitating cancers in wildlife are exceedingly rare under field conditions.

Data gaps - From previous analyses such as HWIR, it is apparent that there will be a number of data gaps in the ecotoxicological database on mammals, birds, and reptiles. In fact, chronic studies on reptiles are generally unavailable. Similarly, there is a paucity of relevant studies on birds that meet the selection criteria described above. Two alternatives will be considered in developing screening factors:

1. **Use of Surrogate Chemicals.** For some classes of constituents, toxicity data exist for only a few, well-studied constituents (e.g., polycyclic aromatic hydrocarbons). Research on qualitative (QSARs) suggests that chemicals with similar molecular or physicochemical properties have similar biological reactivity and toxicity (Donkin, 1994; Nirmalakhandan and Speece, 1988). Therefore, these chemicals may be used as surrogates for other detected members of the chemical class.

2. **Use of Uncertainty Factors.** In screening ecological risk assessments, it is often standard practice to adopt uncertainty factors to derive benchmarks intended to represent chronic exposures. We will use these factors to ensure that critical receptors are not eliminated from the Phase I screening.

Selection of Appropriate Ecotoxicological Studies—Community Inference. The community-based screening factors generally reflect direct exposures to a contaminated medium, which, in the Phase I screening analysis, is represented by actual impoundment concentrations in water and sludge. As shown in Table 2-6, risks to five groups will be estimated based on endpoints relevant to sustainability of community structure and function: soil fauna, terrestrial plants, aquatic biota, algae and aquatic plants, and benthos. It should be noted that the screening factors for communities generally are not based on community-level studies in the sense that they do not reflect endpoints relevant to community dynamics (e.g., predator-prey interactions). Rather, they are based on the theory that protection of 95 percent of the species in the community will provide a sufficient level of protection for the community (see, for example, Stephan et al., 1985, for additional detail). As with the wildlife populations, ecotoxicological data on individual species will be used to infer risks to the community.

Appropriate ecotoxicological studies to derive screening factors for these receptor groups are available in a number of compendia and, as a result, it is often not necessary to conduct primary literature reviews to identify suitable studies. These compendia frequently present threshold concentrations for effects that may be used directly as screening factors with little or no modification. Table 2-8 presents the primary data sources that will be used to support the derivation of screening factors for the community receptors. The selection process for screening factors among different sources and the screening factor calculations are discussed in the following section.

Calculation of Ecological Screening Factors—Receptor Populations. The calculation of ecological screening factors for receptor populations is based on the implicit assumption that

Table 2-8. Examples of Primary Data Sources for Derivation of Screening Factors for Community Receptors

Source	Contents
Plant Community	
Efroymson, R.A., M.E. Will, G.W. Suter II, and A.C. Wooten. 1997a. Toxicological Benchmarks for Screening Contaminants of Potential Concern for Effects on Terrestrial Plants: 1997 Revision.	This document provides effects data for terrestrial plants exposed in soil and solution mediums. Approximately 45 constituents have proposed soil criteria.
PHYTOTOX Database. Office of Research and Development. Environmental Protection Agency.	This database contains over 49,000 toxicity tests on terrestrial plants for more the 1,600 organic and inorganic chemicals and 900 species.
Freshwater Community / Algae and Aquatic Plants	
AQUIRE (AQUatic toxicity Information REtrieval) Database. 1997. Environmental Research Laboratory, Office of Research and Development, U.S. EPA, Duluth, MN	This database contains over 145,000 toxicity tests for more than 5,900 organic and inorganic chemicals and 2,900 aquatic species.
U.S. EPA. *Ambient Water Quality Criteria*. U.S. EPA, Washington, DC.	These chemical-specific documents provide the ecotoxicity data and derivation methodologies used to develop the National Ambient Water Quality Criteria (NAWQC).
U.S. EPA. 1995a. Great Lakes Water Quality initiative Criteria Documents for the Protection of Aquatic Life in Ambient Water. Office of Water. (U.S. EPA, 1996a Update)	For a limited number of constituents, the GLWQI has proposed surface water criteria for aquatic biota using analogous methods as implemented in the derivation of the NAWQC.
Suter II, G.W. and C. Tsao. 1996. Toxicological Benchmarks for Screening Contaminants of Potential Concern for Effects on Aquatic Biota: 1996 Revision	This compendia reference provides acute and chronic water quality criteria for freshwater species including algae.
Soil Community	
Efroymson, R.A., M.E. Will, and G.W. Suter II. 1997b. Toxicological Benchmarks for Contaminants of Potential Concern for Effects on Soil and Litter Invertebrates and Heterotrophic Process: 1997 Revision. Oak Ridge National Laboratory.	This document provides effects data for soil biota (i.e., microbial processes and earthworms). Approximately 35 constituents have proposed soil criteria, and some field studies are included.
CCME (Canadian Council of Ministers of the Environment), 1997. Recommended Canadian Soil Quality Guidelines.	The criteria developed by the CCME are concentrations above which effects are likely to be observed.
Sediment Community	
U.S. EPA. 1993. *Technical Basis for Deriving Sediment Quality Criteria for Nonionic Organic Contaminants for the Protection of Benthic Organisms by Using Equilibrium Partitioning*.	This document supplies toxicological criteria for nonionic hydrophobic organic chemicals using FCVs (final chronic values) and SCVs (secondary chronic values) developed for surface water (Sediment Quality Criteria, SQC).
Long and Morgan. 1991. *The Potential for Biological Effects of Sediment-Sorbed Contaminants Tested in the National Status and Trends Program*. National Oceanic and Atmospheric Administration (NOAA) Technical Memorandum. Update: (Long et al., 1995)	Field measured sediment concentrations are correlated with impacts to sediment biota in estuarine environments. Measures of abundance, mortality, and species composition are the primary toxicity endpoints.
Jones, D.S., G.W. Sutter III, and R.N. Hall. 1997. *Toxicological Benchmarks for Screening Contaminants of Potential Concern for Effects on Sediment-Associated Biota: 1997 Revision.* Oak Ridge National Laboratory.	This document proposes sediment criteria for both organic and inorganic constituents using both field and estimation methodologies.
MacDonald, D.D. 1994. Approach to the Assessment of Sediment Quality in Florida Coastal Waters. Florida Department of Environmental Protection (FDEP), Tallahassee.	This approach applies statistical derivation methods to determine sediment criteria using NOAA data. The resulting criteria are more conservative than NOAA values.

each receptor species forages only within the contaminated area, regardless of the size of its home range. For smaller animals, this assumption has little impact on the estimates of exposure. However, for larger animals with more extensive foraging areas, this assumption may overestimate exposure if the animal's foraging patterns tend to be evenly spread over the home range. Thus, it is important to recognize both the explicit *and* implicit sources of protection in this methodology.

For amphibian populations, a screening factor for water (SF_{water}) will be derived as the geometric mean of acute studies meeting the data requirements discussed above (i.e., relevant endpoint, acute exposure, high effect level). However, it is important to point out that this screening factor should be construed as only "protective" of gross effects to amphibian populations (e.g., lethality to 50 percent of the population). As a result, careful consideration will be given in interpreting the results of the screening results during the risk characterization. The remainder of this section outlines the basic technical approach used to convert avian or mammalian benchmarks (in daily doses) to soil and water screening factors (in units of concentration) that will be compared with surface impoundment sludge and water concentrations, respectively.

Once the appropriate ecotoxicological study is identified for mammals and/or birds,[1] the screening factors will be calculated for each medium of interest using a four-step process:

1. Adjust study benchmark using uncertainty factor.
2. Scale benchmark from test species to receptor species.
3. Identify uptake/accumulation factors.
4. Calculate protective concentration (i.e., screening factor).

STEP 1: Adjust Study Benchmark Using Uncertainty Factor

For benchmarks that are based on acute studies, uncertainty factors may be used to extrapolate from acute exposures to chronic exposures. Based on the review of a toxicity database of over 4,000 records, we propose using the following:

Extrapolation	Uncertainty Factor
Acute LD_{50} to chronic NOAEL	100
Acute LOAEL to chronic NOAEL	50

These uncertainty factors are consistent with DTSC (1996) guidance and an independent review of toxicity data by other authors (Calabrese and Baldwin, 1993; Sample et al., 1996). To convert the acute benchmark to a chronic benchmark, Equation 2-1 will be used:

$$\text{Chronic Benchmark}_{\text{Study Species}} = \text{Acute Benchmark}_{\text{Study Species}} / \text{Uncertainty Factor} \qquad (2\text{-}1)$$

The intent of this conversion is to provide a benchmark for the study species that represents a no observed adverse effects level. Consequently, we refer to this value as the $NOAEL_{SS}$ to indicate the effects level and the fact that it applies to the study species.

[1] Reptiles are not discussed in this section because of the data deficiencies for this receptor group.

STEP 2: Scale Benchmark from Study Species to Receptor Species

The benchmark chosen to represent the mammalian or avian taxa will be extrapolated from the study species to the receptor species ($NOAEL_{RS}$) within the same taxa using a cross-species scaling equation (Sample et al., 1996). For population-inference benchmarks for mammals, the extrapolation is performed using Equation 2-2.

$$NOAEL_{RS} = NOAEL_{SS} \cdot \left(\frac{bw_{SS}}{bw_{RS}} \right)^{1/4} \tag{2-2}$$

where $NOAEL_{SS}$ is the NOAEL for the study species, bw_{RS} is the body weight of the receptor species, and bw_{SS} is the body weight of the study species. This is the default methodology EPA proposed for carcinogenicity assessments and reportable quantity documents for adjusting animal data to an equivalent human dose.

For avian species, new research suggests that the cross-species scaling equation used for mammals is not appropriate (Mineau et al., 1996). Mineau et al. (1996) used a database that characterized acute toxicity of pesticides to avian receptors of various body weights. The results of the regression analysis revealed that applying mammalian scaling equations may not predict sufficiently protective doses for avian species. Mineau et al. (1996) suggested that a scaling factor of 1 provides a better dose estimate for birds, as shown in Equation 2-3. This recommendation will be adopted for avian receptors in this assessment.

$$NOAEL_{RS} = NOAEL_{SS} \cdot \left(\frac{bw_{SS}}{bw_{RS}} \right)^{1} \tag{2-3}$$

STEP 3: Identify Uptake/Accumulation Factors

As suggested in Figure 2-18, movement of contaminants through the food web is an important exposure vector for mammals and birds. Consequently, estimates of chemical accumulation in the tissues of plants and prey items are required. For receptors likely to rely on aquatic systems for food (e.g., kingfisher), bioaccumulation factors and/or bioconcentration factors are required for aquatic biota such as fish, benthos, and aquatic plants. These data may be identified in the open literature or they may be estimated for organic constituents using regression equations such as that shown in Equation 2-4 (Lyman et al., 1990):

$$\log BCF = 0.76 \; [\log (K_{ow})] - 0.23 \tag{2-4}$$

where BCF is the estimated bioconcentration factor for fish and the K_{ow} is the constituent-specific octanol-water partition coefficient.

For receptors found primarily in terrestrial systems, bioconcentration factors are required for terrestrial plants, soil invertebrates (e.g., earthworms), and vertebrates that report the relationship between tissue concentrations and soil concentrations. As with aquatic

accumulation factors, these data may be identified in the literature or estimated using recently developed methods for earthworms and small mammals (Sample et al., 1998a, 1998b).

In short, these values are typically identified in the open literature and EPA references or calculated based on the relationship between log K_{ow} and accumulation in lipid tissue. The primary source of data is the methodology developed for HWIR and described more fully in Section 3 of this technical plan. To ensure that the Phase I ecological screening assessment is protective, a default value of 1 will be assigned to each uptake/accumulation factor that cannot be derived through estimation methods or identified in the literature.

STEP 4: Calculate Protective Concentration for Receptor

Based on the $NOAEL_{RS}$, the screening factor for a receptor that relies on aquatic biota as the primary food source will be calculated as a function of the receptor's body weight, the receptor's ingestion rate for food and water, and the bioaccumulation potential of the constituent. As shown in Equation 2-5:

$$SF_{water} = \frac{NOAEL_{RS} \ x \ bw}{(I_{food} \sum BAF_j \ x \ F_j \ x \ AB_j) + (I_{water})} \qquad (2\text{-}5)$$

where

bw	=	body weight (kg)
I_{food}	=	total daily intake of aquatic biota (kg WW/d)
I_{water}	=	total daily soil intake (kg/d)
BAF_j	=	bioaccumulation factor for food item j (L/kg WW))
F_j	=	fraction of diet consisting of food item j (unitless)
AB_j	=	absorption of chemical in the gut from food item j (assumed = 1).

Equation 2-5 can also be used to derive an “impoundment use only” screening factor for sites that do not have any fishable waterbodies identified in the survey data. For these cases, only I_{water} would be included in the denominator to reflect use of the impoundment as a drinking water source.

For terrestrial systems, Equation 2-6 is simply modified to account for soil or sludge intake:

$$SF_{soil/sludge} = \frac{NOAEL_{RS} \ x \ bw}{(I_{food} \sum BCF_j \ x \ F_j \ x \ AB_j) + (I_{soil/sludge})} \qquad (2\text{-}6)$$

where

bw	=	body weight (kg)
I_{food}	=	total daily food intake of terrestrial biota (kg/d)
BCF_j	=	bioconcentration factor for food item j (assumed unitless)
F_j	=	fraction of diet consisting of food item j (unitless)
AB_j	=	absorption of chemical in the gut from food item j (assumed = 1)
$I_{soil/sludge}$	=	total daily soil intake (kg/d).

Information sources to develop the input values for body weight (bw), ingestion rates (I_{xx}), and dietary fractions (F_j) will generally be taken from the extensive HWIR databases. The HWIR databases were developed using EPA's *Wildlife Exposure Factors Handbook* (U.S. EPA, 1993c) and augmented by substantial literature review and synthesis of a variety of information sources. However, it may be necessary to expand the data collection efforts beyond the current HWIR universe of constituents; in particular, the identification of suitable ecotoxicological studies to support the development of receptor species benchmarks ($NOAEL_{RS}$) will require significant effort. In addition to the review of primary literature, Table 2-9 presents some examples of key data sources that may be used to identify suitable ecotoxicological studies.

Calculation of Ecological Screening Factors—Receptor Communities. The calculation of ecological screening factors for receptor communities relies heavily on existing data sources, many of which have produced peer-reviewed concentrations for soils and surface water presumed to be protective of ecological receptors. Example include

- **Aquatic Biota**: U.S. EPA's National Ambient Water Quality Criteria

- **Sediment-Associated Biota**: National Oceanic and Atmospheric Administration's (NOAA) Effects Range-Low (ER-Ls)

- **Soil Invertebrates**: Dutch National Institute of Public Health and Environmental Protection's (RIVM) Ecotoxicological Intervention Values (EIVs)

To the extent possible, we will rely on existing data sources as well as the ecotoxicity databases developed under HWIR and other studies conducted by EPA. For constituents lacking readily available sources, we will use the following approach to calculate ecological screening factors.

Aquatic community—For aquatic biota in freshwater systems, the final chronic value (FCV) developed for the National Ambient Water Quality Criteria (AWQC) will be chosen as the screening factor. If an AWQC is not available, the continuous chronic criterion (CCC) developed for the Great Lakes Water Quality Initiative (GLWQI) will be used as the screening factor (U.S. EPA, 1995a, 1996a). If neither of these criteria are available, we will calculate a secondary chronic value (SCV) using the Tier II methods developed through the Great Lakes Initiative (Stephan et al., 1985; Suter and Tsao, 1996; RTI, 1995a, 1995b).

The SCV is calculated using methods analogous to those applied in calculating the FCV. However, the Tier II methods: (1) require chronic data on only one of the eight family requirements, (2) use a secondary acute value (SAV) in place of the FAV, and (3) are derived based on a statistical analysis of AWQC data conducted by Host et al. (1991). Host et al. (1991) developed adjustment factors (AFs) depending on the number of taxonomic families that are represented in the database. The Tier II methodology was designed to generate SCVs that are below FCVs (for a complete data set) with a 95 percent confidence limit.

Table 2-9. Selected Sources of Toxicity Data

Databases

- Hazardous Substances Data Bank (HSDB). National Library of Medicine, National Toxicology Information Program. Bethesda, MD.
- PHYTOTOX. Chemical Information System (CIS) Database.
- Registry of Toxic Effects of Chemical Substances (RTECS). National Institute for Occupational Safety and Health (NIOSH), Washington, D.C.

Compilations

- Agency for Toxic Substances and Disease Registry (ATSDR). 1997. *Toxicological Profiles*. On CD-ROM. CRC press. U.S. Public Health Service. Atlanta, GA.
- Devillers, J. and J.M. Exbrayat. 1992. *Ecotoxicity of Chemicals to Amphibians*. Grodon and Breach Science Publishers. Philadelphia, PA.
- Eisler, R. 1985-1993. *Hazards to fish, wildlife, and invertebrates: A synoptic review*. U.S. Fish Wildlife Service Biological Reports
- Hudson, R.H., R.K. Tucker, and M.A. Haegele. 1984. *Handbook of toxicity of pesticides to wildlife*. U.S. Fish and Wildlife Serv. Resour. Publ. 153. 90 pp.
- Sample, B.E., D.M. Opresko, and G.W. Suter II. 1996. Toxicological benchmarks for wildlife: 1996 Revision. Prepared for the U.S. Department of Energy.

Algae and aquatic plants—For algae and aquatic plants, toxicological data are available in the open literature and in data compilations such as the *Toxicological Benchmarks for Screening Potential Contaminants of Concern for Effects on Aquatic Biota: 1996 Revision* (Suter and Tsao, 1996). Studies on freshwater vascular plants are seldom available; however, toxicity data are available from standard algal tests. In order of preference, the screening factors for algae and aquatic plants will be based on either (1) a lowest observed effects concentration (LOEC) for vascular aquatic plants or (2) an effective concentration (EC_{xx}) for a species of freshwater algae, generally a species of green algae.

Benthic community—Two methods will be applied to develop screening factors for the sediment community. The first and preferred method will use measured sediment concentrations that resulted in *de minimis* effects to the composition and abundance of the sediment community. The second derivation method uses the equilibrium partitioning relationship between sediments and surface waters to predict a protective concentration for the benthic community using the chronic FCV. A brief discussion of each method is provided below.

- **Screening Factors from Measured Data:** The premier sources of measured sediment toxicity data are the National Oceanic and Atmospheric Administration (NOAA) and the Florida Department of Environmental Protection (FDEP). These data are used by NOAA to estimate the 10th percentile effects concentration effects range-low (ER-L) and a median effects concentration effects range-median (ER-M) for adverse effects in the sediment community. The FDEP sediment

criteria are developed from the ER-L and ER-M values to approximate a threshold effects level (TEL) (estimated from ER-L data). The TELs are preferable to the ER-L primarily because they have been shown to be analogous to TELs observed in freshwater organisms (Smith et al., 1996).

Predicted Sediment CSCLs. If neither a TEL nor an ER-L is available for nonionic, organic constituents, the screening factor will be calculated using the sediment quality criteria (SQC) method (U.S. EPA, 1993b). This method assumes equilibrium-partitioning between the sediment and water column is a function of the organic carbon fraction (f_{oc}) in sediment and the organic carbon partition coefficient of the constituent. The screening factor is calculated as shown in Equation 2-7, assuming that the f_{oc} is equivalent to 1 percent total organic carbon (Jones et al., 1997).

Terrestrial plant community—For the terrestrial plant community, screening factors for soil will generally be derived according to the methodology presented in the *Toxicological Benchmarks for Screening Contaminants of Potential Concern for Effects on Terrestrial Plants: 1997 Revision* (Efroymson et al., 1997a). The authors derive ecologically relevant benchmarks by rank ordering the phytotoxicity data according to the lowest observed effects concentrations (LOECs). We are proposing to adopt that same approach and select screening factors for constituents with 10 or fewer values at the lowest LOEC. For constituents with more than 10 LOEC values, the 10th percentile LOEC will be selected. Because the toxicity endpoints reflect endpoints such as plant growth and yield reduction, the screening factors are presumed to be

$$SF_{sediment} = f_{oc} \ x \ K_{oc} \ x \ FCV \qquad (2\text{-}7)$$

relevant to sustaining “healthy” plant communities.

Soil community—For the soil community, screening factors will be calculated using the methodology developed under HWIR. In brief, the screening factors for soil fauna are estimated to protect species found in a typical soil community, including earthworms, insects, and other soil fauna. Eight taxa of soil fauna are represented to reflect the key structural (e.g., trophic elements) and functional (e.g., decomposers) components of the soil community. The methodology presumes that protecting 95 percent of the soil species will ensure long-term sustainability of a functioning soil community. The toxicity data on soil fauna will be gleaned from several major compendia and supplemented with additional studies identified in the open literature. The mathematical construct shown in Equation 2-8 was developed by Dutch scientists (i.e., the RIVM methodology) and will be used to calculate screening factors at a 50th percentile level of confidence (Sloof, 1992). For the screening factors for soil biota ($SF_{soil5\%}$), the 50th percentile level of confidence will be selected because the 95th percentile has been shown to be overly conservative (e.g., well below background levels).

$$SF_{soil_5\%} = [x_m - k_l \ s_m] \qquad (2\text{-}8)$$

where

x_m = sample mean of the log LOEC data
k_l = extrapolation constant for calculating the one-sided leftmost confidence limit
s_m = sample standard deviation of the log LOEC data.

When data are insufficient to calculate screening factors using this methodology, two other sources of screening factors will be used. First, the ecotoxicological data presented on indicator species such as earthworms will be used to select a protective soil concentration (Efroymson et al., 1997b). Second, the criteria developed by the Canadian Council of Ministers of the Environment (CCME, 1997) for the protection of soil organisms will be adopted as screening factors.

2.3.1.4 <u>Procedure for Phase I Ecological Risk Screening</u>. In most respects, the ecological risk screening procedure mirrors the framework presented in Figure 2-9 for the risks from noncancer constituents to human health. Therefore, this discussion is intentionally brief to avoid duplicating the technical plan described in Section 2.2. The salient features of the Phase I ecological risk screening are summarized below.

Select Appropriate Screening Factors. The underlying strategy for the Phase I assessment is to identify screening factors that are appropriate for a given facility. Screening factors for terrestrial receptors (e.g., plants, raccoons) will be used routinely at each site since these "common" receptors were selected to be broadly applicable across the contiguous United States. However, surface impoundments are not intended to support aquatic plants, aquatic invertebrates, fish, or sediment-associated biota; therefore, aquatic and sediment-associated biota will be assessed only if a potentially affected waterbody is identified near the surface impoundment. Although not intended to support amphibians, birds, and mammals, surface impoundments are likely to be attractive to these receptors (especially if impoundments support vegetation); therefore amphibians, birds, and mammals will be assessed for all surface impoundments. Consequently, not all screening factors will be applied to each facility.

Select Appropriate Surface Impoundment Concentrations. Whenever possible, reported mean concentrations for impoundment water and sludge will be used in the Phase I ecological screening assessment. If impoundment water concentrations are not reported, available data will be used in the same order of preference as shown in Figure 2-6 to estimate impoundment water concentrations.

If sludge concentrations are not reported for the surface impoundment, available data will be used in the following order of preference as shown in Figure 2-8 to estimate impoundment sludge concentrations.

Calculate Risks. To evaluate the receptor risks (defined as the ratio between the impoundment concentration and the screening factor, or hazard quotient) from exposure to a chemical constituent at a particular surface impoundment, Equation 2-9 will be used:

$$HQ^{i}_{constituent} = \frac{C_{imp_{water}}}{SF_{water}} \quad or \quad \frac{C_{imp_{sludge}}}{SF_{sludge}} \quad or \quad \frac{C_{imp_{soil}(sludge)}}{SF_{soil}} \tag{2-9}$$

where C_{imp_water}, and C_{imp_sludge}, and C_{imp_soil}(sludge) are the impoundment water concentration and the impoundment sludge concentration, respectively; and SF_{water}, SF_{sludge}, and SF_{soil} are the ecological screening factors applicable to that site. The $HQ^{i}_{constituent}$ is the risk to receptor i associated with that impoundment and facility. The HQ values for each receptor i may be summed across the entire facility in generating facility risks because (1) the screening factors for each receptor are based on the same study data (and endpoints) and (2) receptors may be exposed through both terrestrial and aquatic systems.

2.3.1.5 <u>Results of Phase I Risk Screening/Prioritization</u>. Risk estimates generated by the Phase I ecological screening assessment must be suitable to characterize, screen, and prioritize constituents, surface impoundments, and facilities by the following categories of interest (see also Section 2.4, Phase IC Initial Prioritization):

Facility

- Regulatory status
- Industry type

Surface Impoundment

- Treatment type
- Functional class

Constituent

- Constituent type

The facility risk is defined as the maximum surface impoundment risk ro receptor i for a particular facility. Facility risk estimates are used to develop industry type and regulatory type risk distributions.

The surface impoundment risk is defined as the cumulative risk to receptor i from exposure to all constituents at a particular surface impoundment. Surface impoundment risk estimates will be used to develop treatment type- and functional class type-specific distributions.

For the Phase I ecological screening assessment, the constituent risk is defined as risk to the most sensitive receptor across all impoundments at a facility. Constituent risk estimates will be used to develop constituent-specific risk distributions.

Construct Risk Distributions. Separate risk distributions will be constructed from risk estimates to evaluate categories of interest. Proposed Phase I risk distributions will consist of the following five risk intervals (risk bin):

- # < 0.1
- # ≥ 0.1 and < 1
- # ≥ 1 and < 10
- # ≥ 10 and < 100
- # ≥ 100.

A unitary value (1), representing the constituent, surface impoundment, or facility, will be added to the appropriate risk bin. Since sample facilities represent a number of facilities nationwide, unitary values may be weighted by the facility sample weight before being added to the bin. The Agency may modify risk intervals to provide a more suitable distribution of risks to evaluate categories of interest.

The facility- and surface impoundment-related risk distributions will be constructed from risk estimates for all receptors considered at a particular surface impoundment or facility. These risk distributions will be used to screen facilities, surface impoundments, and constituents. Risk distributions constructed from maximum risk estimates (i.e., risk estimate for the most sensitive receptor) will be compared to risk distributions for all receptors to determine if the number of receptors affects the facility- and impoundment-level risk distributions. In addition, risk distributions for each trophic level will be developed to evaluate potential impacts on food webs. These risk distributions for receptor groups and trophic levels will provide useful metrics for the Phase I risk characterization.

Establish Risk Criteria. A risk criterion of 1 is proposed to screen ecological risk estimates. Risk estimates less than 1 (e.g., $HQ^i < 1$) indicate a negligible potential for adverse ecological impacts. Alternatively, risk estimates of 1 or greater indicate a potential for adverse ecological effects. Surface impoundments and facilities with risk estimates of one or greater may be assigned for further evaluation in Phase II, depending on the results of the Phase I human health screening.

Conduct Risk Screening. The ecological risk screening process is outlined in the decision tree shown in Figure 2-19. As expected, the decision tree is very similar to the health risk decision tree illustrated in Figure 2-9. However, there are three distinct differences in the ecological risk screening procedure. First, the decision tree does not include a margin of protection (MP) for ecological receptors. Whereas, the human health risk screening is

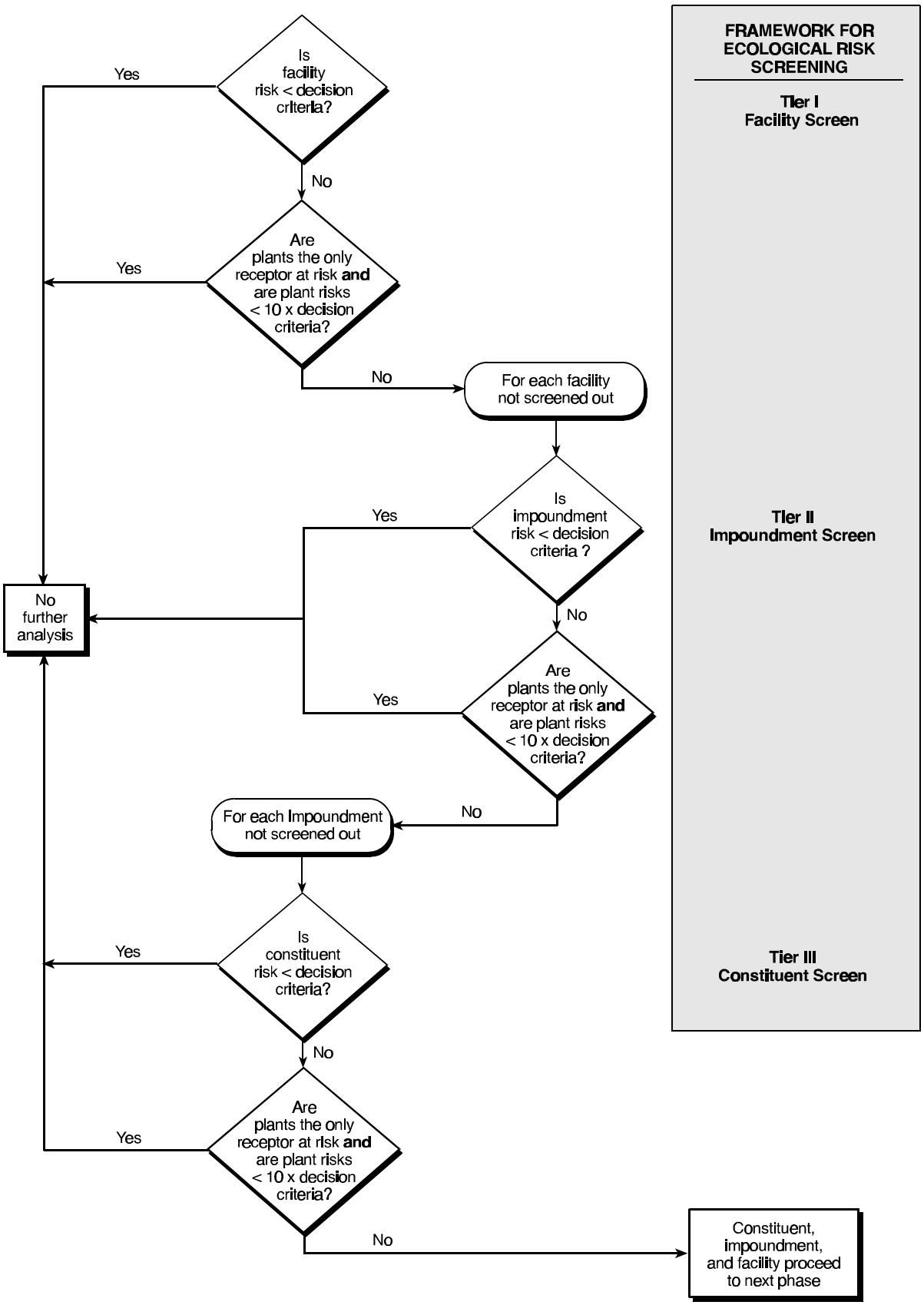


Figure 2-19. Decision tree for performing Phase I ecological risk screening.

intended to protect individuals, the ecological risk screening is intended to protect species populations and communities from adverse effects. Although the Agency considered adding an MP to the risk screening for sites co-located with sensitive habitats (e.g., wildlife refuges), these "special cases" will be considered prior to the conduct of the ecological risk screen, as shown in Figure 2-20. The Agency may consider the use of an MP for ecological risk in special cases in which facilities identify threatened and endangered species located within a 2 km radius of the impoundments. Second, the ecological risk screening does not include cancer effects; only the endpoints described under Section 2.3.1.3 on the development of screening factors will be considered. Third, the figure includes an additional decision point that pertains to the receptor group for which risk is indicated. The results of the surface impoundment pilot study suggested that, for each facility, at least one constituent will fail the ecological risk screening for the terrestrial plant receptor group. Because impoundment sludge/soils are not intended to support terrestrial habitats, and because the screening factors for terrestrial plants are based on a data set that does not reflect adaptation by plant communities, EPA determined that a simple exceedance of the plant screening factor does not provide an adequate basis to determine the potential for adverse ecological effects. Thus, constituents, surface impoundments, or facilities will only proceed to the Phase IC analysis if: (1) the hazard quotient for plants exceeds 10 (indicating a greater potential for adverse effects than a simple exceedance) and (2) the hazard quotient for at least one other receptor group (e.g., amphibians, birds, or mammals) exceeds the risk criterion of 1.

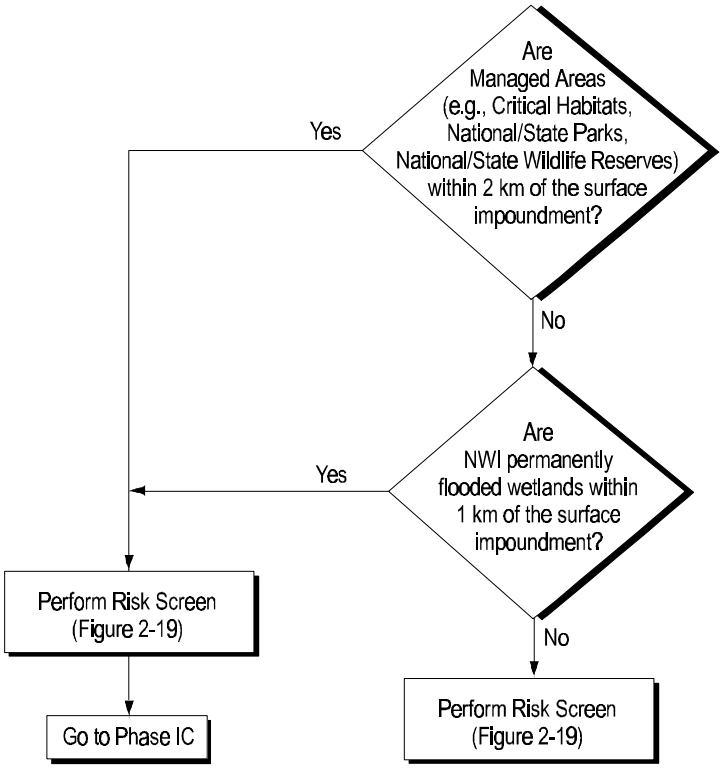


Figure 2-20. Decision diagram for evaluating special cases.

The risk characterization for ecological receptors will be used to determine the priority of facilities, impoundments, and constituents within the context of the human health risk screening results (see discussion on Phase IC). That is, the results of the Phase I ecological risk screening will be used in support of the prioritization, not as an independent screen to identify facilities, impoundments, and constituents for Phase II. The ecological risk characterization will:

- Characterize facility-level risks to address cumulative effects of multiple surface impoundments and constituents

- Characterize impoundment-level risks to address the cumulative effects of multiple constituents at a single surface impoundment.

- Characterize constituent-level risks to address the effects of a single constituent.

The risk estimates (i.e., hazard quotients) will be the primary tool used to prioritize constituents, surface impoundments, and facilities according to the potential for adverse ecological effects. The output from the risk screening will be presented in cumulative frequency histograms similar to those shown in Figure 2-21 to provide EPA with several descriptions of ecological risk that are relevant to ecological receptors as well as the impoundments and facilities. In addition, the presence of protected or potentially sensitive habitats will be considered when prioritizing constituents, surface impoundments, and facilities for further evaluation in Phase IC. These “special cases” will include managed areas and permanently flooded wetlands as designated by the National Wildlife Inventory (NWI). As shown in the decision tree in Figure 2-20, the presence of either managed areas or designated wetlands will be sufficient to assign a high priority risk score to the facility and impoundments found at that site. Notice that the figure allows for the performance of a risk screen for high priority sites as well as those sites that are not co-located with managed areas or designated wetlands. This will support development of risk distributions for this subset of sites and provide a more complete risk distribution for the national data set. A brief description of the criteria for managed areas and designated wetlands is included below.

Managed Areas. Managed areas are specifically protected by law to ensure that plants and wildlife are preserved. Thus, managed areas may need to be evaluated in further detail than that provided in the Phase I ecological screening assessment. A high priority score will be assigned to those facilities and impoundments that are within 2 kilometer of the following areas, irrespective of the risk estimates:

- National or state parks
- National or state wildlife reserves
- Critical Habitats (designated by the U.S. Fish and Wildlife Service)
- Wild and Scenic Rivers (designated by the U.S. Department of the Interior)

GIS coverages from the Managed Areas Database provide the data needed to quickly identify surface impoundments within 2 kilometers of a managed area. A distance of 2 kilometer is proposed because, even for a screening level assessment, the presumption of wildlife use and exposure to a surface impoundment becomes increasingly tenuous as the distance from the

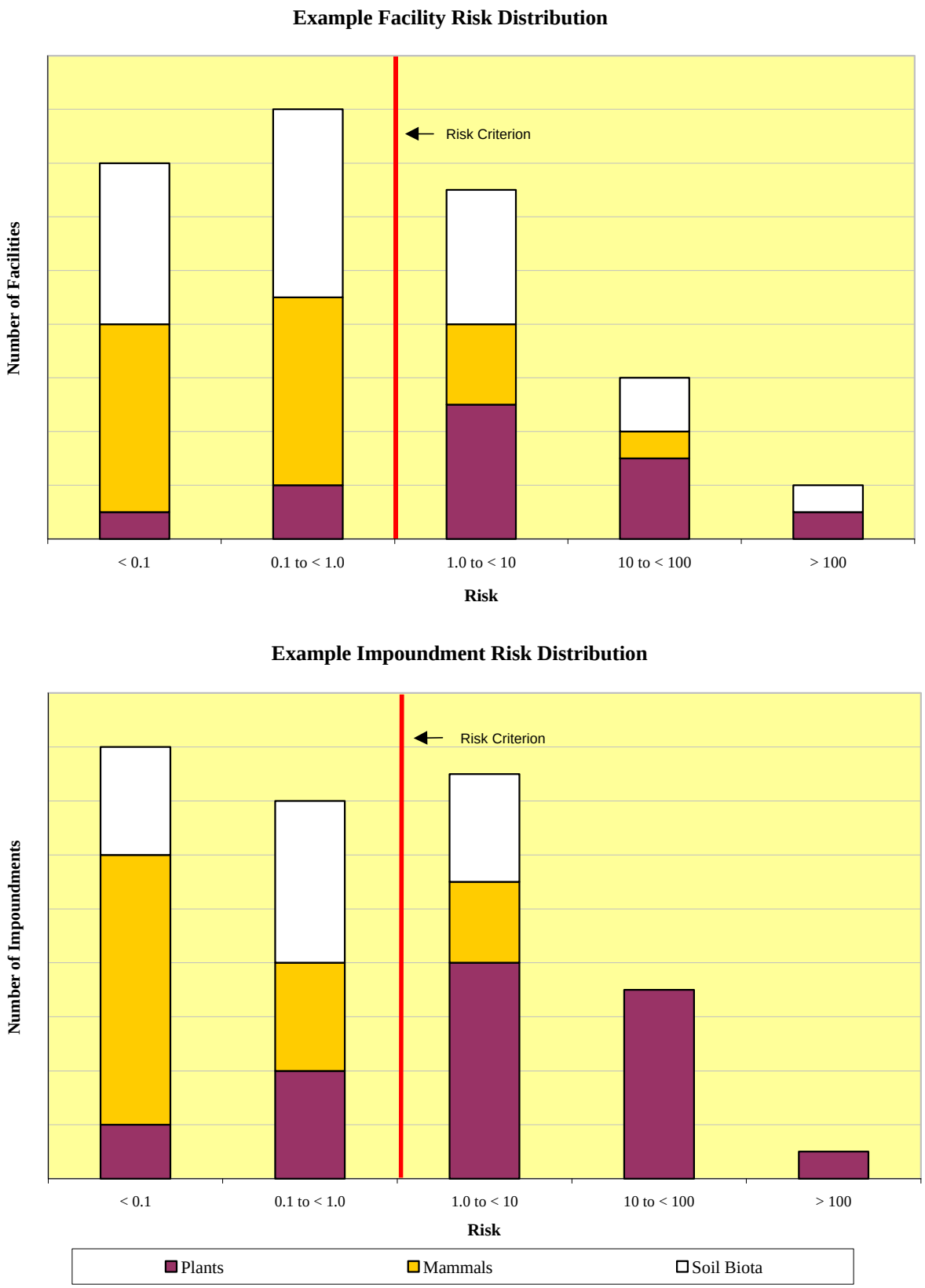


Figure 2-21. Example Phase I ecological screening assessment output.

impoundment increases. In short, it is not possible to determine whether foraging patterns of receptors living in managed areas might include the impoundments at a given facility.

Designated Wetlands. If surface impoundments are located within 1 kilometer of wetlands designated as permanently flooded by the NWI then these surface impoundments and facilities will receive a high priority score for Phase IC. The NWI GIS coverages will provide the data needed to quickly identify surface impoundments within 1 kilometer of a designated wetland. A distance of 1 kilometer is proposed because wetlands near the impoundment are more likely to be influenced through surface water recharge or drainage systems and, as a result, they may be significantly affected by the impoundment.

2.4 Phase IC Initial Prioritization

The Phase IA and IB human health and Phase I ecological risk screening will identify the constituents, impoundments, and facilities that should proceed to Phase II. The screening process, as described in the Phase IA and IB human health and Phase I ecological risk screening (Sections 2.2 and 2.3), defines constituents, impoundments, and facilities that will be considered for proceeding to Phase II analysis as those that have risks greater than the risk decision criteria (risk $\geq 10^{-5}$ and HI ≥ 1). Phase IC provides a method of analyzing the Phase I risk distributions for this subset of constituents, impoundments, and facilities to aid in defining the scope of Phase II given the limited resources of the SI Study. A prioritization scheme is proposed because of concern that the number of constituents, units, and facilities that could move into Phase II will be large (e.g., greater than 25 percent of the study sample) and may exceed the resources allocated for Phase II. If the number of constituents, units, and facilities that could move to Phase II is small and the resulting Phase II effort is within its allocated resources, the prioritization scheme will not be necessary.

2.4.1 Design Goals and Overview

The goal of Phase IC is to prioritize the Phase II analysis of these constituents, impoundments, and facilities. The Phase IC prioritization scheme is based on the risk distributions generated by the Phase I screening analyses. The prioritization scheme consists of five key features:

- Scoring system for facility risks and constituent risks
- Options for combining facility and constituent scores depending on resource limitations
- Separate scores for human health and ecological risks
- Ranking system combining human health and ecological scores
- Prioritization based on a qualitative review of risk distributions for the categories that are of concern to the SI Study (e.g., industry type, treatment type).

Priority will be given to those facilities and constituents with the highest screening risks. Constituents that were not screened in Phase IA and IB because they were considered special cases (e.g., constituents that bioaccumulate) are also given highest priority in the Phase II prioritization scheme.

2.4.2 Approach

The Phase IC prioritization scheme consists of four steps:

- Score facility risks and constituent risks
- Rank facility and constituent scores
- Rank combined human health and ecological scores
- Prioritize based on a qualitative review of risk distributions for the categories that are of concern to the SI Study (e.g., industry type, treatment type).

2.4.2.1 <u>Facility and Constituent Risks Scoring System</u>. The Phase IC prioritization system is based on the Phase IA and IB risk distribution by facility and constituent. The facility risk is the cumulative risk from all constituents and impoundments. For human health, a separate facility risk is provided for both carcinogenic and noncarcinogenic risks for the individual resident. For ecological risk, a single facility risk based on the maximally impacted receptor type is provided. The constituent risk for a facility is the cumulative risk for all impoundments at a facility. For human health, the cumulative risk is a summation of carcinogenic or noncarcinogenic risks by toxic endpoint for the individual resident. For ecological risk, the cumulative risk is the maximum risk from any impoundment for the maximally impacted receptor type. Facility and constituent risk are defined in Sections 2.2 and 2.3.

The risk distributions are risk histograms. For Phase II, only risk bins above the risk decision criteria are of concern. The risk decision criteria are 10^{-5} for excess individual human cancer risk and 1 for human noncancer risk and ecological risk. Each risk bin in the risk histogram that exceeds the risk decision criteria will be given an integer score. A score of 1 is given to the largest numeric risk bin and so forth. The scoring system for both facility risks and constituent risks is shown in Table 2-11.

For example, if a constituent for a facility has a human noncancer hazard index in the $\geq$100 risk bin, then it has a score of 1. If the constituent has a hazard index in the $\geq$10 and <100 risk bin, then it has a score of 2. Finally, if the constituent has a hazard index in the $\geq$1 and <10 risk bin, then it has a score of 3.

If the constituent is considered a human health special case (i.e., a constituent that bioaccumulates), then it receives a score of 1. If the constituent does not receive an ecological score because the risk screening can not be performed due to a lack of suitable toxicity data, then the ecological score is 3.

Table 2-11. Phase IC Prioritization Scoring System

Score	Human Health Individual Excess Cancer Risk Bin	Human Health Noncancer Hazard Index	Ecological Hazard Index
1	$\geq 10^{-4}$	≥ 100	≥ 100
2	$\geq 10^{-5}$ and $< 10^{-4}$	≥ 10 and < 100	≥ 10 and < 100
3	$\geq 10^{-6}$ and $< 10^{-5}$	≥ 1 and < 10	≥ 1 and < 10; NA

NA = Not available.

Human health and ecological risk screening will be scored separately. For human health risk screening, the maximum of the cancer and noncancer risks provides the constituent's score. For ecological risk, the maximum of all receptor types provides the constituent's score.

2.4.2.2 <u>Ranking System for Facility and Constituent Scores</u>. There are currently two options under consideration to rank facilities and constituents:

Option 1: The facility scoring alone will provide the ranking system. The constituent score is not used. This option automatically addresses the issue of cumulative effects of multiple chemicals and multiple impoundments. This approach also recognizes that the resource efforts to set up the modeling evaluation for a facility will be the most resource intensive. Therefore, including all constituents (of all three ranks) will add minimal level of effort to the modeling setup effort.

Option 2: The facility and constituent scores will be combined to provide a single rank. In this option, the constituents that score the highest are given highest priority (see Table 2-12). This option recognizes that some constituents (and impoundments) may constitute more of the facility risk than others. Therefore, the constituent score will be used to prioritize the rank.

2.4.2.3 <u>Ranking System Combining Human Health and Ecological Scores</u>. The Phase 1C ranking will combine the human health and ecological risk scores. The ranking of the nine possible combinations is shown in Table 2-13. This ranking process assumes that the human health score will be the primary ranking factor and the ecological score will be the secondary ranking factor. The ranking system is used only to establish order and priority to our Phase II modeling, not to characterize risks. We expect that high potential risks to ecological receptors will also be captured under this approach; multimedia modeling includes ecological receptors; and prioritization based upon a qualitative review (i.e., special cases) will address high ecological risk scenarios. If resources are limited, then the number of ranks assessed in Phase II could be reduced (e.g., evaluate only Ranks 1 through 5).

Table 2-12. Option 2 Ranking System

Rank	Facility Score	Constituent Score
1a	1	1
1b	2	1
1c	3	1
2a	1	2
2b	2	2
2c	3	2
3a	1	3
3b	2	3
3c	3	3

Table 2-13. Phase IC Ranking System

Rank	Human Health Score	Ecological Score
1	1	1
2		2
3	1	3
4	2	1
5	2	2
6	2	3
7	3	1
8	3	2
9	3	3

2.4.2.4 <u>Prioritization Based on Qualitative Review of Risk Distributions for SI Study Categories</u>. Consideration will also be given to a qualitative review of the Phase IA and IB risk screening distributions for the SI Study categories. The risk distributions may provide interesting conclusions on which EPA may want to focus or reduce attention.

- Example 1: If 95 percent of the risk distribution for a certain industry or treatment type is below the risk decision criteria, then all facilities in the industry or treatment type could be reprioritized with the lowest prioritization **or the industry or treatment type could be omitted entirely** from Phase II. If the same is true for any constituent's risk distribution, then the constituent could be demoted in rank or omitted from Phase II.

- Example 2: If comparison of industry-type risk distributions indicates that a particular industry type (e.g., chemicals and allied products) has a risk distribution that is skewed toward high risks, then facilities that are in that industry type will be given highest priority.

2.4.3 Risk Characterization Outputs

The outcome of Phase IC will be the identification of a subset of surface impoundments, constituents, pathways, and facilities that will be given high priority for further risk characterization during Phase II. The surface impoundments will be profiled according to significant patterns (if any), such as industry type, unit characteristic, and constituent type, using the risk distributions developed during Phase I.

3.0 Phase II Risk Assessment

Phase I of the surface impoundment risk assessment will likely identify a number of units and constituents that need further risk analysis. EPA has designed Phase II to provide that analysis by characterizing risk for constituents, units, and facilities of concern from Phase 1 using state-of-the-science risk assessment models. Phase II will expand the Phase I risk profile of the SI universe based on a true multimedia and multiple exposure pathway model and will take full advantage of site-based data available from the SI Survey results. These data will be supplemented, as necessary and practicable, by site-based, regional, and national data collected using methodologies developed for the Hazardous Waste Identification Rule.

Because of run-time constraints, EPA is considering developing central tendency and high-end risk results during Phase II, with a Monte Carlo analysis conducted as a possible third phase. Thus, EPA still considers Phase II to be a screening analysis. However, the risk estimates generated during Phase II will provide a comprehensive national profile of potential risks posed by the universe of surface impoundments for several reasons:

- It is based on a sample of facilities selected to statistically represent the SI universe.
- It covers the significant exposure pathways and receptors likely to be present at an SI site.
- The potential risks modeled for the major pathways at each site will be based, to the extent possible, on real concentration and exposure data reported by facilities and regions in the survey.
- Because the high-end and central tendency scenarios will be based on real receptors, they will provide a realistic span of potential risks.

The risk profile generated during Phase II will also serve to identify a smaller subset of units and constituents to be characterized, if necessary, using a full Monte Carlo analysis in future analysis.

To develop Phase II risk estimates, EPA has selected the state-of-the-art, multimedia, multiple exposure pathway, multiple receptor risk assessment (3MRA) model it developed for HWIR. This section of the technical plan

- Provides an overview of the Phase II technical framework that summarizes how the risks will be modeled and how the 3MRA modeling system will be implemented (Section 3.1)

- Describes the conceptual model and technical approach for the risk assessment, including sources, exposure pathways, receptors, spatial and temporal scale, and risk benchmarks and metrics (Section 3.2)

- Reviews the modeling system proposed to be used for the Phase II assessment, including summaries of the functionality, inputs, and outputs for each 3MRA component module (Section 3.3)

- Describes modifications to the HWIR 3MRA modeling system and data collection methodologies that may be necessary for SI Study application, including data collection requirements (Section 3.4).

Phase II is based heavily on the HWIR 3MRA model and data collection methodologies; as a result, this writeup depends upon the HWIR 3MRA background documents that are cited throughout. To fully understand the 3MRA model and its many components, the reader is encouraged to review these documents, which may be found at: http://www.epa.gov/epaoswer/hazwaste/id/hwirwste/risk.htm.

3.1 Overview

Phase II of the Surface Impoundment Study risk assessment will include a multimedia, multiple exposure pathway, multiple receptor risk assessment of the management of industrial wastes in surface impoundments. The simulation model EPA selected for this phase is the 3MRA model, which was developed by EPA to support the proposed Hazardous Waste Identification Rule. The 3MRA model provides the core functionality required for the Surface Impoundment Study, including:

- **Spatial scale** - 2-km radius or less

- **Temporal scale** - future risk, extended as needed to capture peak exposure concentrations in media of concern; hourly, daily, monthly, or annual time steps used in specific models as appropriate for source type or exposure pathway

- **Receptors** - human and ecological

- **Exposure pathways** - direct and indirect, including air, surface water, groundwater, soil, and both terrestrial and aquatic food chains

- **Model components** - designed to characterize risk by estimating contaminant release, multimedia fate and transport, exposure, and dose response.

Figure 3-1 shows the Phase II analysis in relation to Phase I.

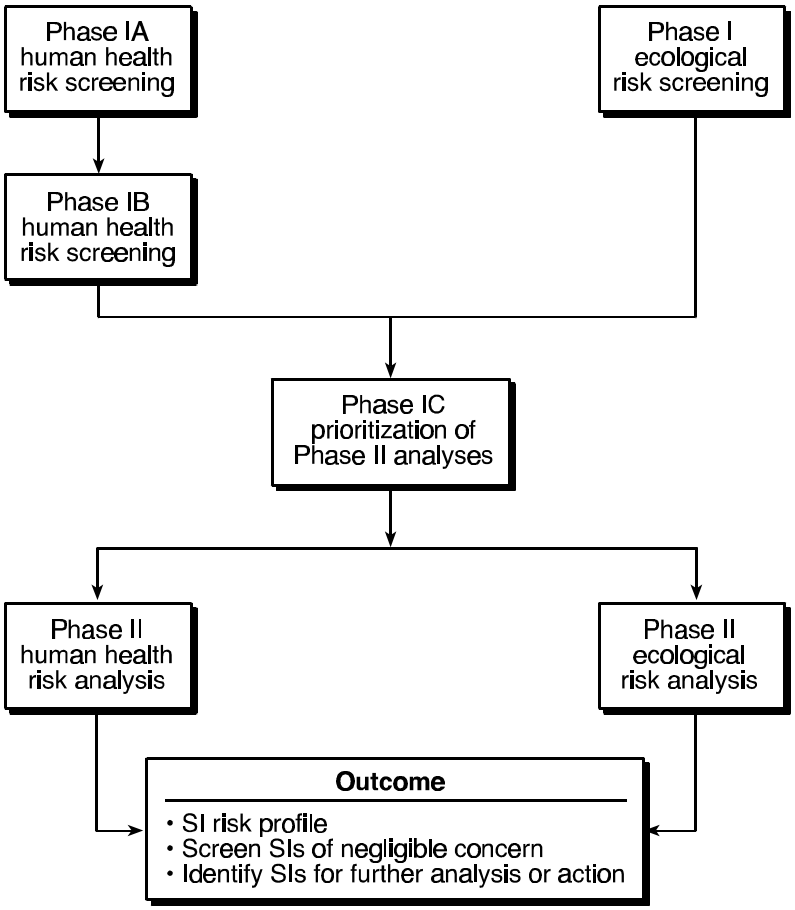


Figure 3-1. Overview of the SI study risk analysis.

3.1.1 Key Features

Key features of human health and ecological risk assessment approach for the SI study include the following.

- Receptor types and exposure pathways are the same as for HWIR (Section 3.2.3).

- Models are the same as for HWIR, except that the SI source module will need specific modifications in use and possibly function to address multiple impoundment, postclosure, and possibly other scenarios (such as catastrophic failures). In addition, the exit level processor (ELP) and 3MRA system will need modification to compile and save risk results in a manner consistent with the study goals (see Sections 3.4.1 and 3.4.2).

- Data collection will begin with the SI survey that will characterize the facilities, units, waste streams, and constituents to be modeled, including receptor locations. HWIR data and data collection methodologies will be applied as needed to supplement these site-specific data with site-based, regional, and national data.

- Modifications to data collection methodologies will be necessary for human receptor placement to update 1990 U.S. Census and land use data with SI Survey, map, and aerial photo data available for each SI site. In addition, modification to HWIR waterbody and watershed delineation methods is recommended to take advantage of newly available hydrography and elevation data sets (see Section 3.4.3).

- Risk metrics will be similar to HWIR (i.e., risk distributions based on risk cumulative frequency distributions [cdfs]), modified as necessary to satisfy SI Study objectives. Concern will be defined by excess cancer risk or HQ above EPA-set action levels (see Sections 3.2.3 and 3.2.4).

- Phase II results will update Phase I risk bins for sites not screened out in Phase I. This will require comparability between phases to be considered during design.

- Two alternative data collection approaches have been developed: representative and site-specific:

  - The representative method uses a limited number of site layouts to represent conditions at a larger number of sites.

  - The site-specific approach develops site layouts for all surface impoundment sites of potential concern.

- Alternatives also exist in terms of necessary modifications to the 3MRA modules and modeling system.

Table 3-1 summarizes options currently envisioned for the alternative approaches to Phase II. The 3MRA will be used for both alternatives; differences in implementation for the second alternative can include changes to the source models and system to better represent SI study objectives and an increase in site-specific resolution for data collection efforts (i.e., all sites represented).

The representative data collection alternative will be needed only if there are a large number of sites to evaluate in Phase II and resources (time or budget) limit the number of site layouts and model revisions that can be developed. Note that because the representative scenarios will be carefully chosen to span the range of conditions reported under the SI Survey, and because the modeling takes advantage of a powerful multimedia model, the results will be more realistic than in Phase I. Still, if undecided between two possible representative scenarios for a given site, EPA intends to choose the one with the more protective assumptions, i.e., the less protective environmental settings.

3.1.2 Decision Methodology

Phase II will follow a similar decision process as Phase I, with facilities routed through Phase II as follows:

Table 3-1. Alternative Stages for Phase II SI Risk Analysis

Activity	Representative Alternative	Site-Specific Alternative
Data Collection	Use representative site layout data, population profiles for a subset of SI Study sites to reflect surface impoundment settings Use existing HWIR regional data for SI Study sites Use SI Survey data as available and practicable.	Collect data and define site layouts for all SI sites Process additional meteorological station data as necessary to cover SI sites. Use SI Survey data as available
Model Revisions	Use 3MRA models "as is" except adjustments to exit level processor to fit SI Study goals/objectives. Model multiple units separately or as mega-units. Model postclosure as land application unit separately for each site.	*(Optional)* Revise SI model and 3MRA system to better fit SI Study goals and objectives. Model revisions could include # Model multiple SIs # Model catastrophic failures # Model postclosure in one run

- Loop over multiple impoundments, multiple chemicals.
- Compare risk against screening criteria.
- Assign facilities, impoundments, and chemicals to risk bins for identifying and prioritizing possible followup activities.

Figure 3-2 pictures the Phase II decision process.

3.1.3 Anticipated Outcome

After the completion of Phase II, the Agency will prepare a report by March 2001 that characterizes the potential risks associated with the SI universe for 256 constituents. This report will include

- Identification of any constituents, unit types, or facility categories for which additional comprehensive analysis may be needed.
- A profile of risks for the SI universe by unit type, industry type, and constituent.
- A descriptive profile of the subset of the universe that is of negligible concern and requires no further risk analysis.

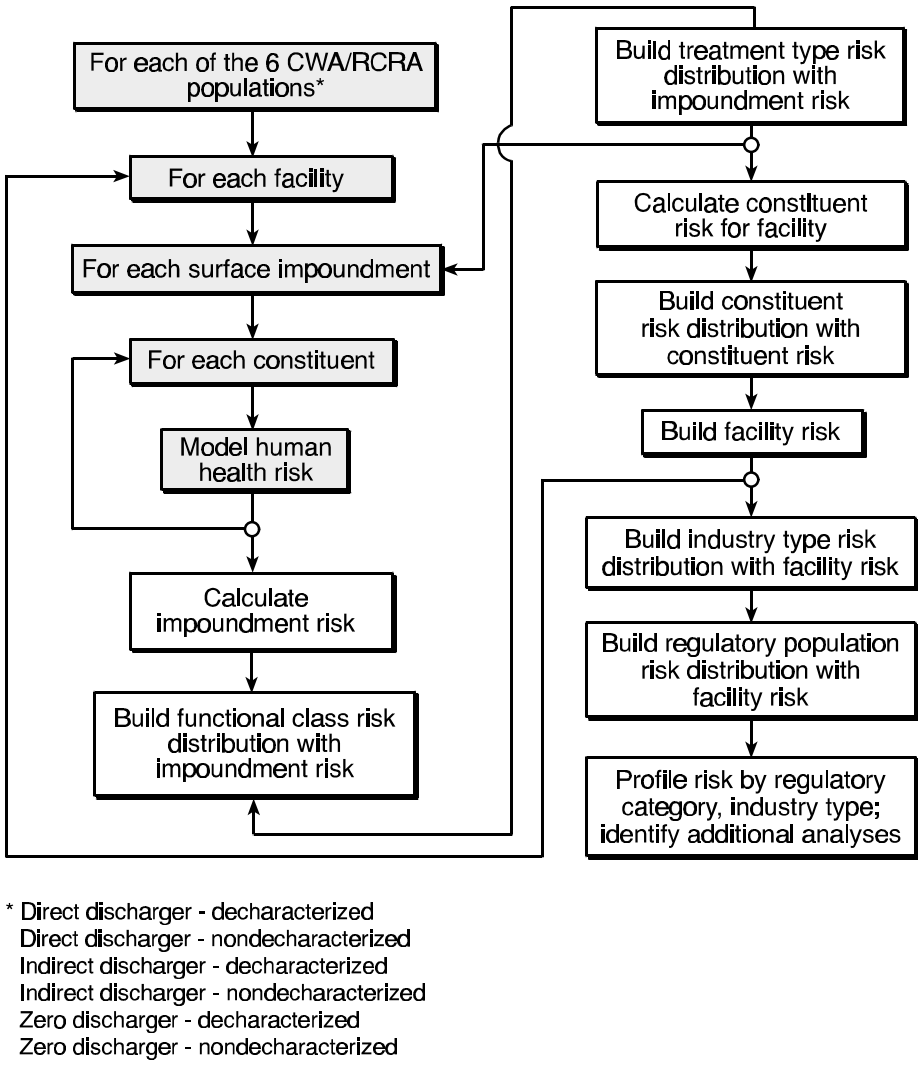


Figure 3-2. Phase II decision process.

Recommendation for additional analysis for the remaining facilities that show significant risks.

The Phase II analysis is designed to provide the risk information necessary to formulate these profiles and risks.

3.2 Conceptual Model and Approach

The approach to conducting the SI Study risk assessment begins with the conceptual model of a surface impoundment site. Figure 3-3 diagrams this conceptual model for human exposure, beginning with the multimedia release of chemicals from a surface impoundment, both during its active life and following closure. Once released, the chemicals travel through environmental media that define the exposure pathways for the analysis: air, vadose zone and groundwater, watershed, and surface water. In addition, plants and animals take up the chemicals

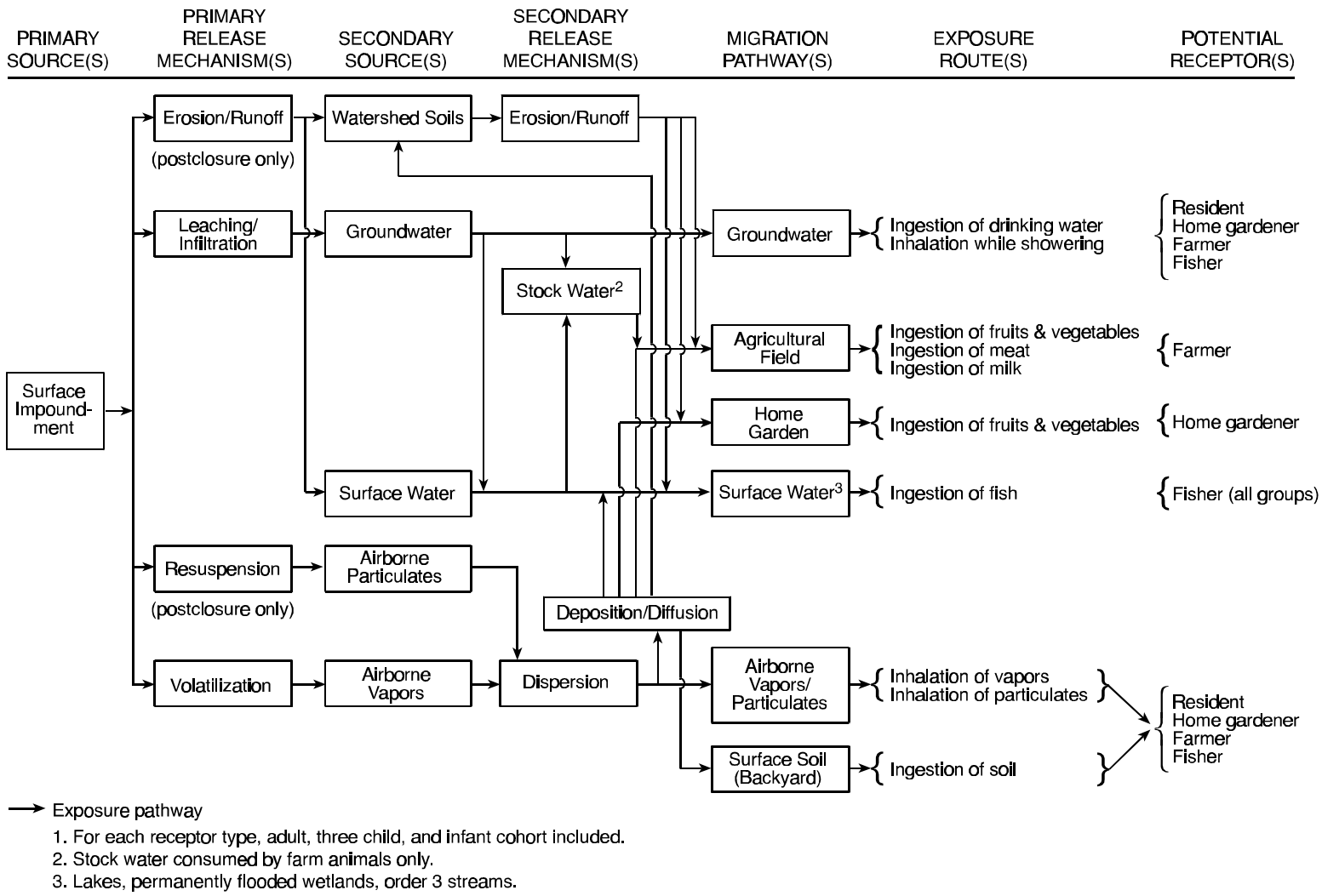


Figure 3-3. Conceptual exposure model for human receptors.

either directly from the different fate and transport media or by bioaccumulation of chemicals in terrestrial and aquatic food webs. Eventually, human and ecological receptors are exposed to chemicals in the environment as a result of inhalation or ingestion of contaminated media and/or biota.

Human receptor types considered in the SI Study include residents, gardeners, farmers, and fishers, each divided into five age cohorts. The conceptual model diagram (Figure 3-3) shows the exposure pathways for each type of receptor. For example, the exposure pathways that will be evaluated for an adult resident include ingestion of soil and groundwater and inhalation of airborne vapors and particulates. Contaminated foodstuffs are considered only for resident gardeners and farmers.

The ecological risk assessment provides descriptions of risk to representative wildlife species in representative habitats. The ecological receptor types include plants, invertebrates, amphibians, reptiles, birds, and mammals. The conceptual exposure model demonstrating the environmental exposure pathways for each type of ecological receptor is shown in Figure 3-4. For example, the exposure pathways that will be evaluated for a mammal include ingestion of soil, water, and terrestrial food items.

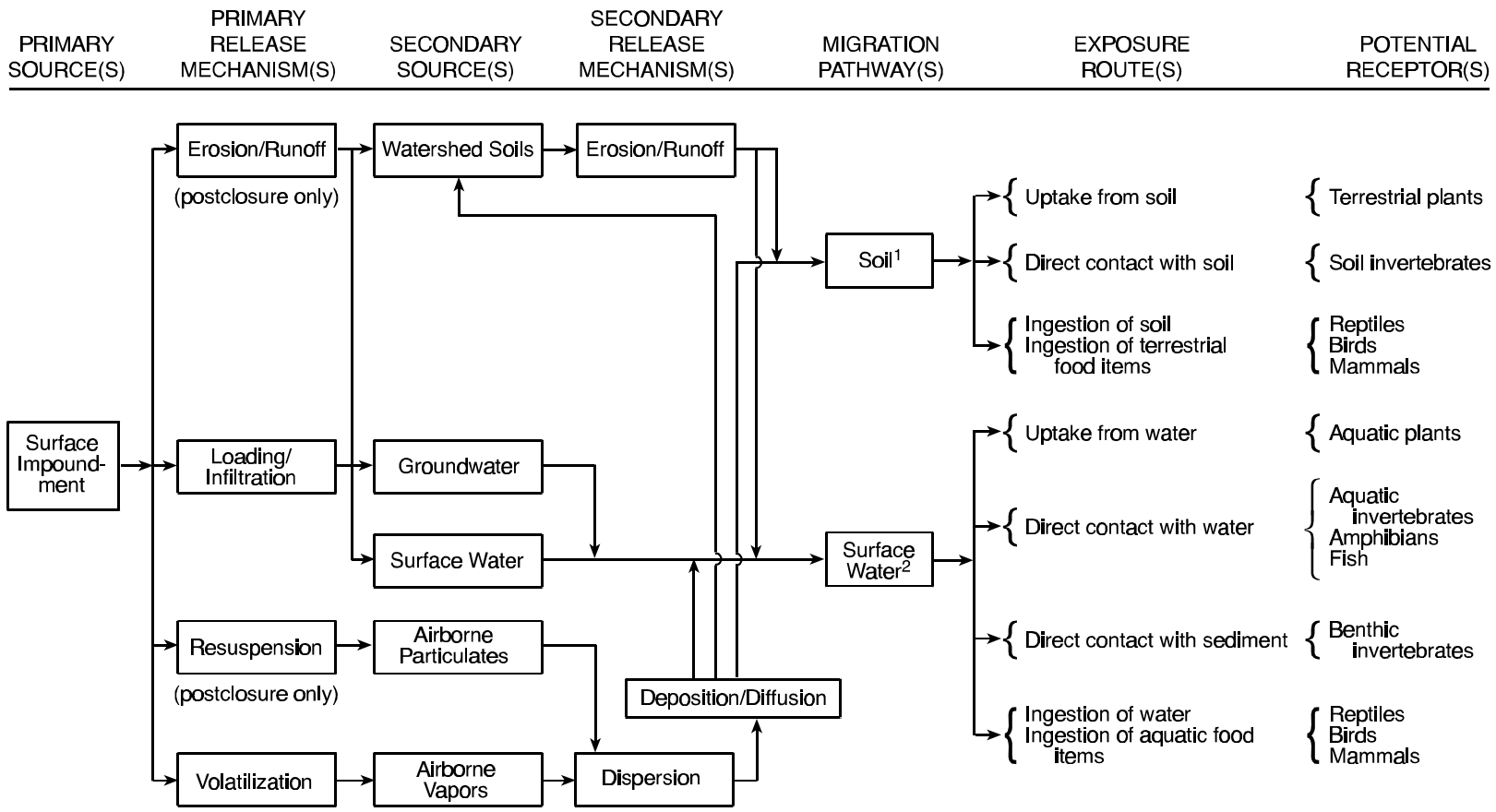
Figure 3-5 itemizes the dimensions of the 3MRA as it will be implemented to address the SI Study conceptual model. These dimensions include 11 major categories:

- Chemicals addressed
- Source type (i.e., surface impoundment)
- Source term characteristics
- Source release mechanisms
- Transport media
- Fate processes
- Intermedia contaminant fluxes
- Food chain/food web components
- Receptors and habitats
- Exposure pathways
- Human and ecological risk measures.

These categories characterize the Phase II analysis that will provide a state-of-the-art representation of risks. A more detailed overview of the 3MRA model, including each component module and its conceptual basis, is provided in Section 3.3 and the HWIR background documents referenced therein.

3.2.1 Spatial Scale and Layout

Phase II of the SI Study will adopt the same spatial scale and site layout framework as used for the HWIR 3MRA. The area of interest (AOI) for the analysis is defined by a 2-km radius from the corner of a square surface impoundment (Figure 3-6). This distance was determined to encompass the area of greatest risk for the air and groundwater pathways. In addition, concentric



→ Complete pathway (evaluated)

Notes:

1. If intermittently flooded wetland, hydric-soil invertebrates are included.
2. If intermittently flooded wetland, aquatic invertebrates and fish are not included.

Figure 3-4. Conceptual exposure model for ecological receptors.

Chemicals
- Organic chemicals (227)
- Metals (17)
- Nonmetallic inorganic chemicals (8)

Source Type
- Surface impoundment (operating and postclosure)

Source Term Characteristics
- Mass balance
- Multiphase partitioning
- First-order degradation
- Source depletion

Source Release Mechanisms
- Volatilization
- Leaching
- Runoff (postclosure, surface failure)
- Erosion (postclosure, surface failure)
- Particle resuspension (postclosure)

Transport Media
- Atmosphere
- Watershed
- Vadose zone/Groundwater
- 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

Source	→	Air (volatilization, resuspension)
Source	→	Vadose zone (leaching)
Source	→	Local watershed soil (erosion, runoff)
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	→	Groundwater (infiltration)
Watershed soil	→	Air (volatilization)
Groundwater	→	Surface water

Food Chain/Food Web Fluxes

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

Receptors and Habitats

Ecological Habitats:
- Terrestrial
- Freshwater aquatic

Human Receptors*:
- Resident
- Home gardener
- Dairy farmer
- Beef farmer
- Fisher**

Ecological Receptors:
- Plants
- Invertebrates
- Amphibians
- Reptiles
- Birds
- Mammals

*For each human receptor type, consider 5 age cohorts
**All receptor types can be fishers.

Exposure Pathways

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

Ecological
- Ingestion (plant, animal, water, soil)
- Direct contact (surface water, sediment, soil)

Human And Ecological Risk Measures
- Cancer (risk probability)
- Noncancer (hazard quotient)
- Human: population
- Ecological: population

Figure 3-5. Dimensions of the 3MRA conceptual model for surface impoundments.

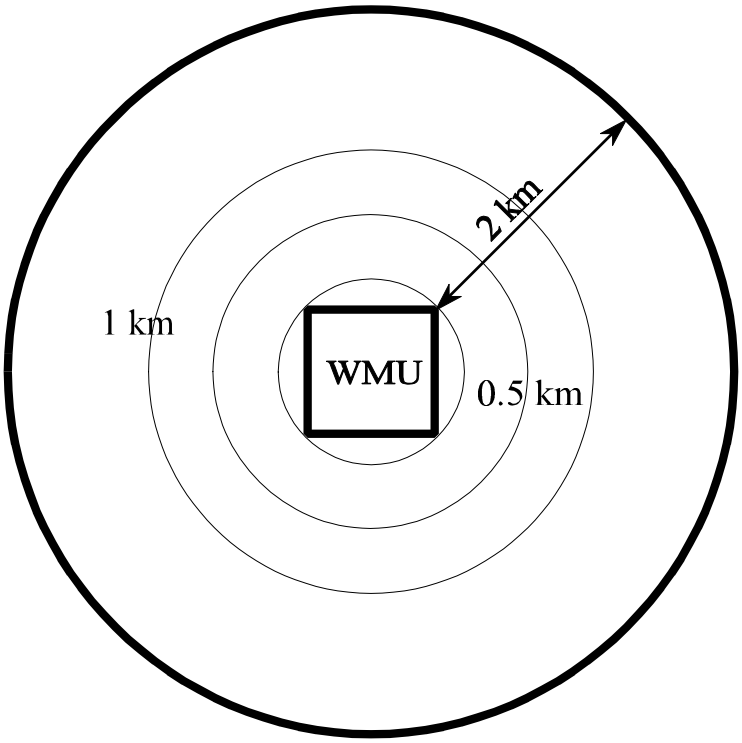


Figure 3-6. Area of interest (AOI) and risk rings for SI Study 3MRA.

risk rings are defined within the 2-km radius (Figure 3-6) to provide additional spatial resolution for the risk results:

- Humans risks are totaled within the 0 to 0.5 km, 0.5 to 1 km, and 1 to 2 km distances from the edge of the SI.

- Ecological risks are totaled with the 0 to 1 km, 1 to 2 km, and 0 to 2 km distances from the edge of the surface impoundment.

Human and ecological risk results will be tracked and maintained for each of these risk rings within the AOI to provide information on the distribution of risk with distance from the SI.

Another important determinant of the spatial scale of the analysis is the size of watershed subbasins delineated across the 2-km AOI. For the 3MRA model, 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 the site, the size of the subbasins subdividing these watersheds is defined during watershed delineation. Currently, these are defined in 3MRA so that there are generally about 10 to 12 watershed subbasins within the AOI at a site, with an average subbasin area of about 1 million

square meters within the AOI (Figure 3-7).[1] This provides adequate spatial resolution to map soil concentration gradients across the site while keeping the total number of watersheds at a given site to a reasonable number from a run-time perspective. This decision could be revisited when watersheds are delineated at the SI sites.

The spatial resolution is also limited by the resolution of the underlying data (topographic, waterbodies, land use, soils) used in the site-based data collection process. Because many of these data sources (i.e., topographic, land use, soils) have a scale of 1:250,000, that scale was used to define a minimum resolution for the coordinate system used to pass spatial data from the geographic information system (GIS) data sources to the 3MRA model. Figure 3-8 shows how the site grid system, based on 100 m × 100 m grid cells, defined the data resolution used to pass watersheds, waterbodies, farms, and ecological habitats.

In HWIR, human receptor locations at a site are defined by the centroids of 1990 U.S. Census blocks or by the ring/block centroid where the blocks cross a risk ring. Figure 3-9 illustrates human receptor locations at a typical HWIR site. Note that the density of receptor points will vary with population density because census blocks are sized by the population they contain. Because some site-specific receptor location data will be available from the SI Survey results, there may be a need to modify receptor point placement for SI sites. There also may be onsite receptors placed within the SI after closure, a scenario not addressed in HWIR. These issues are discussed in Section 3.4 along with other modifications to the HWIR data collection methodologies.

Ecological habitats are defined in the 3MRA primarily by land use and waterbody coverages (see U.S. EPA, 1999n, for description of the habitat delineation methodology). Four receptor home range bins are placed within each habitat in an overlapping fashion, with receptors assigned to the appropriately sized home range bin. Figure 3-10 illustrates a typical habitat and home ranges. This approach will likely be used “as is” to place ecological receptors around the SI Study sites.

3.2.2 Temporal Scale, Frame, and Integration

The SI Study considers in-scope impoundments to be those in active operation on or after June 1, 1990. Selection of this date ensures that the study will be limited to wastes managed according to practices that have become more commonplace in recent years. Therefore, the study will evaluate the release of in-scope constituents starting from June 1, 1990, through the remainder of its active lifetime and, if appropriate, for the postclosure lifetime of the impoundment.

3.2.2.1 <u>Model Temporal Scale</u>. 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

[1] Note that some watershed subbasins extend outside of the AOI in Figure 3-7 to capture the entire drainage area for each watershed draining into the AOI. This is necessary to calculate accurate runoff and solids loads for the 3MRA surface water module.

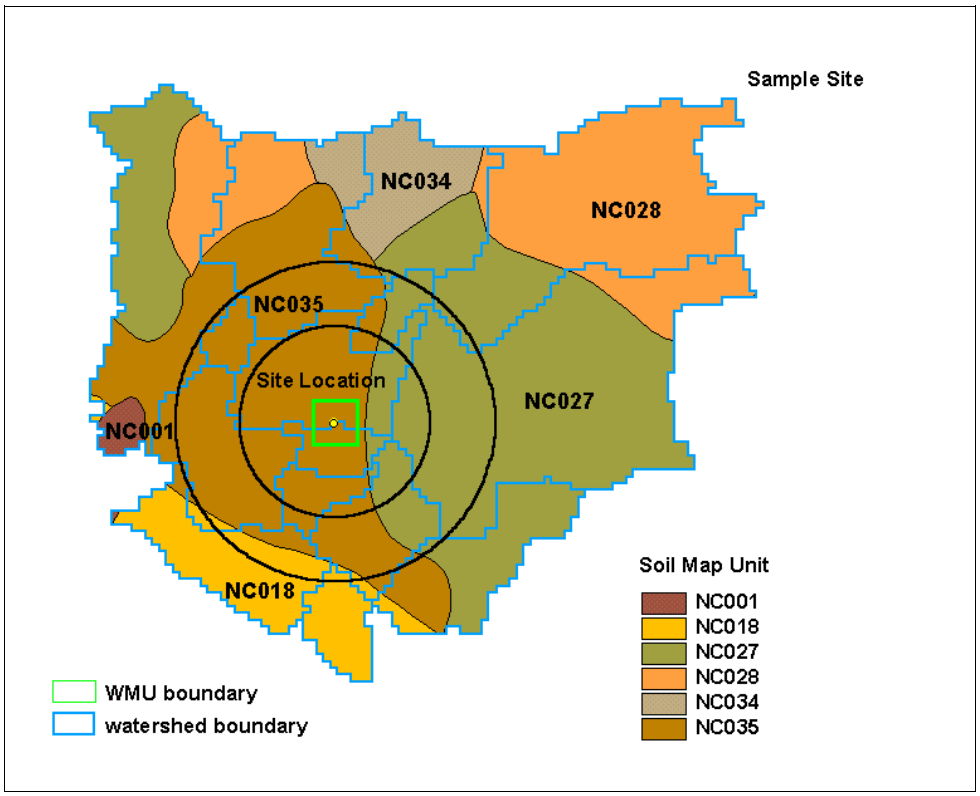


Figure 3-7. Typical watershed layout for HWIR 3MRA.

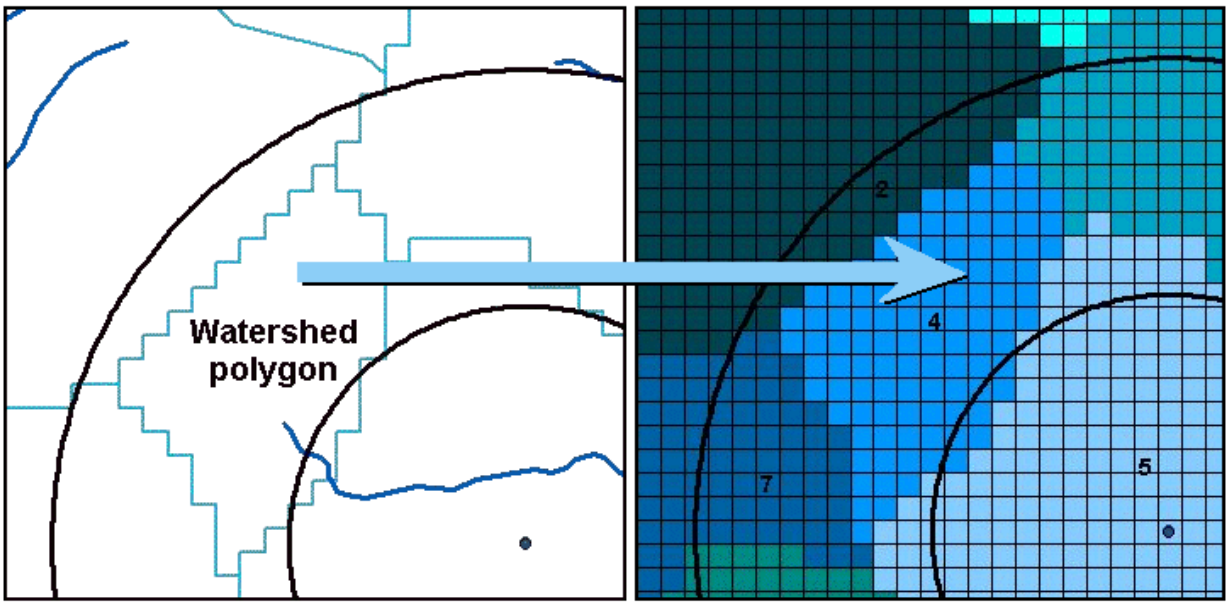


Figure 3-8. Transfer of watershed polygons to 100- by 100-m template grid.

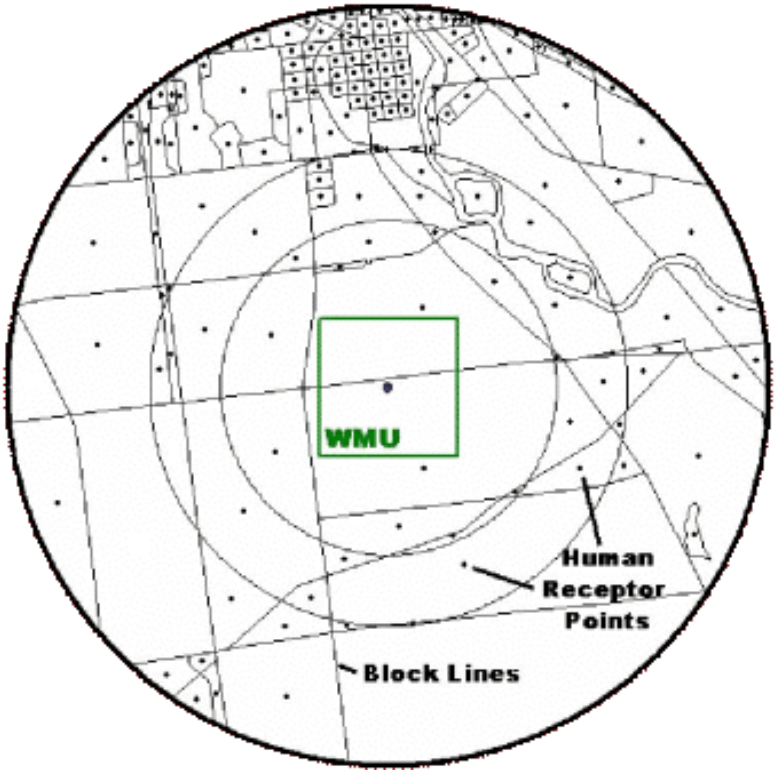


Figure 3-9. Example human receptor placement for HWIR 3MRA.

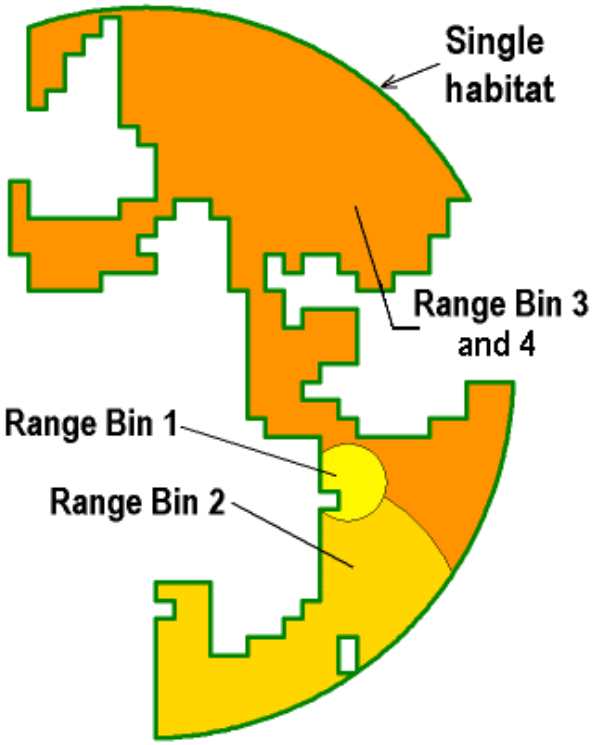


Figure 3-10. Example ecological habitat and home range bins.

Table 3-2. Meteorological Data Time Scales, by 3MRA Model Module

3MRA Module	Hourly	Twice Daily	Daily	Monthly	Annual	Long-term
Surface impoundment				!		
Land application unit			!	!	!	!
Air	!	!				!
Watershed			!	!		!
Surface water						!

what is appropriate for modeling objectives. This is reflected by which type of meteorological data each module reads, shown in Table 3-2. Reasons for departures from annual average conditions include the need for shorter time scales to accurately estimate release or fate and transport in media sensitive to fluctuations in meteorological data. For example, the surface impoundment module needs monthly data to capture temperature extremes that can impact volatilization. The land application unit (LAU)[2] and watershed modules require daily precipitation data to accurately estimate precipitation-driven runoff and erosion events.

3.2.2.2 <u>Study Time Frame</u>. The study time frame for exposure and risk depends on the migration times of the 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 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 study time frame, therefore, varies for each chemical and environmental medium considered for each specific facility and impoundment. A maximum time limit for considering exposure and risk is defined as 5,000 years. This should capture the significant impacts of most chemicals included in the analysis.

3.2.2.3 <u>Temporal Integration</u>. 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. Figure 3-11 illustrates how risks of different time periods will be overlaid and aggregated across exposure pathways for a given receptor and constituent. Note that risks will be aggregated across different exposure routes (i.e., ingestion, inhalation) only after considering current EPA practices for route-to-route extrapolation. In general, combining pathways and routes involves the following considerations:

[2] The LAU module is being used to model a postclosure surface impoundment; see Section 3.3.1.

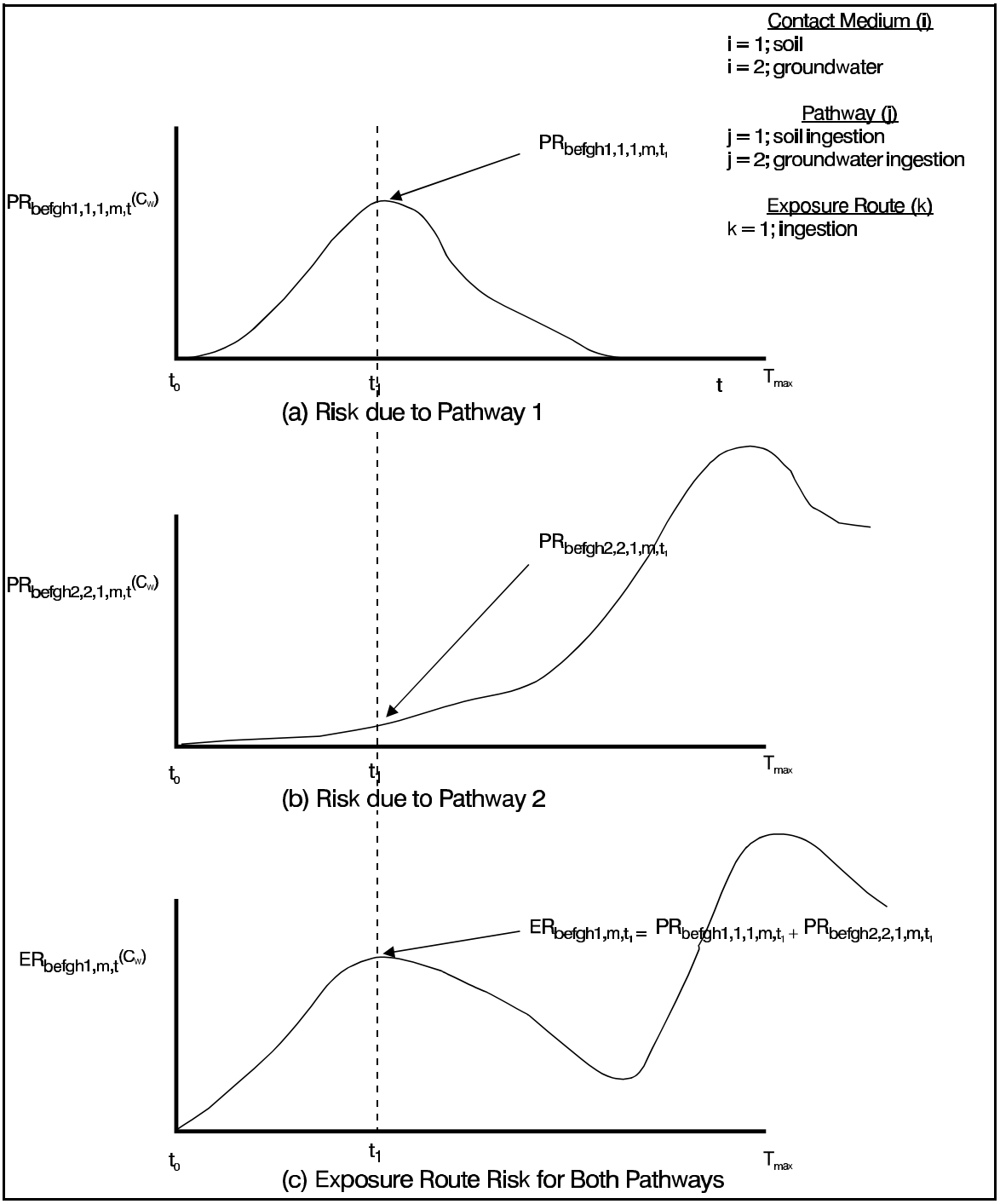


Figure 3-11. Illustration of concurrent time aggregation of risks.

Source: U.S. EPA (1999aa).

- Pathway-specific benchmarks
- All ingestion pathways combined
- All inhalation pathways combined
- Results flagged in database if oral and inhalation routes could be combined
- Cancer risk and hazard quotients not combined.

Once risk estimates are integrated temporally, the 3MRA human risk module determines and outputs that critical year, T_{crit}, during which the maximum cumulative risk and/or hazard quotient occurs across the population for each receptor/cohort combination and for each exposure pathway and pathway aggregation. This process involves adding receptors across all risk bins for each year of the analysis to calculate total risk/hazard for each period. The year with maximum total risk/hazard is T_{crit}. Types of outputs at T_{crit} include population-weighted risk or hazard quotient.

T_{crit} is determined by the following steps:

1. Calculate total risk/hazard for each period

2. Find period with maximum total risk/hazard

   - by nine exposure pathways

     - by route (ingestion or inhalation) or
     - by combined routes

   - by distance (3 risk rings)

   - by four receptor types

   - by five age cohorts.

T_{crit} is determined in a similar fashion in the ecological risk module for receptor types, groups, and distances. An example of a simple T_{crit} determination is shown in Figure 3-12.

3.2.3 Human Health

Example of 2-year analysis with T_{crit} = year 2

	Bin 1 $<10^{-8}$	Bin 2 10^{-8} - $<10^{-7}$	Bin 3 10^{-7} - $<10^{6}$	Bin 4 10^{6} - $<10^{-5}$	Bin 5 10^{-5} - $<10^{-4}$	Bin 6 10^{-4} - 1	Total	
Year 1	10	10	10	10	10	10	5.5E-3	
Year 2	0	0	0	20	20	20	1.1E-2	(T_{crit})

Figure 3-12. Finding T_{crit} (year with maximum risk).

The human health risk assessment (HRA) will evaluate the potential for adverse human health effects that may occur as a result of chemical releases at the surface impoundments investigated as part of the study. The results of the HRA will be used to assess the potential risks associated with the impounded wastes. The HRA for the SI Study is designed to be consistent with EPA guidance (U.S. EPA, 1989, 1991a, 1992c, 1997d, in press) and consists of the following components:

- Identification of chemicals of potential concern
- Identification of potential human receptors
- Assessment of exposure
- Assessment of chemical toxicity
- Characterization of risk
- Analysis of sources of uncertainty in the predicted risk estimates.

3.2.3.1 <u>Chemicals of Potential Concern</u>. Chemicals of potential concern (COPCs) are those identified in the environment that may cause adverse health effects in exposed individuals. The general types of COPCs identified within the scope of the SI Study are listed in Figure 3-5 and include:

- 227 organic chemicals
- 17 metals
- 8 nonmetallic inorganic chemicals
- 4 other.

EPA will select the final list of COPCs based on the results of the SI Survey (i.e., chemicals detected in the SI wastes) as well as policy and regulatory concerns (e.g., the three specific target chemicals beryllium, 1,1,2-trichloroethane, 1,1,2,2-tetrachloroethane). In addition, the Phase II analysis will address only those chemicals that were not screened out in the Phase I analysis.

3.2.3.2 <u>Human Receptor Types</u>. 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 will be used in conjunction with the SI Survey results to identify receptor types and populations that are potentially exposed in the AOI for each SI site. Receptor types and age cohorts to be evaluated using 3MRA are shown in Table 3-3.

EPA risk assessments are expected to address or provide descriptions of individual risk to important subgroups of the population such as highly exposed or highly susceptible groups or individuals, if known. EPA plans to evaluate the risk burden carried by different subgroups of the exposed population, with particular concern over the potentially disproportionate risks to children and subsistence populations (e.g., Native Americans who rely on indigenous fish species as a major portion of their diets) in the study area. EPA believes that these concerns will exhibit themselves on a site-specific basis and plans to address such risk in separate, site-specific analyses.

Table 3-3. Matrix of Human Receptor Types and Age Cohorts[a]

Receptor Type	Age Cohort				
	Infant[b]	**Child (1-5)**	**Child (6-11)**	**Child (12-19)**	**Adult**
Resident[c]	✓	✓	✓	✓	✓
Home gardener[c]	✓	✓	✓	✓	✓
Beef farmer	✓	✓	✓	✓	✓
Dairy farmer	✓	✓	✓	✓	✓
Fishers[d]	✓	✓	✓	✓	✓

[a] There is no overlap between receptor types or age cohorts (unique sets).

[b] Infant is less than 1 year old and is evaluated only for dioxin-like compounds in breast milk.

[c] May include onsite future resident for time periods after closure of an impoundment.

[d] Fishers defined for all four receptor types: resident, home gardener, beef farmer, dairy farmer, and across noninfant age cohorts.

3.2.3.3 <u>Human Exposure Pathways</u>. The human exposure assessment will estimate the type, timing, and magnitude of exposures that receptors may experience due to contact with the chemicals of potential concern (these exposures are calculated using the human exposure module, which is described in Section 3.3.9). Exposures will be evaluated for potentially complete exposure pathways. An exposure pathway describes the course that a chemical 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 that was released from the source of concern (in this case, a surface impoundment).

Exposure routes include uptake mechanisms such as ingestion, dermal contact, and inhalation. When modeling human exposure, the exposure routes that will be 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 impoundment
- Inhalation of particulate emissions from sludge (postclosure in place)

- Indirect exposure through ingestion of produce (gardeners, farmers) and meat and dairy (farmers only) contaminated from air deposition or sludge erosion/runoff to soil and subsequent plant uptake and consumption

- Indirect exposure (all recreational fishers) through ingestion of T3 and T4 fish contaminated through the aquatic food web from air deposition onto or sludge erosion/runoff into surface waterbodies surrounding each SI.

These routes define the exposure media to be modeled in the risk analysis (i.e., groundwater, soil, air, vegetables, meat, dairy products, and fish). OSW considered the inclusion of dermal routes of exposure but decided that health benchmarks for dermal toxicity derived from oral toxicity studies are not sufficiently developed at this time for use in analyses that could support regulatory decisions and, therefore, has decided not to include dermal exposure routes.

The exposure pathways and routes that will be evaluated for each receptor type at each site are shown in Table 3-4. These pathways were previously pictured in the conceptual model diagram (Figure 3-3) for human receptors. Residents are exposed to some level of contaminant in the air (inhalation) and the soil (incidental ingestion) and are assumed to be exposed to potentially contaminated groundwater (inhalation and ingestion) if the house is not on 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 contaminated dairy products (depending on the type of farms present at a site). Recreational fishers are any of the above receptors with the added pathway of eating contaminated fish from local streams or lakes. Thus, some fraction of residents, home gardeners, and farmers also are fishers.

As shown in Figure 3-3, a receptor may be exposed simultaneously via multiple pathways, each involving different combinations of contact media and exposure routes. The human exposure model component will aggregate 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 provide estimates of total exposure for the eight routes listed above. Because human health benchmarks are pathway-specific, pathways and routes are combined in the analysis as follows in the 3MRA model:

- All ingestion pathways are combined.
- All inhalation pathways are combined
- Flag placed in database if oral and inhalation routes could be combined.
- Cancer risk and hazard quotients are not combined.

The evaluation of human exposure must include evaluation of spatial variability 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 HWIR, these age cohort-specific distributions were derived from percentile data for contact rates, body

Table 3-4. Human Exposure Pathways by Receptor Type

	Receptors (as output by Human Risk Module)							
	Resident	**Resident Gardener**	**Fisher**				**Farmer**	
	Receptors (as output by Human Exposure Module)							
Pathway	**Resident**	**Resident Gardener**	**Resident Fisher**	**Resident Gardener Fisher**	**Beef Farmer Fisher**	**Dairy Farmer Fisher**	**Beef Farmer**	**Dairy Farmer**
Air inhalation	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Shower air inhalation	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Soil ingestion	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Water ingestion	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Crop ingestion	No	Yes	No	Yes	Yes	Yes	Yes	Yes
Beef ingestion	No	No	No	No	Yes	No	Yes	No
Milk ingestion	No	No	No	No	No	Yes	No	Yes
Fish ingestion	No	No	Yes	Yes	Yes	Yes	No	No

weight, etc. in the *Exposure Factors Handbook* (U.S. EPA, 1997b), as described in U.S. EPA (1999v). Exceptions include fixed values assumed for exposure duration (9 years for carcinogens, 1 year for noncarcinogens), and medium or food-specific estimates of fraction contaminated.

Lead exposures and risk evaluations will differ from those used with other exposure pathways. This set of evaluations will be developed as a separate model because EPA (FR 56[110]:26460-26564) evaluates lead exposures in terms of potential blood lead (Pb) concentrations (μg/dL-blood) rather than as intake or absorbed doses (i.e., μg/kg-d). The reasons for using this different protocol are discussed in Section 3.2.3.4.

3.2.3.4 <u>Human Health Effect Benchmarks</u>. The health effect benchmarks that will be used in the human health risk assessment are chemical- and exposure pathway-specific and include

Cancer Risk

- Oral cancer slope factor
- Inhalation cancer slope factor

Noncancer (Toxic) Effects

- Oral reference dose (RfD)
- Inhalation reference concentration (RfC).

The Agency has a comprehensive human health benchmark database to support risk assessment projects, which will be used to populate the SI Study database and is based on the following sources, listed in order of preference:

- Integrated Risk Information System (IRIS)
- Health Effects Assessment Summary Tables (HEAST)
- EPA-approved toxicity equivalency factors (TEFs)
- Superfund Technical Support Center Provisional Benchmarks
- Various EPA criteria documents.

When benchmarks are not available from the above sources, alternative sources include the following:

- Agency for Toxic Substances and Disease Control (ATSDR) minimal risk levels (MRLs)

- California Environmental Protection Agency (CalEPA)

- Interim benchmarks developed from primary scientific literature.

Each of these sources is briefly reviewed below.

IRIS is EPA's electronic database containing information on human health effects (U.S. EPA, 1999s). Each chemical file contains descriptive and quantitative information on potential health effects. Health benchmarks for chronic noncarcinogenic health effects include RfDs and RfCs. Cancer classification and oral and inhalation CSFs are included for carcinogenic effects. IRIS is the official repository of Agency-wide consensus of human health risk information.

HEAST is a listing of provisional noncarcinogenic and carcinogenic health toxicity values (RfDs, RfCs, and CSFs) derived by EPA (U.S. EPA, 1997c). Although the health toxicity values in HEAST have undergone review, they have not been updated in several years and do not represent Agency-wide consensus information.

Cancer slope factors for some dioxin-like compounds and polychlorinated aliphatic hydrocarbons (PAHs) were calculated by using the TEF approach. For the TEF approach, the toxicity of a group of chemically related constituents that typically occur in the environment as mixtures is based on estimates of the toxic potency of each constituent as compared with a reference compound within the group. TEF estimates are based on a knowledge of the mechanism of action, available experimental data, and other structure-activity information. TEFs have been established for a number of polychlorinated dibenzodioxins, polychlorinated dibenzofurans, and polychlorinated biphenyl (PCB) congeners thought to have dioxin-like

toxicity (Ahlborg et al., 1994; U.S. EPA, 1998d). TEFs for several PAHs also have been established (U.S. EPA, 1993b).

The Superfund Technical Support Center (U.S. EPA, National Center for Environmental Assessment or NCEA) derives provisional RfCs, RfDs, and CSFs for certain chemicals. These provisional health benchmarks can be found in Risk Assessment Issue Papers. These provisional values have not undergone EPA's formal review process for finalizing benchmarks, and do not represent Agency-wide consensus information.

EPA has also derived health benchmark values in other risk assessment documents such as Health Assessment Documents (HADs), Health Effect Assessments (HEAs), Health and Environmental Effects Profiles (HEEPs), Health and Environmental Effects Documents (HEEDs), Drinking Water Criteria Documents, and Ambient Water Quality Criteria Documents. Evaluations of potential carcinogenicity of chemicals in support of reportable quantity adjustments were published by EPA's Carcinogen Assessment Group (CAG) and may include cancer potency factor estimates. Health toxicity values identified in these EPA documents are usually dated and are not recognized as Agency-wide consensus information or verified benchmarks, however.

The ATSDR minimal risk levels are substance-specific health guidance levels for noncarcinogenic endpoints. An MRL is an estimate of the daily human exposure to a hazardous substance that is likely to be without appreciable risk of adverse noncancer health effects over a specified duration of exposure. MRLs are derived for acute, intermediate, and chronic exposure durations for oral and inhalation routes of exposure. Inhalation and oral MRLs are similar to EPA's RfCs and RfDs, respectively; however, MRLs are intended to serve as screening levels.

CalEPA has developed cancer potency factors for chemicals regulated under California's Hot Spots Air Toxics Program (CalEPA, 1999a). The cancer potency factors are analogous to EPA's oral and inhalation CSFs. CalEPA has also developed chronic inhalation reference exposure levels (RELs), analogous to EPA's RfC, for 120 substances (CalEPA, 1999b). CalEPA used EPA's 1994 inhalation dosimetry methodology in the derivation of inhalation RELs. The cancer potency factors and inhalation RELs have undergone internal peer review by various California agencies and have been the subject of public comment.

Appendix B provides a comprehensive list of EPA and non-EPA benchmarks available for the 256 SI study constituents. At least one benchmark was available from EPA sources for all but the following 25 constituents:

#	Ammonium perchlorate	#	Cyclohexanol
#	Ammonium vanadate	#	tris(2,3-Dibromo propyl)phosphate
#	Chloral hydrate	#	cis-1,3-Dichloropropylene
#	Chlordecone	#	trans-1,3-Dichloropropylene
#	Chloromethyl methyl ether	#	7,12-Dimethyl benz[a]anthracene
#	Copper	#	Dimethylphthalate
#	Cresol mixtures	#	Ethyl methanesulfonate
#	Cyanide (total)	#	Fluoride

- Lead and compounds
- 3-Methyl cholanthrene
- N-Nitrosopiperidine
- Perchlorate
- Safrole
- Styrene-7,8-oxide
- Sulfide
- Thallium
- p-Xylene

Possible benchmark options for several of these constituents are discussed in the remainder of this section.

Alternatives for addressing constituents without EPA benchmarks include omitting them from the quantitative risk assessment, using provisional benchmarks from other sources (e.g., ATSDR, CalEPA), or estimating benchmarks (for screening purposes) if suitable toxicological data are available.

EPA considers that, for a screening-level analysis, it is appropriate to identify or develop and use draft provisional benchmarks where necessary. For 9 of the chemicals listed above, IRIS benchmarks for similar chemicals could be used as their benchmarks. The rationale for these chemicals is as follows:

- Chloral hydrate could be based on chloral. The IRIS RfD for chloral (2E-03 mg/kg-d) was based on a study that used chloral hydrate.

- Chloromethyl methyl ether could be based on bischloromethylether. The IRIS file for chloromethyl methyl ether states that the risk is not likely to be greater than for bischloromethylether (a contaminant of chloromethyl methyl ether). The CSF for bischloromethylether is 220 $(mg/kg\text{-}d)^{-1}$ and the URF is 6.2E-02 $(\mu g/m^3)^{-1}$.

- cis-1,3-Dichloropropylene and trans-1,3-dichloropropylene could be based on 1,3-dichloropropene. The studies cited in the IRIS file for 1,3-dichloropropene used a technical-grade chemical that contained about a 50/50 mixture of the cis- and trans-isomers. The RfD is 3E-04 mg/kg-d and the RfC is 2E-02 mg/m^3.

- Cresol mixtures could be based on m-cresol. Cresol mixtures contain all three cresol isomers; therefore, it is appropriate to use the lowest RfD (5E-02 mg/kg-d for m-cresol) from the cresol isomers to represent the mixture.

- Total cyanide could be based on amenable cyanide. The IRIS RfD is 0.02 mg/kg-d.

- Fluoride could be based on fluorine. The RfD for fluorine (6E-02 mg/kg-d) is based on soluble fluoride.

- Thallium could be based on thallium chloride. There are several thallium salts that have RfDs in IRIS. The lowest value among the thallium salts is routinely used to represent thallium in risk assessments.

- **#** p-Xylene could be based on total xylenes. An RfD of 2 mg/kg-d is listed for total xylenes, m-xylene, and o-xylene in IRIS. Total xylenes contains a mixture of all three isomers; therefore, the RfD likely is appropriate for p-xylene.

Copper and lead present special cases. Although HEAST lists an RfD of 1.3 mg/L for copper, HEAST notes that there is a drinking water standard and that data are inadequate to calculate an RfD. Nevertheless, the drinking water standard is sometimes used to calculate an RfD of 0.037 mg/kg-d (assuming a 70-kg body weight and ingestion of 2 L of water per day). This RfD has previously been used.

Even though lead toxicity has been investigated for decades, the data do not fit into the typical RfD methodology. EPA has determined that lead exposure can result in various health effects, depending on the level of exposure. Also, potential health effects differ, depending on whether exposure occurs to an adult or a child and, at blood-lead levels of 10 to 15 μg/dL or possibly lower, effects may include inhibited activity of enzymes involved in red blood cell metabolism, interference with heme synthesis, interference with vitamin D hormone synthesis, altered brain wave activity, deficits in IQ and other mental indices, early childhood growth reductions, and increases in blood pressure (FR 56[110]:26460-26564). Some of these effects may not have a threshold. The EPA RfD workgroup concluded that it was inappropriate to develop an RfD for lead. Consequently, a biokinetic uptake model was developed to predict blood lead levels in young children exposed to lead. A soil screening guidance level of 400 mg/kg (U.S. EPA, 1996d) was developed based on the lead model. EPA is considering use of a screening value (for sludge) of 400 mg/kg in the surface impoundment study and 10 to 15 mg/L for water.

EPA is in the process of developing a revised RfD for perchlorate. A peer review workshop was held in February 1999 to review the toxicological data used as the basis for the revised RfD (0.0009 mg/kg-d). This value is still undergoing review; however, if it were to be finalized in the near future it could be used in the risk assessment. A provisional RfC of 2.0E-3 mg/m^3 was derived for cyclohexanol in the listing rule for solvents (63 FR 64371) and could be used in the SI study. The Agency will use a screening value (for sludges) of 400 mg/kg in the surface impoundment study.

In summary, EPA benchmarks exist for 240 SI constituents. Of the 24 without benchmarks, suitable draft benchmarks may be readily identified for about one-third and subsequent literature searches may identify suitable studies to develop benchmarks for several others. These special cases will be clearly identified in presenting analytic findings based on draft benchmarks. For the few remaining chemicals for which benchmarks cannot be developed, a quantitative risk assessment will not be possible; however, information concerning the frequency of detection and concentrations should be considered carefully in a qualitative assessment.

3.2.3.5 <u>Human Health Risk Measures</u>. Risk characterization integrates the exposure and toxicity assessments to produce quantitative estimates of potential health risks associated with the chemicals of potential concern. Risks will be determined for individual chemical parameters as well as for additive effects (across pathways) and cumulative effects for multiple

chemicals. The following are key features of the calculation of cancer and noncancer risk in the SI Study:

- Excess cancer risk criterion = 10^{-5}
- HQ criterion = 1
- Cancer risks can be cumulative across chemicals
- HQs can be summed across chemicals if effects are to same target organs.

Because of fundamental differences in the calculation of critical toxicity values, the estimates of potential excess carcinogenic risks and noncarcinogenic health effects are calculated separately.

Risk probabilities determined for each carcinogen generally will be considered to be additive over all exposure pathways so that an overall risk of cancer will be estimated for each group of potentially exposed receptors. Cancer risks will not be summed if inhalation or ingestion of a chemical results in health effects at the point of exposure or has other immediate effects.

Consistent with previous EPA practice in the assessment of human cancer risks from constituents, if an individual's probability of developing cancer due to an exposure to the constituent in question is estimated to be in the range of 1 in 100,000 (1×10^{-5}), with a confidence level consistent with the levels that can be achieved with the existing state of chemical constituent risk assessment methodologies, then that exposure would be of concern.

In a manner similar to carcinogens, HQ values will be summed for chemical exposures causing the same health effect (i.e., affecting the same target organ) to develop hazard indices (HIs). HQs and HIs are not risk probabilities but are accepted by EPA as quantitative levels of risks for noncarcinogens. Consistent with previous EPA practice in the assessment of human noncancer health effects from constituents, if the ratio of the individual's exposure and the applicable toxicity value is greater than 1, again with a confidence level consistent with the levels that can be achieved with the existing state of chemical constituent risk assessment methodologies, then that exposure would be of concern.

Lead Risk Evaluations. A separate model will be developed for risks from potential exposures to lead. Blood-lead levels for potentially exposed receptors will be compared with a selected action level. EPA typically considers that action may be warranted if the 95th percentile of blood-lead levels exceeds 10 μg/dL (i.e., action may be considered if there is a 5 percent chance that a sensitive receptor exposed to lead would have a blood-lead level greater than 10 μg/dL). To be health protective, predicted blood-lead levels exceeding this criterion would be noted for receptors at each facility.

To accommodate this method in the SI Study requires integrating potential lead exposures calculated by the 3MRA model with the EPA model used to estimate blood-lead levels corresponding to different levels of exposure and then comparing the predicted blood-lead levels with a selected action level. A suggested approach to implement this method would be to use the 3MRA model to estimate multimedia lead exposure point concentrations and evaluate risks to children using EPA's Integrated Exposure and Uptake Biokinetic (IEUBK) Model (U.S. EPA,

1994a). The IEUBK Model combines estimates of environmental exposures with pharmocokinetic modeling to predict blood-lead levels in children. Blood lead levels could also be estimated using an EPA method for estimating adult blood lead levels.

Infant Risks. Risk to infants will be estimated only for exposures to dioxin and dioxin-like compounds via the breast milk pathway. This exposure will be calculated on the basis of the total exposure to the adult (maternal) exposures of each receptor type. The risk will be characterized as a margin of error (MOE) using a measure of background exposures for comparison purposes.

Risk Estimates. Carcinogenic risk estimates and noncarcinogenic HI values will be estimated for each receptor type in each exposure area and, as appropriate, for each exposure route in the vicinity of a facility. In the case of carcinogens (or noncarcinogens where inhalation and ingestion act on the same organ), the individual exposure route risks can be aggregated to estimate the aggregate risks. Each set of risk analyses will provide a determination of the contribution of each exposure pathway and the other dimensions for the SI Study risk analysis.

Individual vs. Population-Weighted Risk Estimates. EPA risk assessments are expected to address or provide descriptions of individual risk and population risk. The estimates of the potential distribution of human health risk will be communicated, or described, in terms of the number of individuals who (currently) have or (in the future) can reasonably be expected to incur risks from the constituents from the impoundments in either the central tendency range or the high end of the estimated risk distribution. The risk summary processor will include the proportion of the population whose exposures are modeled who can reasonably be expected to incur risks above the levels described previously for cancer and noncancer effects, the proportion of people within the modeled exposed population with risks estimated to be above those levels, and pathways, receptors, and age cohorts exceeding identified risk levels.

Population-weighted risk estimates will be produced by multiplying the population estimates for each exposure area to the individual risk estimate and summing the adjusted risk estimates for all exposure areas. Normalized population risk estimates will be provided for each receptor type to provide the distribution of risk across all receptors in the study area. The population-weighted risk estimate is shown as

$$PRr = \sum^{Ne} (Rr,e \times Nr) \; / \; \sum^{Ne} Nr \qquad (3\text{-}1)$$

where

PRr	=	Population-weighted risk estimate for receptor type r
Rr,e	=	Risk estimate for receptor type r in exposure area e
Nr	=	Number of receptors of receptor type r in exposure area e
Ne	=	Number of exposure areas in the study area.

3.2.3.6 <u>Uncertainty Analysis</u>. Potential sources of uncertainty and variability will be identified and evaluated using a semiquantitative uncertainty analysis. The uncertainty analysis

will provide an evaluation of the variability in the estimated risks and allow the identification of sources of uncertainty that are potentially reducible.

3.2.4 Ecological Health

The ecological risk assessment (ERA) for the SI Study will evaluate the potential for adverse ecological impacts that may occur as result of chemical releases at surface impoundments. The results of this ERA may provide information to assist in evaluating the need for future regulation of surface impoundments. The ERA for the SI Study is consistent with EPA guidance (U.S. EPA, 1998) and, as such, will be structured around the following main sections:

- Problem formulation
- Analysis phase
- Risk characterization.

3.2.4.1 <u>Problem Formulation</u>. The problem formulation establishes the scope of the ERA by (1) ensuring that ecological receptors (e.g., plants, wildlife) likely to be exposed are evaluated and (2) evaluating exposure scenarios relevant to different habitats. The problem formulation for the SI Study will describe the following elements, which are detailed in this section:

- Representative ecological receptors
- Chemicals of potential concern
- Potential and relevant exposure pathways
- Assessment and measurement endpoints.

Representative Ecological Receptors. In general, ecological receptors are species of plants and wildlife that may be exposed and adversely impacted by chemicals released from surface impoundments. The ecological receptors that will be evaluated in this ERA include the following:

- Terrestrial wildlife using habitats at or near surface impoundments can be exposed by either drinking directly from the surface impoundment and/or consuming plants, soil, or prey items that bioaccumulate chemicals present in the impoundment.

- Aquatic plants and other biota may be exposed to chemicals that are transported from surface impoundments to nearby aquatic habitats.

- Vascular plants and other terrestrial biota may be exposed to chemicals that are transported from the surface impoundment to nearby terrestrial habitats (e.g., surficial soils).

Because all potentially affected species cannot be individually assessed, ecological receptors will be identified by organizing potentially affected plants and wildlife into guilds of taxonomically and functionally related organisms (e.g., herbivorous birds, insectivorous birds,

carnivorous mammals). Receptors will be 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 an impoundment because (1) it is a bird, (2) it eats insects and worms, (3) it is one of many thrushes observed at or near the impoundment, and (4) wildlife exposure factors have been established (U.S. EPA, 1993d).

For the SI Study, a 2-km radius around the impoundment is considered a conservative estimate of the habitat area in which receptors may be affected by the surface impoundment. Habitats within the 2-km radius of the site will be characterized and assigned based on site-specific and regional data. Risks to aquatic biota (i.e., fish and aquatic invertebrates) living in surface impoundments will not be evaluated in the SI Study since impoundments are expected to provide poor habitat for these organisms, and impoundments are not intended to support freshwater aquatic biota. Habitats that will be considered in the SI Study include

Terrestrial Habitats

- Grasslands
- Shrub/scrub
- Forest
- Crop fields and pastures
- Residential

Freshwater Habitats

- Rivers/streams
- Ponds
- Lakes

Wetland Habitats

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

These habitats are intended to represent habitats across the United States that may be found at or near surface impoundments and that support wildlife receptors. Although estuarine and marine ecosystems may potentially be impacted, evaluating these systems would require substantial effort in data collection on estuarine receptors (e.g., ecotoxicity data) as well as in adapting the multimedia modeling construct to simulate the complex environmental behavior of chemicals in the brackish and marine waters of estuarine systems. Currently, there is no system developed to support this type of assessment; as such, these habitats will not be included in the analyses.

Once site-specific habitats are identified, representative ecological receptors will be assigned to appropriate habitats based on documented foraging and feeding behavior and habitat

usage. Representative ecological receptors for the following groups of taxa will be used to populate habitats:

Terrestrial Habitats

- Terrestrial plants
- Soil invertebrates
- Reptiles
- Herbivorous birds, soil invertebrate-consuming birds, and carnivorous birds
- Herbivorous mammals, soil invertebrate-consuming mammals, and carnivorous mammals

Freshwater Habitats

- Aquatic plants
- Aquatic invertebrates
- Benthic invertebrates
- Fish
- Amphibians
- Herbivorous birds, benthic invertebrate-consuming birds, piscivorous birds, and carnivorous birds (including migratory birds and waterfowl)
- Herbivorous mammals, benthic invertebrate-consuming mammals, and carnivorous mammals

Wetland Habitats

- Wetland plants
- Hydric soil-associated invertebrates
- Aquatic invertebrates (permanently flooded wetlands only)
- Fish (permanently flooded wetlands only)
- Amphibians

- Reptiles
- Herbivorous birds, invertebrate-consuming birds, and carnivorous birds (including migratory birds and waterfowl)
- Herbivorous mammals, piscivorous mammals, and carnivorous mammals.

Chemicals of Potential Concern. Chemicals of potential concern are detected chemicals in exposure media (e.g., soil, surface water, prey tissue) that may adversely impact ecological receptors. Specific COPCs within the study scope are discussed in Section 3.2.3.1.

Ecological Exposure Pathways. The complete exposure pathways to be evaluated in this analysis must conform to the following elements:

- A source and mechanism of COPC release
- A transport medium
- A point or area where ecological receptors may be exposed to COPCs
- An exposure route through which COPC uptake occurs.

Figure 3-4 graphically presents the risk conceptual model and potentially complete exposure pathways for ecological receptors. Table 3-5 lists the media and exposure routes that will be evaluated in the analysis.

Direct contact to COPCs by terrestrial wildlife will not be evaluated because (1) dense undercoats or down effectively prevents chemicals from reaching the skin of wildlife species and significantly reduces the total surface area of exposed skin (Peterle, 1991; U.S. ACE, 1996) and (2) results of exposure studies indicate that exposures due to dermal absorption are insignificant compared to ingestion for terrestrial wildlife (Peterle, 1991). Similarly, inhalation of volatile organic chemicals (VOCs) will not be evaluated because (1) concentrations of volatile chemicals released from soil to aboveground air are drastically reduced, even near the soil surface (U.S. ACE, 1996) and (2) VOC concentrations in soils would have to be great to induce noncarcinogenic effects in wildlife based on inhalation toxicity data for laboratory rats and mice (U.S. ACE, 1996). In addition, availability of inhalation benchmarks for ecological receptors is limited.

Assessment and Measurement Endpoints. Assessment endpoints describe attributes of ecological receptors that are considered environmentally important and that reflect environmental values to be protected. Assessment endpoints are selected to reflect regulatory and policy goals as well as the environmental conditions addressed by the risk assessment. In selecting assessment endpoints, it is crucial to establish the relationship between the assessment endpoints (i.e., the ecological values to be protected) and the measures of effect (e.g., the ecotoxicity data used to support benchmarks). The measures of effect generally reflect toxicity to individual organisms while the assessment endpoints represent ecological values that go beyond the individual receptor.

Table 3-5. Ecological Exposure Routes Evaluated by Receptor Type

Receptor	Root Uptake		Direct Contact			Ingestion		
	Surface Water	Soil	Surface Water	Sediment	Soil	Surface Water	Soil	Food
Plants								
Aquatic plants	x							
Terrestrial plants		x						
Invertebrates								
Aquatic invertebrates			x					
Sediment-associated invertebrates				x				
Soil invertebrates					x			
Wildlife								
Fish			x					
Amphibians			x					
Reptiles						x	x	x
Birds						x	x	x
Mammals						x	x	x

Assessment endpoints are defined based on the identification of potentially exposed ecological receptors and potentially complete exposure pathways. Development of assessment endpoints is based on the assumption that protection of a population or community can be inferred from protection of developmental and reproductive functions in individuals. Toxicity endpoints that can reasonably be assumed to influence the potential of a population to sustain itself (e.g., developmental and reproductive effects) are used to infer a level of protection to populations. This inference, however, has yet to be validated from field or microcosm studies on exposed populations. This is currently a limitation in the state-of-the-science and limits our ability to interpret ecological risk results.

3.2.4.2 <u>Analysis</u>. The analysis phase for the SI Study will estimate COPC exposures and establish toxicity benchmarks for ecological receptors.

Exposure Assessment. Estimates of exposure (doses or medium concentrations) for each representative receptor will be calculated according to EPA guidance (U.S. EPA, 1993d).

Exposure Point Concentrations. Concentrations in accessible media (including food items) are needed to estimate exposures to representative species. Because the risk assessment is intended to be an evaluation of receptors at large (rather than of the maximally exposed receptor), estimates of the mean exposure point concentrations in accessible environmental media will be predicted using the 3MRA fate and transport models described in Section 3.3.

For receptors that receive significant exposures through their food, simple food webs will be constructed to show the major trophic levels and pathways through which chemicals are transferred up the food chain. Estimates of COPC concentrations in terrestrial and aquatic food items will be calculated using COPC concentrations in environmental media and biological uptake factors such as bioaccumulation factors, bioconcentration factors, and biotransfer factors. Estimates of exposure will include evaluations of spatial and temporal variability in exposure point concentrations.

Wildlife Exposure Factors. Species-specific wildlife exposure factors will be established for each representative receptor. These factors include body weight; food, soil, and water ingestion rates; dietary preferences; and foraging range. For receptors with foraging areas smaller than the habitat, the foraging area will be randomly located within the habitat boundaries. For receptors with foraging areas larger than the habitat, the estimated dose is weighted as the ratio of the habitat area to the foraging area (habitat area/foraging area). This weighting is used to adjust the dose for the fraction of the receptor's diet taken from the habitat that is potentially affected by the surface impoundment.

The exposure assessment will include an algorithm to construct a unique, randomly selected diet for each receptor species at each site where it occurs, thus reflecting the variability in receptor species' dietary composition. The algorithm requires dietary preference data consisting of a list of potential diet items for each species and the maximum and minimum proportion of the species' diet that each item can constitute. The prey preference algorithm ranks diet items by maximum potential dietary fraction, and then constructs the diet from these ranges, starting with the most preferred food item (largest maximum) and randomly selecting dietary fractions from within the given ranges. The dietary composition is habitat-specific because the same species (e.g., raccoon) may be assigned to aquatic and terrestrial habitats, resulting in different dietary preferences.

Because the risk assessment is intended to be an evaluation of receptors at large (rather than of the maximally exposed receptor), estimates of the mean wildlife exposure factors will be used in the SI Study. Ingestion rates are a function of body weight and, thus, will also reflect central tendency values.

Effects Assessment. Ecological benchmarks based on the toxicological effects of chemicals on representative ecological receptors will be used to evaluate whether estimated exposures are likely to result in adverse ecological effects. Population-level effects will be inferred from benchmarks developed from toxicity studies examining reproductive, developmental, or mortality endpoints. Community-level effects will be inferred from toxicity benchmarks established to protect a specified percentage of the community (e.g., ambient water quality criteria).

Benchmark Development. The specific methods used to calculate the protective level (i.e., benchmarks and chemical stressor concentration limits [CSCLs]) are taken from the HWIR methodology and vary with the receptor taxa.[3] For the HWIR analysis, protective CSCLs were derived (in ppm) for specific communities and populations in direct contact with contaminated media (i.e., terrestrial plants, soil biota, sediment biota, fish/aquatic invertebrates, and herpetofauna). Protective benchmark doses (mg/kg-d) were developed for mammals and birds based on exposure through the food web by ingestion of contaminated prey items.

Ecological Benchmarks for Representative Receptors (ChemEBRec). Ecological benchmarks (EBs), derived in units of dose (mg/kg-d), were developed for representative taxa of mammals and birds. The EBs were appropriate for upper-trophic-level consumers because the primary exposure route occurs through ingestion of contaminated prey items. The approach adopted for HWIR uses a hierarchy for the selection of ecotoxicity data and extrapolates from a test species to the species of interest (in this case, wildlife).

Benchmark studies for mammals and birds were selected using a few key guidelines. These guidelines represent the minimum requirements for a study to be of sufficient rigor for benchmark derivation.

- *Measurement Endpoints*—Studies containing measurement endpoints reported as either a no-observed-adverse-effect level (NOAEL) or a lowest-observed-adverse-effect level (LOAEL) in units of daily dose were preferred. From these results, the geometric mean between the NOAEL and the LOAEL (i.e., maximum acceptable toxicant concentration [MATC]) was calculated. The MATC was the preferred benchmark for representative mammalian and avian species.

- *Toxicity Endpoints*—Because population viability in mammals and birds was selected as the assessment endpoint, the benchmarks were developed from toxicity endpoints of reproductive or developmental success or, if unavailable, other effects that could conceivably impair population dynamics.

- *Methods*—No specific test methodologies were required in studies used for benchmark derivation. Standard laboratory practices (e.g., control dose groups), however, were required. Field data may not be appropriate to develop a daily dose exposure.

- *Receptor Requirements*—Ecotoxicity data for wildlife species were preferred (e.g., mallards or mink); however, because of the paucity of studies exposing wildlife species, rats and mice were typically the surrogate species exposed in benchmark studies.

[3] For this analysis, CSCLs refer to constituent concentrations (e.g., mg/kg soil) in environmental media that are presumed to cause de minimis effects on ecological receptors. Benchmarks, in mg/kg-d, provide protective ingestion doses that are estimated to cause de minimis effects to mammalian and avian receptors.

- *Durations*—Studies were selected that reflected chronic or subchronic exposure durations extending over a large percentage of the test species' lifetime, over multiple generations, or over a particularly sensitive life stage of a species.

- *Exposure Routes*—Studies indicating oral exposure (e.g., dietary, gavage) were preferred to studies using other exposure routes (e.g., intraperitoneal injection). Mammals and birds in the field are typically more highly exposed through ingestion of contaminated prey than through inhalation or direct contact, although there are exceptions (e.g., burrowing animals).

- *Dosing Scheme*—Dose-response curves characterized by at least three data points were selected over studies exposing animals to one dose level. This helped identify both a NOAEL and a LOAEL for MATC calculations.

Mammalian and avian benchmarks represent population-inference benchmarks. By developing benchmarks from NOAELs and LOAELs in mammals and birds, benchmarks were estimated to provide protection from ingested doses that may inhibit the reproductive capacities of these populations. The ability of the population to sustain itself (within normal biological variation) was inferred from individual effects such as fecundity. This inference, however, has yet to be validated from field or microcosm studies on exposed populations. Without validation, it is likely that some benchmarks are overprotective and others are underprotective of wildlife populations. Although this method does not confirm protection of populations, by protecting individuals from adverse effects to reproductive and developmental endpoints, some level of protection is provided to populations.

Once the benchmark study was identified, a scaled benchmark was calculated for representative receptors of mammals. This method used an allometric scaling equation based on body weight to extrapolate test species doses to estimate wildlife species doses. For mammals, a scaling factor of 3/4 was used (Equation 3-2). This is the default methodology EPA proposes for carcinogenicity assessments and reportable quantity documents for adjusting animal data to an equivalent human dose (U.S. EPA, 1992b). For birds, recent research suggests that the cross-species scaling equation used for mammals is not appropriate for avian species (Mineau et al., 1996). Using a database that characterized acute toxicity of pesticides to avian receptors of various body weights, Mineau et al. (1996) concluded that applying mammalian scaling equations may not sufficiently predict protective doses for avian species. Benchmarks scaled for small-bodied avian species using the mammalian equation generated scaled doses that were not protective enough for small birds. Mineau et al. (1996) suggested that a scaling factor of 1 provided a better dose estimate for birds. Therefore, a scaling factor of 1 was applied for avian receptors (Equation 3-3).

$$EB_w = MATC_t \, x \left(\frac{bw_t}{bw_w} \right)^{1/4} \qquad (3\text{-}1)$$

$$EB_w = MATC_t \, x \left(\frac{bw_t}{bw_w} \right)^0 \tag{3-2}$$

where

EB_w	=	scaled ecological benchmark for species w (mg/kg-d)
$MATC_t$	=	maximum acceptable toxicant concentration (mg/kg-d)
bw_t	=	body weight of the surrogate test species (kg)
bw_w	=	body weight of the representative wildlife species (kg).

Total Surface Water CSCLs. The CSCLs developed for surface water based on total concentrations of the constituent covered the following receptor taxa: freshwater community (i.e., fish and aquatic invertebrates), algae/aquatic plants, and herpetofauna.[4] The methods used to derive CSCLs are reviewed here for each receptor taxon. The CSCL developed for the freshwater community was derived to reflect both total and dissolved water concentrations.

Freshwater community – The freshwater community CSCL was developed to protect species of fish and aquatic invertebrates. The CSCL does not extend to protect species of mammals and birds that may forage in freshwater ecosystems. The methods adopted to develop freshwater community CSCLs are consistent with those supported across EPA offices. The CSCLs were derived using methodologies founded through the development of the National Ambient Water Quality Criteria (NAWQC). These methods require the compilation of appropriate acute and chronic ecotoxicity data reporting effects to survival, growth, and reproduction in aquatic biota for specific members of the freshwater community. The NAWQC method uses a list of ecotoxicity data requirements for eight taxonomic families that represent typical freshwater species (see text box). Whether a final chronic value (FCV) or a secondary chronic value (SCV) is calculated depends on how well the eight taxonomic families are represented by the data.

Data Requirements for FCV Calculation

- The family *Salmonidae* in the class Osteichthyes
- One other family (preferably a commercially or recreationally important warmwater species) in the class Osteichthyes (e.g., bluegill, channel catfish)
- A third family in the phylum Chordata (e.g., fish, amphibian)
- A planktonic crustacean (e.g., a cladoceran, copepod)
- A benthic crustacean (e.g., ostracod, isopod, amphipod)
- An insect (e.g., mayfly, dragonfly, damselfly, stonefly, midge)
- A family in a phylum other than Arthropoda or Chordata (e.g., Rotifera, Annelida, Mollusca)
- A family in any order of insect or any phylum not already presented.

[4] Herpetofauna includes species of amphibians and reptiles. Insufficient ecotoxicity data were identified to derive CSCLs for reptiles. Therefore, continued discussions only review amphibians.

For populations of the freshwater community (e.g., fish, aquatic invertebrates), the FCV developed for the NAWQC or the criterion continuous concentration (CCC) developed for the Great Lakes Water Quality Initiative (GLWQI) was the preferred CSCL to use for this analysis (U.S. EPA, 1995a, 1996f). If neither a CCC nor an FCV was available, an SCV was calculated using Tier II methods developed through the GLWQI (Stephan et al., 1985; Suter and Tsao, 1996).

Algae and aquatic plants – For algae and aquatic plants, toxicological benchmarks were identified in the open literature or from data compiled in *Toxicological Benchmarks for Screening Potential Contaminants of Concern for Effects on Aquatic Biota: 1996 Revision* (Suter and Tsao, 1996). For most contaminants, studies were not available for aquatic vascular plants, but lowest-effects concentrations were identified for algae. The criteria for algae and aquatic plants were based on a lowest-observed-effect concentration (LOEC) for vascular aquatic plants or an effective concentration (EC_{xx}) for a species of freshwater algae, frequently a species of green algae (e.g., *Selenastrum capricornutum*). Because of the lack of data in this receptor group and the differences between vascular aquatic plants and algae sensitivity, usually the lowest value of those identified was used. In instances where only a median effective concentration (EC_{50}) was identified to characterize effects to algae growth and survival, a safety factor of 5 was applied to generate an estimated low effects concentration.

Amphibians – Amphibians appear to be highly sensitive to a number of toxicants (e.g., trace metals) during the developmental stages of their life cycle. Amphibians are essential parts of a number of food webs (particularly wetlands) and are likely to provide a fairly sensitive indicator for chemical stressors relevant to higher levels of biological organization. Though amphibians are a significant ecological receptor, ecotoxicity data characterizing the chronic dose-response relationship for chemicals of concern are limited. After a review of several compendia presenting amphibian ecotoxicity data (e.g., Devillers and Exbrayat, 1992; Power et al., 1989; U.S. EPA, 1996g) as well as primary literature sources, no suitable subchronic or chronic studies were identified that reported effects to reproductive or developmental endpoints in amphibian species. Therefore, a CSCL based on chronic endpoints and exposure durations was not derived. Instead, the CSCL was developed from a geometric mean of acute (i.e., LC_{50}, lethal water concentration resulting in 50 percent mortality) amphibian ecotoxicity data. A few general guidelines were followed in selecting analogous acute studies for developing the CSCL:

- Test duration was usually less than 15 d.
- Toxicity endpoints included mortality (LC_{50})
- Exposure occurred during early life stages (i.e., embryo, larvae, and tadpole).

Because the criteria are based on acute data (i.e., lethality), the severity of the potential adverse effects that this criterion indicates is significant. Incorporating the amphibian data into the NAWQC within the data requirement categories is currently under consideration. Because amphibian species are more likely to breed in standing waters such as wetlands, ponds, or temporary puddles, the appropriateness of combining protection of amphibian receptors with the freshwater community CSCL is unclear.

Dissolved Surface Water CSCLs. Conversion factors were available for several of the metal constituents to convert total metal concentrations in the water column to total dissolved concentrations (U.S. EPA, 1999y). Although the total concentrations supplied by the NAWQC and GLWQI are still deemed scientifically defensible by EPA, the Agency recommends the use of dissolved metal concentrations when they are available (Prothro, 1993).

Methods are currently available to develop dissolved CSCLs only for metals in the freshwater community. Dissolved CSCLs were derived from total water CSCLs using a conversion factor. The conversion factors applicable to chronic criteria in freshwater are presented in Table 3-6. The conversion factors were developed by EPA using a series of filtration experiments that measured the difference between filtered and unfiltered concentrations of metals in surface waters. Dissolved CSCLs were derived by multiplying the total CSCL by the conversion factor (Equation 3-4).

$$Metal\ \ CSCL_{dissolved} = (Metal\ \ CSCL_{total})\ x\ (Conversion\ \ Factor) \qquad (3\text{-}4)$$

where

Metal CSCL $_{total}$ = either an FCV or an SCV in freshwater
Conversion Factor = the fraction of dissolved metal.

Sediment CSCL. Two methods were applied in developing the CSCL for the benthic community (e.g., worms, amphipods). The first and preferred method used measured sediment concentrations that resulted in minimal effects to the composition and abundance of the sediment community. The sediment criteria were derived from the upper limit of the range of sediment contaminant concentrations that are derived from no-effects data, species diversity, and abundance endpoints. Measurements to derive the CSCLs were taken at the national scale and reflected a variety of sediment types and benthic community species. The second CSCL derivation method used the equilibrium partitioning (EqP) relationship between sediments and surface waters to predict a protective concentration for the benthic community. This method was used only for nonionic organic constituents. For the benthic community, the approach used to establish CSCLs was based on a complete assessment of several sources proposing protective sediment CSCLs. A discussion of each method (i.e., measured and estimated CSCLs) is provided.

Measured sediment CSCLs – The premier sources of measured sediment CSCLs are the National Oceanic and Atmospheric Administration (NOAA) and the Florida Department of Environmental Protection (FDEP) sediment documents. NOAA annually collects and analyzes sediment samples from sites located in coastal marine and estuarine environments throughout the United States as part of the National Status and Trends (NS&T) Program. Data collected by NOAA include measured sediment concentrations and the corresponding measures of toxicity in resident species such as amphipods, arthropods, and bivalves on a variety of community-based endpoints (e.g., abundance, mortality, species composition, and species richness). These data are used by NOAA to estimate the 10th percentile effects concentration (ER-L) and a median effects concentration (ER-M) for adverse

Table 3-6. Conversion Factors for Dissolved Metal[a]

Constituent	Conversion Factor
Arsenic	1.00
Cadmium[b]	1.1017-[(ln hardness)(0.04184)]
Chromium III[b]	0.860
Chromium VI	0.960
Lead[b]	1.4620-[(ln hardness)(0.14571)]
Mercury	0.850
Zinc[b]	0.986

[a]Conversion factor for chronic CSCLs in freshwater.
[b]Dependent on the water hardness (assumed to be 100 mg $CaCO_3$/L for this analysis).

effects in the sediment community. These values are not NOAA standards; rather, they are used to rank sites based on the potential for adverse ecological effects. In contrast, the FDEP sediment criteria were developed from the ER-L and ER-M data to approximate a probable effects level (PEL, estimated from ER-M data) and a threshold effects level (TEL, estimated from ER-L data). PELs and TELs correspond to the statistically derived upper limit of contaminated sediment concentrations that demonstrate probable effects and no effects to the benthic community, respectively. Generally, FDEP values are more conservative than NOAA values. Even though these criteria were developed for a marine community, researchers have demonstrated that marine TELs have good correlation with no-effects levels found for freshwater systems (Smith et al., 1996). In order of preference, TELs were adopted as CSCLs if available; if not, ER-L values were used. The FDEP criteria were chosen above the NOAA criteria for the following reasons:

- The same database was used for both the NOAA criteria and the FDEP criteria development.
- In most cases, the FDEP criteria were more conservative than the NOAA criteria because a larger portion of the low-effects data was used in benchmark development.
- The marine TELs developed by the FDEP were found to be analogous to TELs observed in freshwater organisms (Smith et al., 1996).

***Estimated sediment CSCLs*.** When measured effects data were not available for organic constituents using the TEL or ER-L approach, the value was derived using the EqP approach to estimate the sediment CSCL (U.S. EPA, 1993c). The surface water FCV or SCV was used to generate a sediment CSCL using the partitioning relationships among surface water, pore water,

and organic carbon in sediment. This method assumes that the equilibrium partitioning between the sediment and the water column is a function of the organic carbon. Equations 3-5 and 3-6 were used to calculate the sediment CSCL depending on whether an FCV or an SCV was available. In calculating sediment CSCL for nonionic chemicals, the fraction organic carbon (f_{oc}) was assumed to be 1 percent total organic carbon and K_{oc}s (organic carbon partitioning coefficients) were adopted as reported in Jones et al. (1997). However, because sediment CSCLs were derived for organic constituents based on site-specific f_{oc}, some of the CSCLs were recalculated within the HWIR modeling framework on a site-specific basis.

$$Sediment\ \ CSCL = f_{oc} \times K_{oc} \times FCV \tag{3-5}$$

$$Sediment\ \ CSCL = f_{oc} \times K_{oc} \times SCV \tag{3-6}$$

Soil CSCLs. Soil CSCLs were derived for the terrestrial plant community and the soil community. Each of the specific methods, including the rationale and the derivation methods, is outlined in the following sections.

Terrestrial plants – For the terrestrial plant community, toxicological benchmarks were identified from a summary document prepared at the Oak Ridge National Laboratory (ORNL): *Toxicological Benchmarks for Screening Potential Contaminants of Concern for Effects on Terrestrial Plants: 1997 Revision* (Efroymson et al., 1997). The measurement endpoints were generally limited to growth and yield parameters for the following reasons:

- They are the most common class of responses reported in phytotoxicity studies and, therefore, allow for criterion calculations for a large number of constituents.
- They are ecologically significant responses, both in terms of plant populations and, by extension, the ability of producers to support higher trophic levels.

As presented in Efroymson et al. (1997), criteria for phytotoxicity were selected by rank-ordering the LOEC values and then approximating the 10th percentile. If there were 10 or fewer values for a chemical, the lowest LOEC was used. If there were more than 10 values, the 10th percentile LOEC was used.

Soil community – Two methods were used in deriving soil community CSCLs: a community-based CSCL and an earthworm/microbial CSCL.

- **Community-Based CSCL**—The first, and preferred, method was based on a community-level approach similar to that applied in deriving the NAWQC. This method developed a CSCL based on NOECs to reproductive and development endpoints in a number of key functional taxa in the soil community. The CSCL was designed to protect the structure and function of the soil community and its critical role in the overall nutrient processing that occurs in the terrestrial food web.

Two key uncertainties were noted in the development of community-based CSCLs. First, the ecotoxicity data used in the method are based on NOECs. The CSCLs developed using the earthworm/microbial method for the soil community were based on low-effects levels. Because these CSCLs are based on no-effects soil concentrations, some added conservatism was generated in the soil community CSCLs for lead and cadmium. Second, the species taxa groups designed to represent key compartments in the soil community did not include microbes. This introduces some uncertainty in the soil CSCL because microflora make up approximately 80 to 90 percent of the biomass in soil and microflora are responsible for the majority of the biological activity in soil (e.g., N mineralization).

Earthworm and Microbial CSCLs—The second method used to derive soil CSCLs required the identification of LOECs for earthworms and microbial endpoints. However, because a single species alone cannot predict the potential toxicological impacts to the soil community, the community-based method was preferred over using an earthworm or microbial CSCL.

Earthworms have been recognized to play important roles in promoting soil fertility, releasing nutrients, and providing aeration and aggregation of soil, as well as being an important food source for higher trophic level organisms. In addition, their constant contact with soil media and permeable epidermis makes them more susceptible to contaminant exposures. Likewise, microbial communities play a key functional role in soil fertility, decomposition processes, and nutrient cycling, providing nutrients in available forms to plants. Microbial CSCLs were only used when they indicated a significantly higher sensitivity to a particular constituent than the corresponding earthworm toxicity data.

The earthworm and microbial CSCLs were developed using the ER-L approach, which was also applied to develop terrestrial plant CSCLs. When more than 10 studies were identified reporting LOECs, then the 10th percentile of the values was derived as the CSCL. When less than 10 values were identified, however, the lowest LOEC was selected as the CSCL.

3.2.4.3 <u>Risk Characterization</u>. Risk characterization integrates the results of the analysis phase to evaluate the likelihood of adverse ecological impacts associated with exposures to COPCs (U.S. EPA, 1992b). The potential for adverse ecological impacts will be characterized using hazard quotients HQs. HQ is the ratio of the estimated exposure dose to the toxicity benchmark for ecological receptors:

An HQ less than 1 (HQ < 1) indicates a negligible potential for adverse ecological impacts due to exposure to a particular COPC; whereas, an HQ of 1 or greater (HQ $\geq$ 1) indicates a potential for adverse ecological impacts due to exposure to a particular COPC.

Risk results will be considered in the context of two additional site-specific

$$Hazard\ Quotient = \frac{Estimated\ Exposure\ Dose}{Toxicity\ Benchmark}. \qquad (3\text{-}7)$$

characteristics:

- **#** Presence or proximity of managed areas (e.g., state or national parks, wildlife refuges, or wild and scenic rivers

- **#** Presence or proximity of federally listed threatened or endangered (T&E) species.

Locations of managed areas will be determined using the Managed Area Database. At sites where significant managed areas are potentially impacted, ecological risks may be considered greater than equivalent risks at other sites. Presence of T&E species can be determined from U.S. Fish and Wildlife Service (U.S. FWS) data or from State Natural Heritage Program data. In either case, precise locations of T&E populations are not likely to be available. Therefore, the significance of relevant T&E documentation will be weighed on a case-by-case basis.

Uncertainty Analysis. Where wildlife exposure factors, biological uptake factors, and/or toxicity benchmarks are not available, HQs will not be evaluated. Representative ecological receptors and chemicals that cannot be assessed using HQs will be identified. A methodology for a qualitative analysis of uncertainty was developed for the HWIR analysis and will be applied to the surface impoundments ecological risk assessment.

For ecological risks, the constituent-specific concentrations in wastes generated in the HWIR assessment that are determined to pose de minimis risk (i.e., the exemption criteria) were based on two types of risk metrics: (1) the ecological hazard quotient, that is, the ratio between exposure concentrations or dose and appropriate ecological benchmarks,[5] and (2) the probability of protection for ecological receptors. However, the ecological benchmarks include a variety of receptors (e.g., soil fauna, mammals, plants), and, because the quality and quantity of relevant data vary widely across receptors, the ecological exemption criteria represent different levels of knowledge regarding the exposure and toxicity of chemical stressors. The variability in supporting data suggests that the level of confidence in the exemption criteria is dependent on the quantity and quality of available data. In short, the ecological exemption criteria do not reflect a standard data set; rather, they reflect a continuum of data on toxicity and exposure (e.g., bioaccumulation factors) of varying levels of quality. To provide an effective tool to characterize where on the continuum a given exemption criterion falls, a framework was developed to assign confidence indicators based on the sufficiency of the data set supporting an exemption criterion. Sufficiency, in this framework, is determined according to how well an exemption criterion (1) captures risks to all relevant receptor groups in a habitat, (2) is supported by ecotoxicity data of high quality, and (3) represents all significant routes of exposure to ecological receptors. Consequently, the confidence indicators reflect all three of these “attributes” of an ecological exemption criterion.

[5] The term “ecological benchmarks” is used here in a broad sense to refer to two descriptors that were used to identify protective levels: ecotoxicological benchmarks and chemical stressor concentration limits. Briefly, this distinction was made to clearly represent the differences in the level of biological organization. Ecotoxicological benchmarks are threshold doses intended to protect wildlife populations from significant adverse effects from the ingestion of contaminated media and prey and are expressed in units of mg/kg-d. In contrast, chemical stressor concentration limits are medium-specific concentrations (e.g., sediment) intended to protect assemblages of species in contact with a contaminated medium.

The development of confidence indicators must address the completeness of the data set with regard to receptors of concern (in each type of habitat), as well as the confidence in data on toxicity and on uptake and accumulation. Consequently, the confidence indicator consists of three parts: (1) the habitat confidence indicator, (2) the benchmark confidence indicator, and (3) the exposure confidence indicator. A brief discussion is provided here of each of these three parts; a more extensive treatment of the confidence indicators and methods used in their development is provided in *Data Requirements and Confidence Indicators for Ecological Benchmarks Supporting Exemption Criteria for the Hazardous Waste Identification Rule (HWIR99)* (U.S.EPA, 1999z).

Habitat Confidence Indicator. The confidence indicator for habitats is a qualitative statement used to convey the relationship between chemical properties and data availability on receptor groups in terrestrial and aquatic habitats, respectively. For example, to achieve a high level of confidence in assessing a persistent, bioaccumulative constituent, we would require ecotoxicological data on all receptor groups assigned to a habitat. In contrast, we may achieve a high level of confidence in assessing a readily biodegradable constituent that does not bioaccumulate with data on fewer receptor groups because: (1) the spatial impact of the constituent will be extremely limited by rapid breakdown (assuming nontoxic daughter products) and (2) food web exposures are unlikely to be significant. Three habitat confidence indicators were used to establish the data requirements for all combinations of persistence and bioaccumulation potential: “A” indicates high confidence, “B” indicates moderate confidence, and “C” indicates low confidence in the data set. Hence, a habitat confidence indicator of “B” means that, given the persistence and bioaccumulation rating for the constituent, there is moderate confidence in the ability of the data set to assess all appropriate receptors. To afford the maximum flexibility in this indicator, terrestrial and aquatic habitat indicators are reported separately for each constituent.

Benchmark Confidence Indicator. The secondary confidence indicator reflects specific criteria for ecotoxicological data used to develop ecological benchmarks (EBs) and chemical stressor concentration limits (CSCLs). For each EB and CSCL, a data quality confidence indicator was established: a “1” indicates high confidence in the study data, a “2” indicates moderate confidence in the study data, and a “3” indicates low confidence in the study data. For those receptors for which data are available, an average confidence indicator is calculated and assigned to the exemption criterion for the terrestrial and aquatic habitats, as appropriate. This is a critical distinction in interpreting the benchmark confidence indicator. The indicator only refers to the confidence in those data that were actually used to support the development of EBs and CSCLs; it does not address the quantity of receptors for which data are available. For instance, a confidence indicator of “C1” for an aquatic habitat means that, although we have low confidence in the data set to represent a sufficient number of receptors in freshwater systems, we have high confidence in the benchmarks (or CSCLs) that were developed.

Exposure Confidence Indicator. The tertiary confidence indicator reflects the quality of the data and models that are available to predict exposures through the food chain. In addition, this indicator also acknowledges the importance of these pathways given the bioaccumulation potential and persistence of a constituent. For instance, lack of empirical data on bioaccumulation for a constituent rated as having low potential for bioaccumulation should not necessarily result in a lower indicator of confidence. If exposure via the food web is determined

to be insignificant, the data requirements on uptake and accumulation in plants and prey may be lower. Thus, the exposure confidence indicator addresses our ability to evaluate the exposure pathways of concern that are likely to be of concern and acknowledges that, for certain constituents, exposure pathways through the food chain may not be completed. A confidence indicator of "exp-1" indicates that we have high confidence in our ability to evaluate relevant exposure pathways. However, this indicator may be applied to bioaccumulative as well as nonbioaccumulative constituents. For example, an overall confidence indicator of "B2exp-1" could describe two different situations: (1) moderate confidence in sufficiency of the data set across receptors as well as in the toxicity data, and high confidence in the bioaccumulation data for use in terrestrial systems, or (2) moderate confidence in sufficiency of the data set across receptors as well as in the toxicity data and low potential for exposure via the food web. In either case, our confidence is high that we are able to evaluate relevant exposure pathways of concern. In contrast, an "exp-3" indicator would suggest that the data/models are insufficient to evaluate potential exposure pathways of concern and that our confidence in the exposure profile is low.

3.2.5 Risk Metrics

Risk metrics for Phase II will be shaped by current capabilities of the 3MRA system, output needs for the SI study, and EPA decisions to modify the 3MRA system. These metrics represent the outputs of the risk analysis. The 3MRA system currently contains the exit level processor to store, process, and display risk metrics. The ELP contains three components:

- The ELP-I reads the human health and ecological risk/hazard results from the human risk and ecological risk modules and stores these results in a series of Risk Summary Output Files (RSOFs).

- The Risk Visualization Processor graphically displays the RSOFs.

- The ELP-II provides chemical-specific waste stream concentrations that meet a prespecified level of protectiveness.

Additional detail on each of these components can be found in U.S. EPA (1999v, 1999w), including example outputs.

Because the objective of the SI study is to characterize risk from impoundments in the SI universe rather than calculate protective waste concentrations, the ELP-II will not be required in its current form. EPA will decide on whether to modify the 3MRA RVP and ELP-II to meet SI Study objectives or develop a different system to process and analyze the 3MRA RSOFs depending on resources and system capabilities.

3.2.5.1 <u>Risk Bins</u>. The Phase II analysis will use the same risk bins as those used in Phase I. This will allow the Phase II results to be used to update risk bins used in Phase I. The human health risk bins currently under consideration include:

- **Excess Cancer Risk (6 bins):** $< 10^{-8}$, $\geq 10^{-8}$ and $< 10^{-7}$, $\geq 10^{-7}$ and $< 10^{-6}$, $\geq 10^{-6-}$ and $< 10^{-5}$, $\geq 10^{-5}$ and $< 10^{-4}$, $\geq 10^{-4}$.

- **Noncancer HI (6 bins, by target organ):** < 0.01, ≥ 0.01and < 0.1, ≥ 0.1 and < 1, ≥ 1 and < 10, ≥ 10 and < 100, ≥ 100).

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

The current HWIR risk bins are not quite compatible with the bins above - additional resolution is available in the 10^{-7} to 10^{-5} cancer risk range and there are only four human HQ bins. HWIR risk bins are as follows:

- **Excess Cancer Risk (7 bins):** < 10^{-8}, ≥10^{-8} and < 5×10^{-7}, ≥ 5×10^{-7} and < 10^{-6}, ≥ 10^{-6} and < 5×10^{-5},≥ 5×10^{-5} and < 1×10^{-5}, ≥ 10^{-5} and < 10^{-4}, ≥10^{-4}.

- **Noncancer HQ (4 bins, by target organ):** <0.1, ≥0.1 and <1, ≥1 and <10, ≥ 10)

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

However, the number of bins and the bin ranges are specific inputs to the HWIR 3MRA model and can be easily adjusted to meet SI Study objectives.

3.2.5.2 <u>Reporting and Maintenance of Results</u>. As with Phase I, all Phase II risk cumulative probability functions (cdfs) will be reported and maintained according to the SI Study risk attributes:

- Five regulatory status categories
- Three functional classes (storage, treatment, and disposal)
- Ttreatment types (e.g., biological, settling)
- Iindustry types
- Contaminants.

These represent five dimensions by which risk outputs will need to be organized and compiled and will require modifications to the 3MRA system as described below. Additional categories can be included and maintained as necessary (prior to the analysis) to support regulatory decision-making.

Human Health Risk Summary Output. For human risk, the HWIR 3MRA 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 (currently 0%, 5%, 25%, 50%, 75%, 85%, 90%, 95%, 98%, and 99%) for each "risk bin/waste concentration" pair by distance, pathway, receptor, cohort,[6] and critical-year (T_{crit}) method. The ELP2 takes these results and determines the Protective Summary Output File (PSOF) that specifies which waste concentrations will provide risks below the target risk level for the selected 95 percent receptors for the exposure at 80

[6] Note that the 3MRA ELP1 rolls the 5 age cohorts into 4 age cohorts by combining the age 1-6 and 7-12 child age ranges.

percent of the sites. The SI Study does not need this functionality, and, furthermore, needs to segment the SI universe into the five categories or dimensions listed above. For these reasons, a new exit level processor may be needed to produce the human risk summary outputs needed for the SI study.

The population risks estimated across facilities will be summarized for each CWA population. The aggregation will include the facility weighting for the statistically sampled CWA populations (direct and zero dischargers). For each CWA population, multiple ways of viewing the risk summaries may be needed to answer the study objectives. Most of the ways to view the risk summaries, called dimensions, are provided by the existing HWIR model (see above). These include: by exposure pathway, by receptor type, and by chemical. The five additional dimensions needed to address the SI Study study objectives (by regulatory status category, industry, treatment type, and chemical) represent a new functionality that will be needed in the 3MRA ELP. In addition, there may be the need to adjust the 3MRA RVP to graphically display risk summaries for ease of interpretation of SI risk results.

Ecological Risk Summary Output. For ecological risks, the current 3MRA ELP1 produces RSOFs with ecological hazard quotient bins that 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. As with the ELP1 human risk RSOFs, these outputs should be adequate for SI Study purposes, but a new ELP2 and possibly RVS will be needed to accommodate the five additional dimensions needed to address the SI Study study objectives.

3.3 Overview of Simulation Modules

The SI Study will use the 3MRA model for the Phase II risk assessment. To address multiple exposure simultaneously, the 3MRA model includes 17 functional modules. Figure 3-13 shows the 14 component modules of the 3MRA model that will be applied to the SI Study risk assessment.[7] These modules are briefly described in this section, with assumptions and limitations, detailed input and output requirements, and functionality provided for each module in Appendix A.

[7] Three 3MRA source modules are not needed for the SI Study risk assessment: landfill, wastepile, and aerated tank.

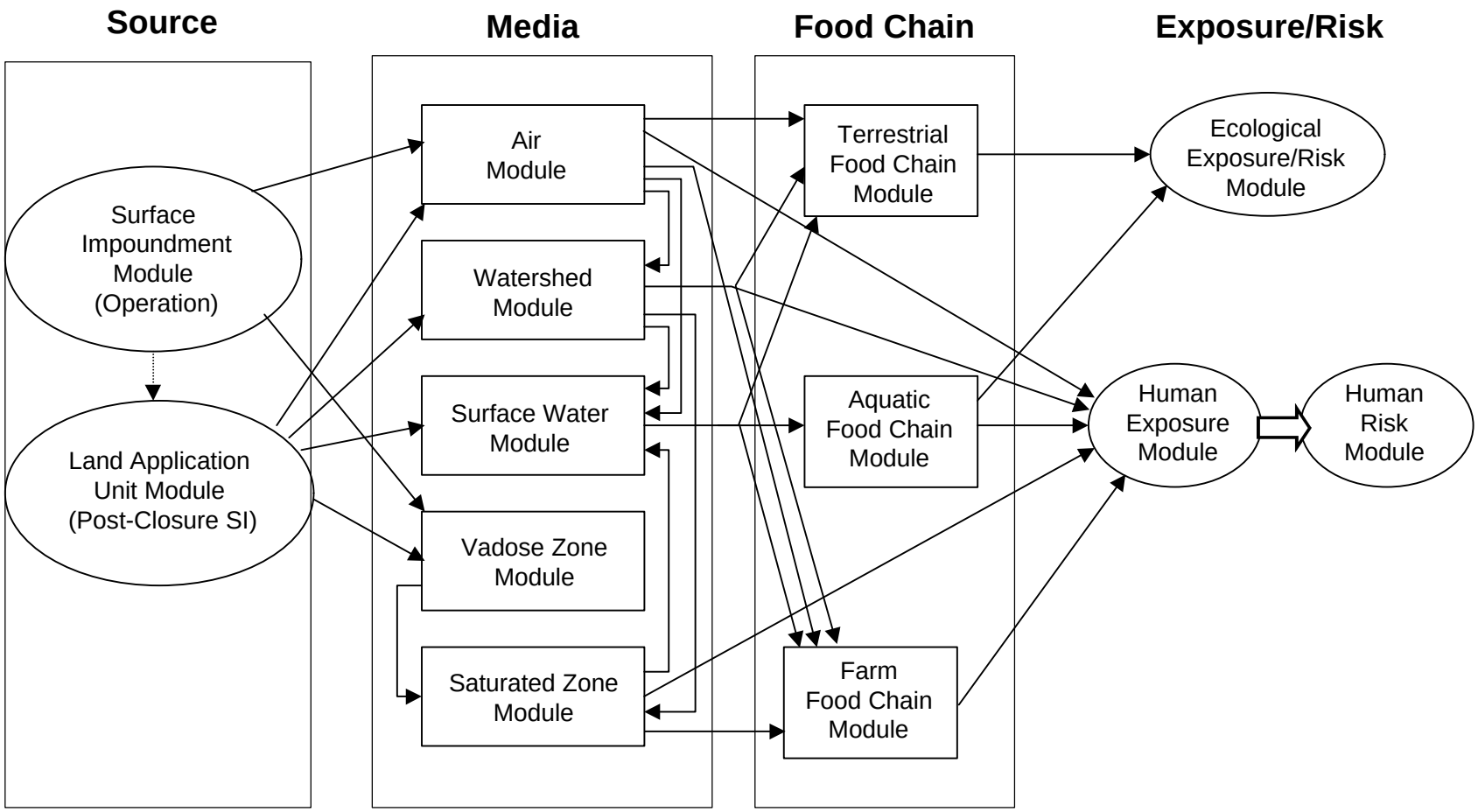


Figure 3-13. Diagram of 3MRA Model as applied to surface impoundments.

3.3.1 Source Modules

The source module employed for the SI Study risk analysis must model multimedia releases both before and after closure of the impoundment. The SI module currently in the 3MRA model only models releases up to closure. For the SI Study risk assessment, sludge from SI operation will be assumed to be left in place after closure where it is subject to volatilization, wind and water erosion, and leaching. Currently, the best option to model these processes is the 3MRA land application unit module, which includes all needed release mechanisms and can be adapted to the SI postclosure scenario simply by adjusting input variables.

The remainder of this section provides an overview of the 3MRA SI and LAU modules to be used in the SI Study risk analysis. This information was extracted and adapted from the HWIR 3MRA background documents for source modules (U.S. EPA, 1999a, 1999b), which contain additional detail, including all assumptions, governing equations, boundary conditions, solution techniques, and supporting references.

3.3.1.1 <u>Overview - SI Operating Module</u>. The SI module divides an operating SI into two primary compartments: a "liquid" compartment and a "sediment" compartment. Mass balances are performed on these primary compartments at time intervals small enough that the hydraulic retention time in the liquid compartment is not significantly impacted by the solids settling and accumulation. Figure 3-14 provides a general schematic of a module construct for an SI.

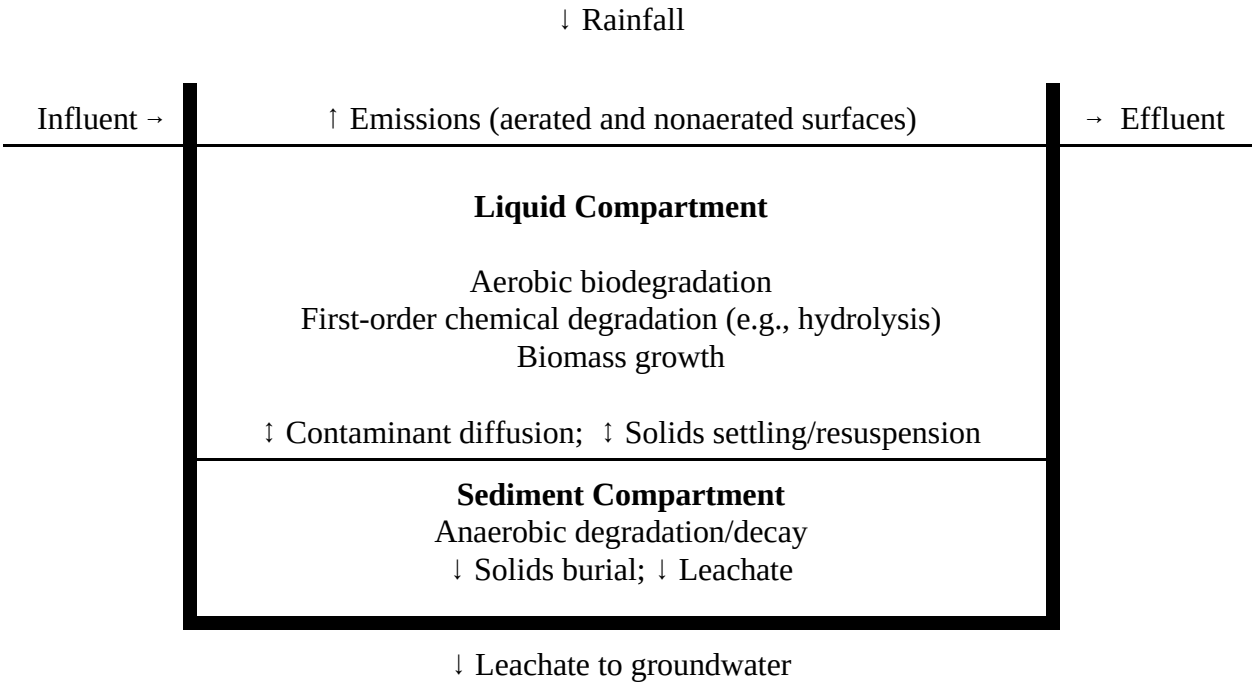


Figure 3-14. Schematic of general surface impoundment module construct.

In the liquid compartment, there is flow both in and out of the waste management unit. There is also a leachate flow to the sediment compartment and out the bottom of the surface impoundment. The leachate flow rate is estimated from liquid depth and from the hydraulic conductivities and thicknesses of the sediment compartment, the clogged native soil layer, and the underlying soil layer.

Within the liquid compartment, there is contaminant loss through volatilization, hydrolysis, biodegradation (presumably aerobic), and particle burial (net sedimentation). The sediment compartment has contaminant losses due to (anaerobic) biodegradation and hydrolysis. Some contaminant mixing between the liquid and sediment compartments occurs due to contaminant diffusion and due to particle sedimentation and resuspension.

Solids generation occurs in the liquid compartment due to biological growth; solids destruction occurs in the sediment compartment due to sludge digestion. Using a well-mixed assumption, the suspended solids concentration within the WMU is assumed to be constant throughout the WMU. However, some stratification of sediment is expected across the length and depth of the WMU so that the effective total suspended solids (TSS) concentration within the tank is assumed to be a function of the WMU's TSS removal efficiency rather than equal to the effluent TSS concentration. The liquid (dissolved) phase contaminant concentration within the tank, however, is assumed to be equal to the effluent dissolved phase concentration (i.e., liquid is well mixed). Consequently, the term "mostly well mixed" describes the liquid compartment.

The procedure used to determine the leaching rate follows the method outlined in *EPA Composite Module for Leachate Migration with Transformation Products (EPACMTP) Background Document* (U.S. EPA, 1996a). There are two important differences: (1) the liquid depth is known and (2) there is a sediment layer between the liquid and the liner.

3.3.1.2 <u>LAU (SI Postclosure) Module</u>. At the end of its operating life, an SI may be closed with sludges removed or in place. After that, remaining contaminants in the sludge and/or subsoil solid matrices are subject to release and migration through leaching, volatilization, erosion, and transport by wind and water. Although the current 3MRA SI module currently cannot model these processes from a solid matrix, the LAU module does, and can be adapted to model the SI post-closure period by modifying the model inputs.

The watershed including an LAU (or postclosure SI) is termed here the “local” watershed and is illustrated in Figure 3-15. A local watershed is defined as that drainage area that just contains the LAU (or a portion thereof — there can be multiple local watersheds where a LAU crosses a drainage divide) in the lateral (perpendicular to runoff flow) direction. The local watershed extends downslope to the point that runoff flows and eroded soil loads would enter a waterbody. Areas downslope of the LAU within the local watershed are subject to chemical contamination from the LAU through overland runoff and soil erosion.

Figure 3-16 illustrates how the local watershed is conceptualized within the LAU module, that is, as a two-dimensional, two-medium system. The dimensions are longitudinal, i.e., downslope or in the direction of runoff flow, and vertical, i.e., through the soil column. The media are the soil column

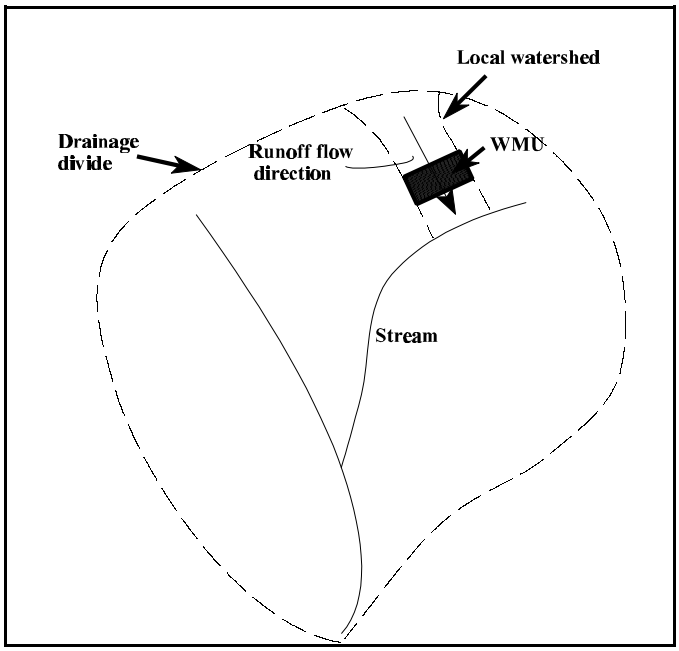


Figure 3-15. Local watershed containing WMU.

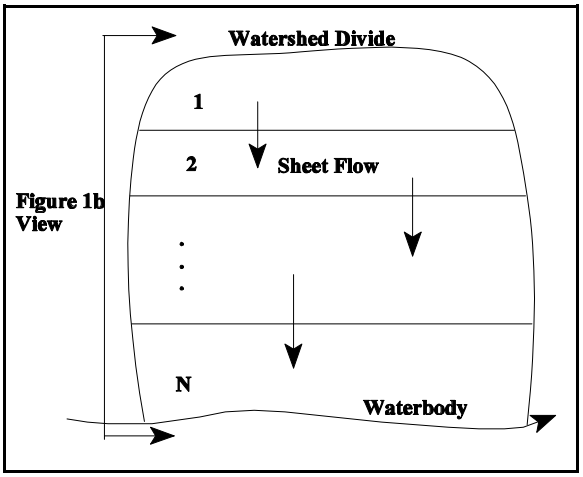


Figure 3-16a. Local watershed.

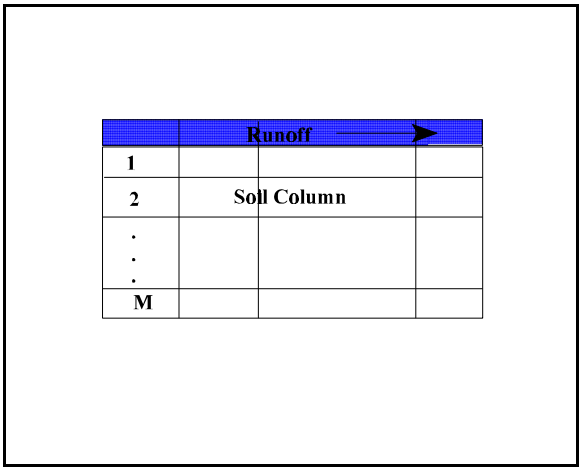


Figure 3-16b. Cross-section view.

and, during runoff events, the overlying runoff water column. The local watershed is assumed to be made up of, in the longitudinal direction, an arbitrary number of land subareas that may have differing surface or subsurface characteristics, e.g., land uses, soil properties, and chemical concentrations. For example, subarea 2 might be a WMU, subarea 1 would then represent an upslope area, and subareas 3 through N would be downslope buffer areas extending to the waterbody.

3.3.2 Air Module

The purpose of the atmospheric modeling for the 3MRA is to estimate, at various receptor points in the area of interest, the annual average air concentration of dispersed 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. Additional detail on the air module can be found in U.S. EPA (1999c and 1999d).

The atmospheric module simulates the transport and diffusion of chemical constituents, which are in the form of volatilized gases or fugitive dust emitted from area sources. The simulated air concentrations are used to estimate bio-uptake from plants and human exposures due to direct inhalation. The predicted deposition rates are used to determine chemical loadings to watershed soils, farm crop areas, and surface waters.

The atmospheric concentration and deposition of constituents can be determined in several ways. However, the selected procedure has to be computationally efficient to satisfy the HWIR requirements of numerous simulations within a Monte Carlo framework. Because the modeling is site-based, the steady-state Gaussian plume modeling approach was considered to be appropriate and, the ISCST3 model was selected. The model provides estimates of contaminant concentration, dry deposition (particles only), and wet deposition (particles and gases) for user-specified averaging periods (i.e., annually).

ISCST3 is used as legacy code in the 3MRA framework. That is, the model is left intact and the necessary interfacing to the framework 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 environment are referred to as the Air Module. The pre- and postprocessing code also provides additional functionality to support other 3MRA framework requirements.

3.3.3 Watershed Module

Chemical mass can be released from a surface impoundment in the form of volatile emissions from an operating impoundment or volatile and particulate emissions from a closed unit (modeled by the source module, Section 3.3.1). These emissions can then be transported and deposited onto the soils of nearby land areas as wet or dry deposition (modeled by the air module, Section 3.3.2). Once deposited, a chemical is then subject to fate and transport processes within the watershed on which it is deposited and it is available either for direct exposure to human or ecological receptors or indirect exposure through a food chain. It is the purpose of the watershed module to model these fate and transport processes. Additional detail, including all governing equations, can be found in U.S. EPA (1999f).

Fate and transport processes simulated by the watershed module are volatilization, leaching, runoff, erosion, and biological and/or chemical degradation. Transport of chemical by runoff and erosion is 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 (see Section 3.3.1.2), 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; that is, no spatial chemical concentration gradients are simulated within a given watershed.

3.3.4 Groundwater (Vadose and Aquifer) Modules

The HWIR 3MRA vadose and aquifer modules are a modified version of EPACMTP (U.S. EPA, 1996a,b,c). This code simulates the fate and transport of contaminants released from land-based waste management units through the underlying unsaturated or vadose zone (soil) and saturated zone (surficial aquifer). EPACMTP replaced EPACML (U.S. EPA, 1993a) as the best available tool to predict potential exposure at a downstream receptor well. EPACMTP offers improvements to EPACML by considering: (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 module that simulates infiltration and dissolved constituent transport through the vadose zone, which is coupled with a three-dimensional saturated zone module. The saturated zone module consists of a three-dimensional groundwater flow submodule and three-dimensional transport submodules. The saturated zone groundwater flow submodule 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 submodule accounts for three-dimensional advection and dispersion and linear or nonlinear equilibrium sorption.

Interrelationships between the vadose and saturated zone modules and other modules (through water and chemical mass fluxes) under the 3MRA framework are shown in Figure 3-17. As shown in the figure, the vadose zone module receives infiltration and solute mass fluxes from the source module. The migration of contaminants in the vadose zone is terminated at the water table where the contaminant fluxes, in the form of concentrations, are transferred to the saturated zone module. The SZM also receives areal recharge from the watershed module. The SZM provides time-dependent, annual average contaminant concentrations at receptor wells and annual average contaminant fluxes at an intercepting stream located somewhere in the modeled domain.

Detailed descriptions of both modules, including their purpose and scope of application, mathematical formulations, and use in HWIR99, are provided in U.S. EPA (1999g). Additional information relating to the EPACMTP and its verification is provided in the background documents for EPACMTP (U.S. EPA, 1996a,b,c, 1997a).

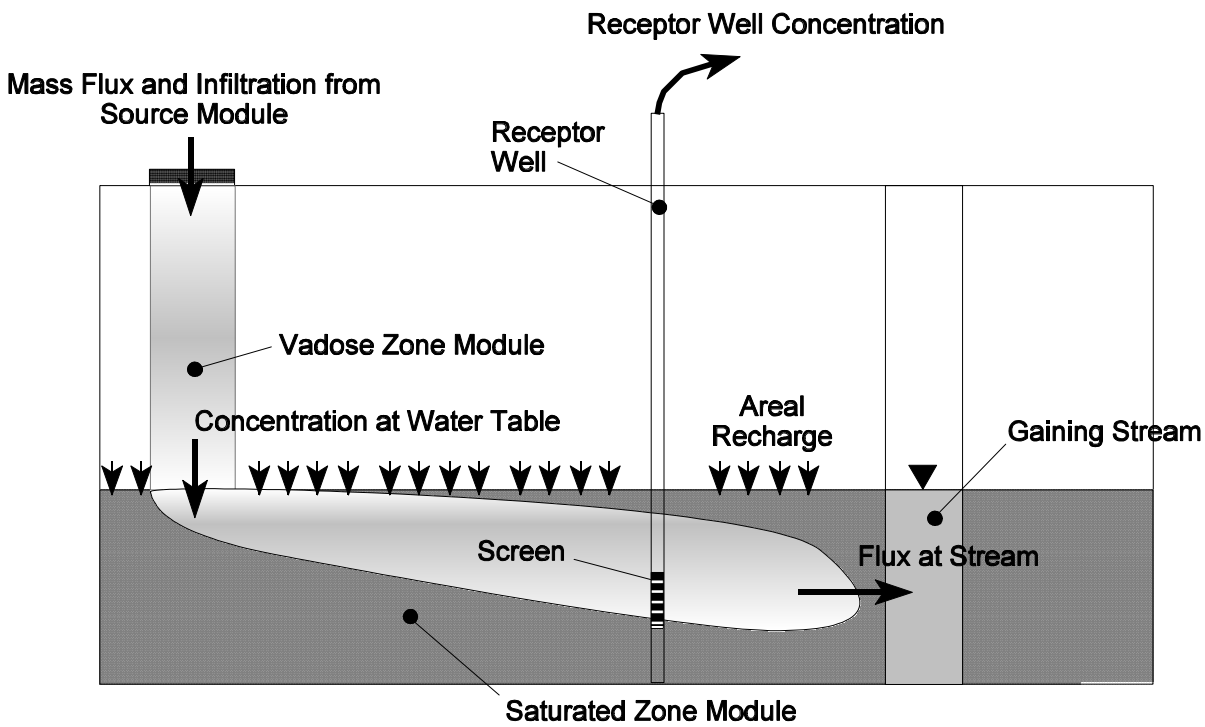


Figure 3-17. Conceptual model of vadose zone and saturated zone.

3.3.5 Surface Water Module

The 3MRA surface water module models streams, lakes, ponds, and wetlands. Chemical mass released from a WMU can enter a nearby surface waterbody network in runoff and erosion directly from the WMU, from atmospheric deposition to the water surface, in runoff and erosion from adjoining watershed subbasins, and by interception of contaminated groundwater. 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 in the 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 3MRA surface water module consists of the core model EXAMS II (Burns, 1997; Burns et al., 1982) and the interface module ExamsIO. More detailed documentation can be found in U.S. EPA (1999u), from which the following material was extracted.

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.

In the HWIR 3MRA, stream reaches of orders 3 to 5 are evaluated, as defined by the Strahler ordering system (Strahler, 1957). Order three reaches are assumed to support fish populations. Reaches of order greater than 5 are assumed to carry sufficient annual average dilution flow that concentrations of chemicals of interest can be reasonably assumed to be at background levels (U.S. EPA, 1999u).

3.3.6 Farm Food Chain Module

The farm food chain (FFC) 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 FFC module is based on recent and ongoing research conducted by EPA's Office of Research and Development (ORD) and presented in *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (U.S. EPA, in press). Additional detail about the background and implementation of the model is available in U.S. EPA (1999i).

The FFC module is designed to predict the accumulation of a contaminant in the edible parts of a plant 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 (e.g., 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 FFC 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 module was designed with this functionality because not all study areas contain farms, and the methodology developed for farms is different than that developed for the home gardener. The program for home gardeners uses point estimates of air and soil concentrations at the residential receptor location assigned to each census block. In contrast, the program 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.

Because the behavior of each chemical constituent is, to a large degree, determined by chemical properties, the module includes a series of chemical-specific switches that turn on the appropriate subroutines, depending on whether the chemical is an organic (O), metal (M), special

(S), or dioxin-like (D). For most organic chemicals, the industrial exposure 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. Metals, dioxin-like chemicals, and special chemicals generally use literature values for these various biotransfer factors, when available. For dioxin-like compounds and special chemicals, the biotransfer factors are calculated in the same way as for organics if literature values are not available.

3.3.7 Terrestrial Food Web Module

The terrestrial food web module (TerFW) 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 (EcoEx) 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 5 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. Supporting detail about the background and implementation of the model is available in U.S. EPA (1999j).

The conceptual approach used in developing the TerFW 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 TerFW 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 the 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.[8]

As with the Farm Food Chain module, the TerFW 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, in press). The model subroutine distinguishes among different types of chemicals, using empirically derived algorithms for some chemicals and bio-uptake data from field or greenhouse studies for other chemicals. The TerFW 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. Specific differences exist between the FFC module and the TerFW module in predicting plant concentrations.

[8] Exposures are prorated depending upon the relationship of the home range to the habitat contained within the area of interest. For details, see U.S. EPA, 1999l.

To estimate the concentrations in other categories of terrestrial prey items (e.g., earthworms, small birds), the TerFW 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., 1998). A thorough discussion of these data is provided in the data collection documentation for the FFC and TerFW modules.

3.3.8 Aquatic Food Web Module

The aquatic food web (AqFW) module calculates chemical concentrations in aquatic organisms that are consumed by human and ecological receptors (e.g., fish filet, 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 cold water and warm water aquatic habitats. Supporting detail about the background and implementation of the model is available in U.S. EPA (1999k).

The underlying framework for the AqFW 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/rivers, permanently flooded wetlands, ponds, and lakes. Simple food webs were constructed for each of the eight freshwater habitats (four cold water and four warm water) 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). Prey preferences are based on optimal foraging theory (Gerking, 1994). For each freshwater habitat, the feeding guilds for various types and sizes of fish (e.g., medium benthivore) were used to construct a simple food web and to map dietary preferences for organisms in each habitat (U.S. EPA, 1999o). The habitat types are less important for some constituents (e.g., metals) for which empirical data are used to relate the water concentration to tissue concentration. However, the food web structure and species assignments are critical in determining concentrations of hydrophobic constituents in aquatic organisms.

The AqFW methodology introduces several new approaches to modeling representative aquatic systems. First, the AqFW module uses a probabilistic algorithm that cycles through the database on prey preferences to select dietary fractions for TL3 and TL4 fish for predicting tissue concentrations. Second, the AqFW module implements a flexible matrix that allows for the simultaneous solution of all compartments (e.g., benthos, zooplankton, fish) in the system. This functionality allows the module to perform calculations efficiently and provides the flexibility for adding additional compartments and/or interactions to the food web structure.

3.3.9 Human Exposure Module

The human exposure module calculates the applied dose (milligram of constituent per killogram 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.[9]

[9] See Section 3.3.10 for the list of receptors and cohorts and applicable exposure pathways.

The human exposure module calculates exposures for two basic receptor types: residential receptors (residents and home gardeners) and 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. The subcategories within residential receptors and farmers differ in the particular exposures they incur. For example, a resident (only) differs from a home gardener in that home gardeners are exposed to contaminated fruits and vegetables, but residents are not. 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). Additional detail about the background and implementation of the model is available in U.S. EPA (1999q).

For HWIR, the human exposure module uses distributions for most exposure factors (e.g., contact rates, body weight) that are derived from data in the *Exposure Factors Handbook* (U.S. EPA, 1997b). Exceptions include exposure duration (9 years for carcinogens, 1 year for noncarcinogens) and "fraction contaminated," specified as point estimates for each medium/feed item.

3.3.10 Human Risk Module

The essence of the 3MRA 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 two basic human receptor types: residential receptors (residents and home gardeners) and 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. These receptor categories were developed considering the exposure pathways of concern, and the category names suggest the associated exposure pathway(s). For example, a resident is exposed only to the baseline exposure pathways, i.e., inhalation via ambient air and shower along with soil and groundwater ingestion, with the home gardener being exposed through these exposure pathways plus ingestion of homegrown produce. Additional detail about the background and implementation of the model is available in U.S. EPA (1999r).

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 risks and/or HQs for each category. However, to maintain output storage at reasonable levels, it aggregates results into four[10] composite receptor categories (resident, resident gardener, fisher, and farmer) to develop the cumulative population[11] frequency histograms and critical years. These three basic human risk module functions (calculating risk/HQ, building cumulative frequency histograms, and

[10] The 3MRA Exit Level Processor (ELP) preserves this receptor resolution, but also aggregates these four receptors into a fifth, "all receptors" category.

[11] Site-specific receptor populations identified as part of HWIR data collection activities are specified by receptor category, exposure area (farm or census block), and distance ring (U.S. EPA, 1999t).

determining critical year) are performed for each radial distance in a series of nested loops, as illustrated in Figures 3-18a through 3-18c.[12]

For example, the composite "fisher" receptor population consists of subpopulations from the resident fisher, resident gardener fisher, beef farmer fisher, and dairy farmer fisher receptor categories. Similarly, beef farmers and dairy farmers are aggregated into a single, composite "farmer." A complete mapping of the eight receptor categories as output by the Human exposure module to their composited receptor categories as output by the human risk module is presented in Table 3-7. Table 3-7 also shows the applicable exposure pathways for the receptor categories. In this section, the term "receptor" is used to mean either one of the eight most disaggregated receptor categories, or one of the four composited receptor categories, as appropriate to the context. In addition, a cohort is defined as a receptor subpopulation based on age. Five cohort classes are considered in the human risk module[13]: Child 1 (0 to 1 year old), Child 2 (1 to 5 years old), Child 3 (6 to 11 years old), Child 4 (12 to 19 years old), and adult (greater than 19 years old).

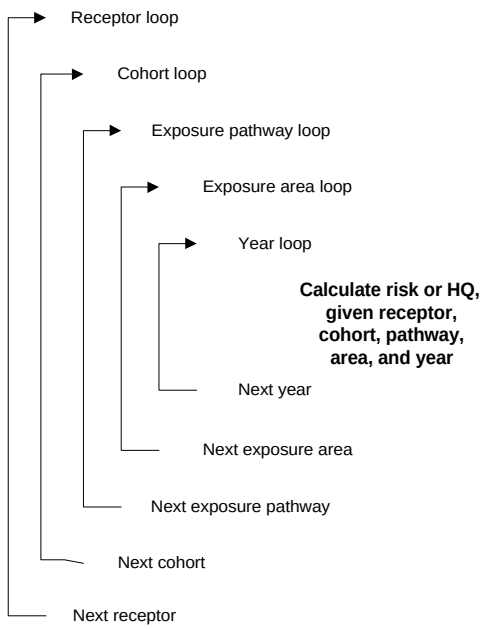


Figure 3-18a. Looping structure to calculate risk or HQ.

[12] These illustrations are intended only to facilitate overall understanding of the module; the implementing computer code is significantly different to optimize performance.

[13] For purposes of storage efficiency, the ELP combines the Child 2 and 3 cohort classes as output by the human risk module into a single composite cohort class (ages 1 to 11). Child 4 is also combined with the adult cohort class by the ELP.

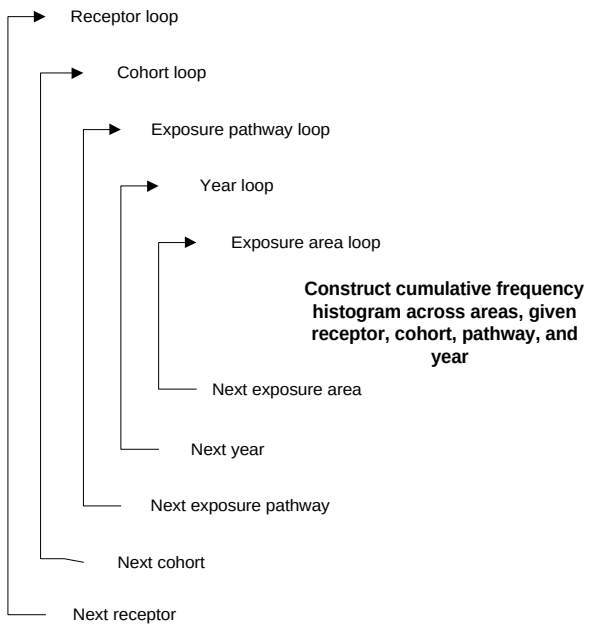


Figure 3-18b. Looping structure to build cumulative frequency histograms.

Table 3-7. Applicable Receptor/Pathway Combinations

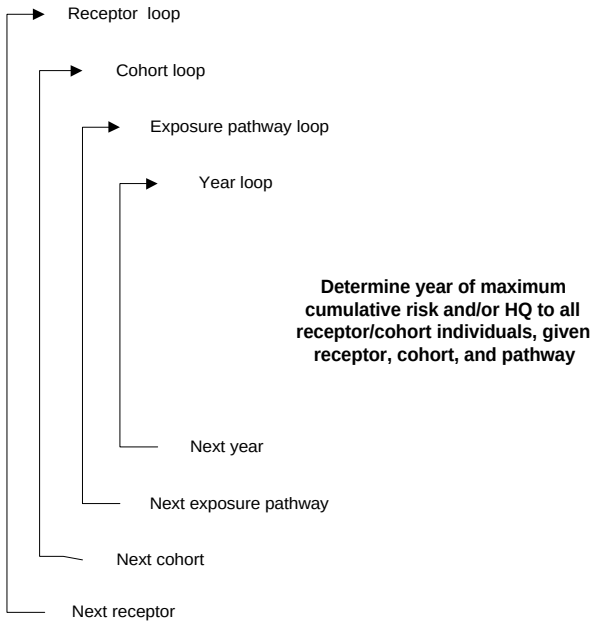


Figure 3-18c. Looping structure to determine critical year.

Pathway	Receptors (as output by Human Risk Module)							
	Resident	**Resident Gardener**	**Fisher**				**Farmer**	
	Receptors (as output by Human Exposure Module)							
	Resident	**Resident Gardener**	**Resident Fisher**	**Resident Gardener Fisher**	**Beef Farmer Fisher**	**Dairy Farmer Fisher**	**Beef Farmer**	**Dairy Farmer**
1. Air inhalation	yes	yes	yes	yes	yes	yes	yes	yes
2. Soil ingestion	yes	yes	yes	yes	yes	yes	yes	yes
3. Water ingestion	yes	yes	yes	yes	yes	yes	yes	yes
4. Crop ingestion	no	yes	no	yes	yes	yes	yes	yes
5. Beef ingestion	no	no	no	no	yes	no	yes	no
6. Milk ingestion	no	no	no	no	no	yes	no	yes
7. Fish ingestion	no	no	yes	yes	yes	yes	no	no
8. Shower inhalation[a]	yes	yes	yes	yes	yes	yes	yes	yes
9. Infant breast milk[b]	yes	yes	yes	yes	yes	yes	yes	yes

[a] Shower inhalation applies only to child 4 and adult cohorts. All other pathways shown apply to all noninfant cohorts.
[b] Applies only to child 1 (infant) cohorts.

The nine individual exposure pathways considered by the human risk module are shown in Table 3-7. All exposure pathways do not apply to all receptors; those that are applicable are indicated by “yes” in the table. With respect to applicability among receptor cohorts, if a pathway applies to a receptor, then it applies to all cohorts of that receptor, with two exceptions: (1) shower inhalation applies only to child 4 and adult cohorts (younger children are assumed to bathe as opposed to shower), and (2) the infant breast milk pathway applies only to breastfeeding infants.[14, 15]

Because the essence of a multipathway risk assessment is the evaluation of total risks incurred as a result of simultaneous exposure from different pathways, the human risk module considers four different pathway aggregations as shown in Table 3-8. The inhalation route aggregates over the two inhalation pathways. The ingestion route aggregates over all ingestion

[14] For HWIR99, the infant breast milk pathway is evaluated only for a single chemical, the dioxin species 2,3,7,8 -TCDD TEQ [CAS No. 1746-01-6]. (That is, the logical flag *ChemBreastMilkExp* will be set to “true” only for this chemical in the chemical properties input file, cp.ssf.)

[15] For the infant breast milk pathway, the margin of exposure [MOE] (mg/kg-d) is analogous to HQ for infant breast milk exposure. Hereinafter, HQ will be understood to mean "MOE" for the Child 1 cohort and breast milk pathway.

Table 3-8. Pathway Aggregations

Pathway	Inhalation Route	Ingestion Route	Groundwater	Multipathway
1. Air inhalation	✓			✓
2. Soil ingestion		✓		✓
3. Water ingestion		✓	✓	✓
4. Crop ingestion		✓		✓
5. Beef ingestion		✓		✓
6. Milk ingestion		✓		✓
7. Fish ingestion		✓		✓
8. Shower inhalation	✓		✓	✓

pathways. The groundwater aggregation includes the two groundwater-based pathways (drinking water ingestion and shower inhalation). Finally, the multipathway aggregation includes all combinable[16] pathways. (The infant breast milk pathway is a separate pathway that is not relevant to the route aggregations and is not included in the table.)

The radial distance rings are set at 500 meters, 1,500 meters, and 2,000 meters from a circle circumscribing the (square) WMU (Figure 3-19). Thus, the first set of risk and/or HQ results is applicable only to those receptors residing within 500 meters of the WMU boundary. The second set applies to **all** receptors within 1,000 meters, including those previously considered within 500 meters. The third set applies to all receptors within 2,000 meters, which includes all receptors within the overall Area of Interest.

3.3.11 Ecological Exposure Module

The ecological exposure (EcoEx) module, initially developed in support of the HWIR 3MRA, 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 EcoEx 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: (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.

[16] The feasibility of pathway additivity is chemical-specific and is specified by the logical variables *ChemC_add* and *ChemNC_add* in the chemical properties input file.

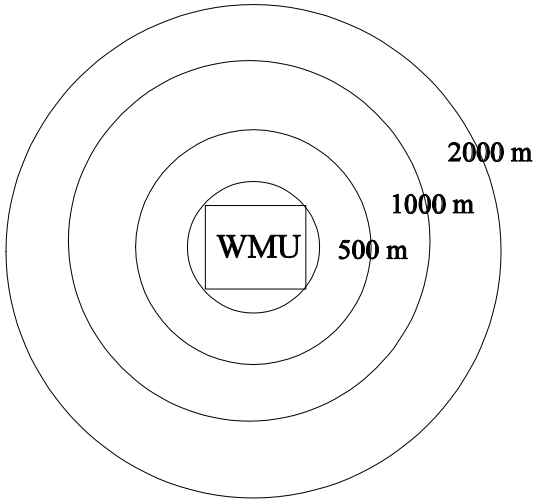


Figure 3-19. WMU with three radial distance rings.

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). Additional detail about the background and implementation of the model is available in U.S. EPA (1999l).

The conceptual approach in developing the ecological exposure assessment for HWIR was to reflect 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 EcoEx module is based on a representative habitat scheme to increase the resolution of general terrestrial and freshwater systems. The spatial characteristics of the site-based database were determined using a geographic information system (GIS) delineation tool to define habitat boundaries and linkages, home ranges, wetland areas, and surface waterbodies. A cross-referencing database was developed to automate the selection of receptors and assign them to habitats based on habitat characteristics and ecological region. A complete description of the habitats, home ranges, receptors, and delineation scheme implemented in the GIS format is found in U.S. EPA (1999n).

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. 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 chemical type and, therefore, contaminant concentrations in some food items may be near zero for chemicals 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 over 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.

3.3.12 Ecological Risk Module

The ecological risk (EcoRisk) module calculates HQs[17] for a suite of ecological receptors assigned to habitats delineated for study 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 the EcoRisk module is, to a large degree, determined by both the home ranges and habitats delineated at each site. Additional detail about the background and implementation of the ecological risk module is available in U.S. EPA (1999m).

Home range areas are defined in terms of species-specific foraging area size as well as the habitat and predator-prey interactions, that is, the home ranges are constrained by habitat boundaries[18] and represent predator-prey interactions. Spatially averaged concentrations in media, plants, and prey items are calculated for each home range and used to estimate the applied dose to receptors in the ecological exposure (EcoEx) module. In addition, soil concentrations for each home range are compared to threshold concentrations for adverse effects in plants and soil biota.

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 EBs) and media concentrations (for comparison with CSCLs).

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. The HQ risk bins are used in developing cumulative distribution functions of risk and are defined as: (1) below 0.1, (2) between 0.1 and 1, (3) between 1 and 10, (4) between 10 and 100, and (5) above 100. Each of the HQs calculated by the EcoRisk 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.

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[17] Hazard quotients are defined as: (1) the ratio between applied dose received from the ingestion of contaminated media and food items and an ecological benchmark (EB in units of dose), and (2) the ratio between the concentration in the medium of interest (soil, sediment, or surface water) and a chemical stressor concentration limit (CSCL in units of concentration).

[18] If the home range area is larger than the area of the habitat, the home range is presumed to extend beyond the 2-km radius that defines the area of interest; that is, habitats are exclusive. If the home range is smaller than the habitat, the entire home range is presumed to fall within the habitat boundaries within the area of interest.

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)
- Rreceptor group (e.g., mammals, amphibians, soil community)
- Ttrophic level (i.e., producers, TL1, TL2, TL3 top predators).

The maximum HQ across the site is also reported along with its ecological risk attributes. This metric was added for use in "pass/fail" analyses that may be needed to prioritize sites for additional analyses.

In calculating receptor-specific HQs, the EcoRisk module does all of the necessary accounting to develop distributions based on the specific receptor and habitat groupings of interest. The EcoRisk module reads in information about the chemical concentrations that each receptor is exposed to, calculates hazard quotients based on the EB or CSCL and the chemical exposure information, and provides summaries of ecological risk information for the simulation to determine when critical years with maximum HQs are experienced. For any given year, the set of HQ data is stored as a series of distributions along with their attributes. As indicated above, 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 receptors with HQ values in the range defined for the given bin.

Each site is constructed as a set of habitats, each located within one or more distance rings at the site, and a set of receptors inhabiting ranges within each of those habitats. Habitats have a variety of characteristics, including a unique index identifier, a habitat type and group, a number of reaches, a number of ranges containing receptors, and the receptors associated with each range. Reaches, habitats, and ranges also have chemical concentrations associated with them. Each receptor has an index, type, name, group, trophic level. To a large degree, the habitats reflect differences in vegetative communities based on various land use and land cover data layers. Home ranges are assigned to each habitat based on the median size of receptor species' foraging and feeding ranges. Ecological receptors were grouped into four different home range sizes: 1,000,000,000, 10,000,000, 1,000,000, and 100,000 square meters. These home ranges were approximated for size (by an expanding a circular polygon) and randomly placed within each habitat polygon so that they overlap to reflect predator-prey relationships.

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). It is important to note that 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.

3.4 3MRA Modifications and Data Collection Requirements

As described previously, the 3MRA Model has the basic functionality and features necessary to characterize risks for the purposes of the SI Study. However, because the specific needs of the SI Study are somewhat different than those for HWIR, there will be some necessary modifications to the 3MRA component models and modeling system. In addition, data availability is better for the SI Study, both in terms of site-specific data from the SI Survey and better, more complete data from other sources. Using these improved data sources in the 3MRA model for the SI Study will require some modifications to the HWIR data collection methodologies.

This section summarizes the model and data collection modifications that may be necessary to implement the 3MRA model for the SI Study. It is intended to outline the major topic areas and alternatives for planning purposes. Although this represents the major areas to be addressed, other changes may be necessary as the analysis evolves. As the Phase I screening analysis progresses, EPA will continue to investigate and expand on these modifications, addressing those necessary before Phase II modeling begins.

3.4.1 Model Modifications

The basic functionality of the 3MRA model will be maintained for the SI Study. Modifications of the HWIR modeling construct for the SI Study that can be handled with simple changes in model inputs (e.g., risk bins, risk distance rings) are not addressed here. More substantive revisions to the current model construct are needed to address the following limitations.

- The current 3MRA system cannot model multiple units at a site.
- The current surface impoundment model cannot model a postclosure scenario or catastrophic failures.
- The Exit Level Processor 2 (ELP2), which produces exit level waste concentrations from the ELP1 risk database, does not meet SI Study objectives.

Current objectives require that the SI Study Phase II risk results be organized in terms of the SI Study risk attributes that are beyond the dimensions currently addressed by 3MRA.

3.4.1.1 <u>Multiple Surface Impoundments</u>. Multiple surface impoundments cannot be modeled simultaneously by the 3MRA Model, and modifying the current system to allow this would require an extensive, system-wide redesign that is well beyond the scope of this effort. To address risks from multiple units will require running the model separately for each unit and combining risk results after modeling during postprocessing. This will require cognizance of this need during data collection and site layout definition (i.e., an identical site layout for all units at a site), as well as consideration of this need during the development of postprocessing techniques for Phase II SI Study risk results.

3.4.1.2 <u>SI Postclosure Scenario</u>. As discussed in Section 3.3.1, the postclosure scenario for the SI Study will be handled by using the LAU module to model a closed SI with sludge left

in place. The LAU module has the functionality necessary to model a closed SI with just changes in module inputs. Currently envisioned alternatives for using the LAU module in this context include

- Combining the SI and LAU modules into a single source module
- Modification of the 3MRA Site Definition Processor to run the LAU module after the SI module to model the SI post closure period and to combine results of the two modules into a single source module output file
- Separate 3MRA model runs for operating and postclosure periods.

The latter option could be problematic because SI module outputs (i.e., sludge concentrations) will be needed as inputs for the LAU module.

3.4.1.3 SI Catastrophic Failure. The SI Survey is collecting data on occurrences of catastrophic failures within the SI universe. EPA will evaluate these results in deciding whether to analyze the risks that could result from such events.

3.4.1.4 ELP - Postprocessing Options. The postprocessing functionality of the ELP2 is not needed for the SI Study and this module will not be used during Phase II modeling. The ELP1 does provide and access a database of the results needed for the SI Study objectives, but additional data processing will be required to summarize results by the SI Study risk attributes:

- Multiple impoundments at a site
- Five regulatory status categories
- Three functional classes (storage, treatment, and disposal)
- Treatment types (e.g., biological, settling)
- Industry types
- Contaminants.

These represent additional dimensions to those currently provided by the 3MRA ELP1. Risk outputs will need to be organized and compiled by these dimensions; this will require either modifications to the 3MRA system or separate postprocessing of the Access database (ouput by the ELP1) containing the Protective Summary Output Files (PSOFs). EPA will decide on the best option, considering the need for automation (i.e., system modifications) in light of the number of SI facilities modeled and data analyses necessary to meet decision-making needs.

3.4.2 Data Collection Requirements

In general, data collection methods developed and documented for the HWIR implementation of 3MRA will be adequate for the SI Study. National and regional data collected for HWIR will likely be suitable for SI Study purposes, although it may be necessary to employ automated HWIR methodologies to collect data to characterize regions with SI sites not covered for the HWIR sites. The main effort necessary for the SI Study will be the collection of site-based

data to characterize the SI Study sites. Specific issues associated with this effort are discussed in the following section.

3.4.2.1 Utilization of SI Survey Data. The SI Survey provides a rich source of data for the Phase II analyses, providing accurate facility locations, SI dimensions and operating characteristics, waste properties and constituents, soil and hydrogeologic information, and receptor locations. Incorporation of these data will require some modification to current 3MRA data collection methods, but will result in a more robust and accurate dataset. EPA is currently designing the survey data coding and database to be compatible with 3MRA data needs. Most of the following points relate to the use of these data.

3.4.2.2 Modificationof the Area of Interest (AOI). Because multiple SIs are present at many facilities, and because the SI Study design requires risks to be combined for such multiple units, a single AOI will be needed so that receptors and other aspects of the site layout will be identical for all units at the site. This, and knowledge of the exact shape of each SI will require an irregular AOI, as shown in the example in Figure 3-20. This is not a problem from the system standpoint, but does represent a change from the circular 3MRA AOI.

3.4.2.3 Receptor Locations. Ecological receptors and habitats will be delineated as they were for the HWIR analysis. Human receptor data are being collected in the survey as residence locations on topographic maps. Initial evaluation of the survey results suggests that these data are variable in extent, quality, and time frame from respondent to respondent. It is possible that the 3MRA automated data collection methodologies for U.S. Census data will be needed to supplement the survey receptor data. The combined dataset will provide improved resolution and accuracy of receptor locations over the use of the Census data alone, especially in sparsely populated areas where residences are far apart. In more populated areas, the Census data will be valuable in providing additional information on the number of households in dense residential areas. The combination of these data at an SI site with varying residential densities is shown in Figure 3-20.

3.4.2.4 Watershed and Waterbody Delineation. Limited resolution and data quality problems of the topographic and hydrographic base data posed a challenge during watershed and waterbody delineation for the HWIR 3MRA. Fortunately, higher-resolution, better-quality data are now available as the National Elevation Dataset (NED) and the National Hydrography Dataset (NHD), as well as in the topographic maps available for every SI facility. These data, combined with the now finalized 3MRA site layout system, should greatly improve the efficiency of waterbody and watershed delineations for the SI Study sites addressed in the Phase II analysis.

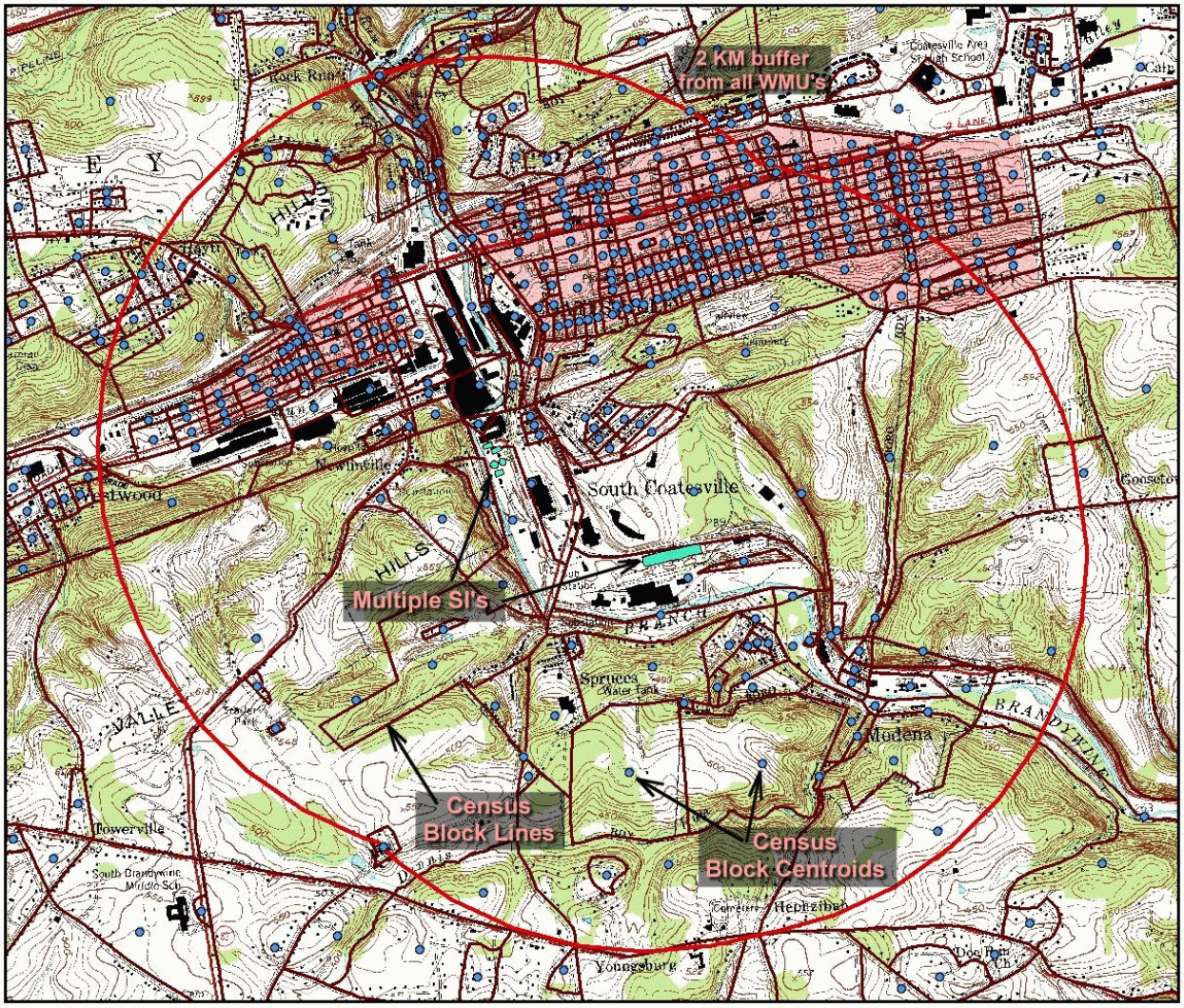

Figure 3-20. Area of interest for multiple SI site illustrating overlay of topographic and U.S. census data.

4.0 References

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Appendix A

Comprehensive List of Toxicity Benchmarks for Human Health Risk Assessment

Table A-1. Comprehensive List of Toxicity Benchmarks

Constituent Name	CAS No.	Benchmarks Selected for Use in Deriving Phase 1A Screening Levels					
		Oral (RfD)	RfC (mg/m^3)	Oral CSF (food) (per mg/kg/d)	Oral CSF (H2O) (per mg/kg/d)	Inh URF (per ug/m^3)	Inh CSF (per mg/kg/d)
Acenaphthene	83329	6.0E-02					
Acetaldehyde	75-07-0		9.0E-03			2.2E-6	
Acetone	67641	1.0E-01					
Acetonitrile	75-05-8		6.0E-02				
Acetophenone	98-86-2	1.0E-01					
Acrolein	107-02-8	2.0E-02	2.0E-05				
Acrylamide	79-06-1	2.0E-04		4.5E+0	4.5E+0	1.3E-3	4.5E+0
Acrylic acid	79-10-7	5.0E-01	1.0E-03				
Acrylonitrile	107-13-1	1.0E-03	2.0E-03	5.4E-1	5.4E-1	6.8E-5	2.4E-1
Aldicarb	116-06-3	1.0E-03					
Aldrin	309-00-2	3.0E-05		1.7E+1	1.7E+1	4.9E-3	1.7E+1
Allyl alcohol	107-18-6	5.0E-03					
Allyl chloride (3-chloropropene)	107-05-1		1.0E-03				
Ammonium vanadate	7803-55-6						
Amonium perchlorate	7790-98-9						
Aniline	62-53-3		1.0E-03	5.7E-3	5.7E-3		
Anthracene	120-12-7	3.0E-01					
Antimony	7440-36-0	4.0E-04					
Antimony trioxide	1309-64-4	4.0E-04	2.0E-04				
Aramite	140-57-8	5.0E-02		2.5E-2	2.5E-2	7.1E-6	2.5E-2
Arsenic, inorganic	7440-38-2	3.0E-04		1.5E+0	1.5E+0	4.3E-3	
Barium	7440-39-3	7.0E-02	5.0E-04				
Benz(a)anthracene	56-55-3			7.3E-01	7.3E-01		
Benzene	71-43-2			2.9E-2[a]	2.9E-2[a]	8.3E-6[a]	2.9E-2[a]
Benzidine	92-87-5	3.0E-03		2.3E+2	2.3E+2	6.7E-2	2.3E+2
Benzo(a)pyrene	50-32-8			7.3E+0	7.3E+0		
Benzo(b)fluoranthene	205-99-2			7.3E-01	7.3E-01		
Benzyl alcohol	100-51-6	3.0E-01					
Benzyl chloride	100-44-7			1.7E-1	1.7E-1		
Beryllium	7440-41-7	2.0E-03	2.0E-05			2.4E-3	8.4E+0
Bis(2-chloroethyl)ether	111-44-4			1.1E+0	1.1E+0	3.3E-4	1.1E+0
Bis(2-chloroisopropyl)ether	39638-32-9	4.0E-02		7.0E-2	7.0E-2	1.0E-5	3.5E-2
Bis(2-ethylhexyl)phthalate (DEHP; also di-)	117-81-7	2.0E-02		1.4E-2	1.4E-2		
Bis(chloromethyl)ether	542-88-1			2.2E+2	2.2E+2	6.2E-2	2.2E+2
Bromoform	75-25-2	2.0E-02		7.9E-3	7.9E-3	1.1E-6	3.9E-3
Bromomethane (methyl bromide)	74-83-9	1.4E-03	5.0E-03				
Butadiene, 1,3-	106-99-0					2.8E-4	1.8E+0
Butanol, n- (n-butyl alcohol)	71-36-3	1.0E-01					

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	Benchmarks Selected for Use in Deriving Phase 1A Screening Levels					
		Oral (RfD)	RfC (mg/m^3)	Oral CSF (food) (per mg/kg/d)	Oral CSF (H2O) (per mg/kg/d)	Inh URF (per ug/m^3)	Inh CSF (per mg/kg/d)
Butyl benzyl phthalate	85-68-7	2.0E-01					
Cadmium	7440-43-9	5.0E-04				1.8E-3	
Carbon disulfide	75-15-0	1.0E-01	7.0E-01				
Carbon tetrachloride (tetrachloromethane)	56-23-5	7.0E-04		1.3E-1	1.3E-1	1.5E-5	5.3E-2
Chloral	75-87-6	2.0E-03					
Chloral hydrate [trichloroacetaldehyde hydrate]	302-17-0						
Chlordane	57-74-9	5.0E-04	7.0E-04	3.5E-1	3.5E-1	1.0E-4	1.3E+0
Chlordecone	143-50-0						
Chlorine cyanide (cyanogen chloride)	506-77-4	5.0E-02					
Chloro-1,3-butadiene, 2- (chloroprene)	126-99-8	2.0E-02	7.0E-03				
Chloroaniline, 4- (p-)	106-47-8	4.0E-03					
Chlorobenzene	108-90-7	2.0E-02	2.0E-02				
Chlorobenzilate	510-15-6	2.0E-02		2.7E-1	2.7E-1	7.8E-5	2.7E-1
Chlorodibromomethane (dibromochloromethane)	124-48-1	2.0E-02		8.4E-2	8.4E-2		
Chloroform (trichloromethane)	67-66-3	1.0E-02		6.1E-3	6.1E-3	2.3E-5	8.1E-2
Chloromethane (methyl chloride)	74-87-3			1.3E-2	1.3E-2	1.8E-6	6.3E-3
Chloromethyl methyl ether	107-30-2						
Chloronaphthalene, beta-	91-58-7	8.0E-02					
Chlorophenol, 2-	95-57-8	5.0E-03					
Chromium (III), insoluble salts	16065-83-1	1.5E+00					
Chromium (VI)	18540-29-9	3.0E-03				1.2E-2	4.1E+1
Chromium (VI) - chromic acid mists & dissolved Cr aerosols	18540-29-9		8.0E-06				
Chromium (VI) - Cr particulates	18540-29-9		1.0E-04				
Chrysene	218-01-9			7.3E-03	7.3E-03		
cis-1,3-Dichloropropylene	10061-01-5						
Cobalt (and cmpds)	7440-48-4	6.0E-02					
Copper	7440-50-8						
Cresol mixtures	1319-77-3						
Cresol, m- (3-methylphenol)	108-39-4	5.0E-02					
Cresol, o- (2-Methylphenol)	95-48-7	5.0E-02					
Cresol, p- (4-methylphenol)	106-44-5	5.0E-03					
Cumene	98-82-8	1.0E-01	4.0E-01				
Cyanide (amenable)	57-12-5	2.0E-02					
Cyanogen bromide	506-68-3	9.0E-02					

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	Benchmarks Selected for Use in Deriving Phase 1A Screening Levels					
		Oral (RfD)	RfC (mg/m^3)	Oral CSF (food) (per mg/kg/d)	Oral CSF (H2O) (per mg/kg/d)	Inh URF (per ug/m^3)	Inh CSF (per mg/kg/d)
Cyclohexanol	108-93-0						
Cyclohexanone	108-94-1	5.0E+00					
DDD (p,p'-dichlorodiphenyldichloroethane)	72-54-8			2.4E-1	2.4E-1		
DDE (p,p'-dichlorodiphenyldichloroethylene)	72-55-9			3.4E-1	3.4E-1		
DDT (p,p'-dichlorodiphenyltrichloroethane)	50-29-3	5.0E-04		3.4E-1	3.4E-1	9.7E-5	3.4E-1
Diallate	2303-16-4			6.1E-2	6.1E-2		
Dibenzo(a,h)anthracene	53-70-3			7.3E+00	7.3E+00		
Dibromo-3-chloropropane, 1,2- (DBCP)	96-12-8		2.0E-04	1.4E+0	1.4E+0	6.9E-7	2.4E-03
Dibromoethane, 1,2- (ethylene dibromide)	106-93-4		2.0E-04	8.5E+1	8.5E+1	2.2E-4	7.6E-1
Dichlorobenzene, 1,2- (o-)	95-50-1	9.0E-02	2.0E-01				
Dichlorobenzene, 1,4-	106-46-7		8.0E-01	2.4E-2	2.4E-2		
Dichlorobenzidine, 3,3'-	91-94-1			4.5E-1	4.5E-1		
Dichlorobromomethane (bromodichloromethane)	75-27-4	2.0E-02		6.2E-2	6.2E-2		
Dichlorodifluoromethane [CFC-12]	75-71-8	2.0E-01	2.0E-01				
Dichloroethane, 1,1-	75-34-3	1.0E-01	5.0E-01				
Dichloroethane, 1,2- (ethylene dichloride)	107-06-2			9.1E-2	9.1E-2	2.6E-5	
Dichloroethylene, 1,1-	75-35-4	9.0E-03		6.0E-1	6.0E-1	5.0E-5	2.0E-1
Dichloroethylene, 1,2- (cis)	156-59-2	1.0E-02					
Dichloroethylene, 1,2- (trans)	156-60-5	2.0E-02					
Dichlorophenol, 2,4-	120-83-2	3.0E-03					
Dichlorophenoxyacetic acid, 2,4- (2,4-D)	94-75-7	1.0E-02					
Dichloropropane, 1,2-	78-87-5		4.0E-03	6.8E-2	6.8E-2		
Dieldrin	60-57-1	5.0E-05		1.6E+1	1.6E+1	4.6E-3	1.6E+1
Diethyl phthalate	84-66-2	8.0E-01					
Diethylstilbestrol	56-53-1			4.7E+3	4.7E+3		
Dimethoate	60-51-5	2.0E-04					
Dimethoxybenzidine, 3,3'-	119-90-4			1.4E-2	1.4E-2		
Dimethylbenz[a]anthracene, 7,12-	57-97-6						
Dimethylbenzidine, 3,3'-	119-93-7			9.2E+0	9.2E+0		
Dimethylformamide, N,N-	68-12-2	1.0E-01	3.0E-02				
Dimethylphenol, 2,4-	105-67-9	2.0E-02					
Dimethylphenol, 3,4-	95-65-8	1.0E-03					
Dimethylphthalate	131-11-3						
Di-n-butyl phthalate	84-74-2	1.0E-01					

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	Benchmarks Selected for Use in Deriving Phase 1A Screening Levels					
		Oral (RfD)	RfC (mg/m^3)	Oral CSF (food) (per mg/kg/d)	Oral CSF (H2O) (per mg/kg/d)	Inh URF (per ug/m^3)	Inh CSF (per mg/kg/d)
Dinitrobenzene, 1,3- (m-)	99-65-0	1.0E-04					
Dinitrophenol, 2,4-	51-28-5	2.0E-03					
Dinitrotoluene, 2,4-	121-14-2	2.0E-03					
Dinitrotoluene, 2,6-	606-20-2	1.0E-03					
Di-N-octyl phthalate	117-84-0	2.0E-02					
Dinoseb	88-85-7	1.0E-03					
Dioxane, 1,4-	123-91-1			1.1E-2	1.1E-2		
Diphenylamine, N,N-	122-39-4	2.5E-02					
Diphenylhydrazine, 1,2-	122-66-7			8.0E-1	8.0E-1	2.2E-4	8.0E-1
Direct Black 38	1937-37-7			8.6E+0	8.6E+0		
Direct Blue 6	2602-46-2			8.1E+0	8.1E+0		
Direct Brown 95	16071-86-6			9.3E+0	9.3E+0		
Disulfoton	298-04-4	4.0E-05					
Endosulfan	115-29-7	6.0E-03					
Endothall	145-73-3	2.0E-02					
Endrin	72-20-8	3.0E-04					
Epichlorohydrin	106-89-8	2.0E-03	1.0E-03	9.9E-3	9.9E-3	1.2E-6	4.2E-3
Epoxybutane, 1,2-	106-88-7		2.0E-02				
Ethoxyethanol acetate, 2-	111-15-9	3.0E-01					
Ethoxyethanol, 2- (ethylene glycol monoethyl ether)	110-80-5	4.0E-01	2.0E-01				
Ethyl acetate	141-78-6	9.0E-01					
Ethyl chloride (chloroethane)	75-00-3		1.0E+01				
Ethyl ether	60-29-7	2.0E-01					
Ethyl methacrylate	97-63-2	9.0E-02					
Ethyl methanesulfonate	62-50-0						
Ethylbenzene	100-41-4	1.0E-01	1.0E+00				
Ethylene glycol	107-21-1	2.0E+00					
Ethylene oxide	75-21-8			1.0E+0	1.0E+0	1.0E-4	3.5E-1
Ethylene thiourea	96-45-7	8.0E-05		1.1E-1	1.1E-1		
Fluoranthene	206-44-0	4.0E-02					
Fluorene	86-73-7	4.0E-02					
Fluoride	16984-48-8						
Formaldehyde	50-00-0	2.0E-01				1.3E-5	4.5E-2
Formic acid	64-18-6	2.0E+00					
Furan	110-00-9	1.0E-03					
Furfural	98-01-1	3.0E-03	5.0E-02				
Glycidaldehyde	765-34-4	4.0E-04	1.0E-03				
Heptachlor	76-44-8	5.0E-04		4.5E+0	4.5E+0	1.3E-3	4.5E+0
Heptachlor epoxide	1024-57-3	1.3E-05		9.1E+0	9.1E+0	2.6E-3	9.1E+0
Hexachlorobenzene	118-74-1	8.0E-04		1.6E+0	1.6E+0	4.6E-4	1.6E+0

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	Benchmarks Selected for Use in Deriving Phase 1A Screening Levels					
		Oral (RfD)	RfC (mg/m^3)	Oral CSF (food) (per mg/kg/d)	Oral CSF (H2O) (per mg/kg/d)	Inh URF (per ug/m^3)	Inh CSF (per mg/kg/d)
Hexachlorobutadiene	87-68-3	2.0E-04		7.8E-2	7.8E-2	2.2E-5	7.8E-2
Hexachlorocyclohexane, alpha-	319-84-6			6.3E+0	6.3E+0	1.8E-3	6.3E+0
Hexachlorocyclohexane, beta-	319-85-7			1.8E+0	1.8E+0	5.3E-4	1.8E+0
Hexachlorocyclohexane, gamma- (lindane)	58-89-9	3.0E-04		1.3E+0	1.3E+0		
Hexachlorocyclopentadiene	77-47-4	7.0E-03	7.0E-05				
Hexachloroethane	67-72-1	1.0E-03		1.4E-2	1.4E-2	4.0E-6	1.4E-2
Hexachlorophene	70-30-4	3.0E-04					
Hexane, n-	110-54-3	6.0E-02	2.0E-01				
Hydrazine	302-01-2			3.0E+0	3.0E+0	4.9E-3	1.7E+1
Ideno[1,2,3-cd]pyrene	193-39-5			7.3E-01	7.3E-01		
Isobutyl alcohol	78-83-1	3.0E-01					
Isophorone	78-59-1	2.0E-01		9.5E-4	9.5E-4		
Lead and cmpds (inorganic)	7439-92-1						
Maleic anhydride	108-31-6	1.0E-01					
Maleic hydrazide	123-33-1	5.0E-01					
Manganese	7439-96-5	1.4E-01	5.0E-05				
Mercuric chloride	7487-94-7	3.0E-04					
Mercury (elemental)	7439-97-6		3.0E-04				
Methacrylonitrile	126-98-7	1.0E-04	7.0E-04				
Methanol	67-56-1	5.0E-01					
Methomyl	16752-77-5	2.5E-02					
Methoxychlor	72-43-5	5.0E-03					
Methoxyethanol acetate, 2-	110-49-6	2.0E-03					
Methoxyethanol, 2- (ethylene glycol methyl ether)	109-86-4	1.0E-03	2.0E-02				
Methyl ethyl ketone	78-93-3	6.0E-01	1.0E+00				
Methyl isobutyl ketone	108-10-1	8.0E-02	8.0E-02				
Methyl mercury	22967-92-6	1.0E-04					
Methyl methacrylate	80-62-6	1.4E+00	7.0E-01				
Methyl parathion	298-00-0	2.5E-04					
Methyl tert-butyl ether	1634-04-4		3.0E+00				
Methylaniline, 2- (o-toluidine)	95-53-4			2.4E-1	2.4E-1		
Methylcholanthrene, 3-	56-49-5						
Methylene bromide	74-95-3	1.0E-02					
Methylene chloride (dichloromethane)	75-09-2	6.0E-02	3.0E+00	7.5E-3	7.5E-3	4.7E-7	
Methylene-bis(2-chloroaniline), 4,4'- (MBOCA)	101-14-4	7.0E-04		1.3E-1	1.3E-1	3.7E-5	1.3E-1
Molybdenum	7439-98-7	5.0E-03					
Naphthalene	91-20-3	2.0E-02	3.0E-03				
Nickel subsulfide	12035-72-2					4.8E-4	1.7E+0

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	Benchmarks Selected for Use in Deriving Phase 1A Screening Levels					
		Oral (RfD)	RfC (mg/m^3)	Oral CSF (food) (per mg/kg/d)	Oral CSF (H2O) (per mg/kg/d)	Inh URF (per ug/m^3)	Inh CSF (per mg/kg/d)
Nickel, soluble salts	7440-02-0	2.0E-02					
Nitrobenzene	98-95-3	5.0E-04	2.0E-03				
Nitropropane, 2-	79-46-9		2.0E-02			2.7E-3	9.4E+0
N-Nitrosodiethylamine	55-18-5			1.5E+2	1.5E+2	4.3E-2	1.5E+2
N-Nitrosodimethylamine (N-methyl-N-nitroso-methanamine)	62-75-9			5.1E+1	5.1E+1	1.4E-2	5.1E+1
N-Nitroso-di-n-butylamine	924-16-3			5.4E+0	5.4E+0	1.6E-3	5.4E+0
N-Nitrosodi-n-propylamine	621-64-7			7.0E+0	7.0E+0		
N-Nitrosodiphenylamine	86-30-6			4.9E-3	4.9E-3		
N-Nitroso-N-methylethylamine	10595-95-6			2.2E+1	2.2E+1		
N-Nitrosopiperidine	100-75-4						
N-Nitrosopyrrolidine	930-55-2			2.1E+0	2.1E+0	6.1E-4	2.1E+0
Octamethylpyrophosphoamide	152-16-9	2.0E-03					
Parathion	56-38-2	6.0E-03					
Pentachlorobenzene	608-93-5	8.0E-04					
Pentachlorodibenzofuran, 1,2,3,7,8-	57117-41-6			7.5E+3	7.5E+3	1.7E+0	7.5E+3
Pentachlorodibenzofuran, 2,3,4,7,8-	57117-31-4			7.5E+4	7.5E+4	1.7E+1	7.5E+4
Pentachlorodibenzo-p-dioxin, 1,2,3,7,8-	40321-76-4			1.5E+5	1.5E+5	3.3E+1	1.5E+5
Pentachloronitrobenzene	82-68-8	3.0E-03		2.6E-1	2.6E-1		
Pentachlorophenol	87-86-5	3.0E-02		1.2E-1	1.2E-1		
Perchlorate	14797-73-0						
Phenol	108-95-2	6.0E-01					
Phenylenediamine , m-	108-45-2	6.0E-03					
Phorate	298-02-2	2.0E-04					
Phthalic anhydride	85-44-9	2.0E+00	1.2E-01				
Polychlorinated biphenyls	1336-36-3			2	0.4	0.0001	see note
Pronamide	23950-58-5	7.5E-02					
Propylene oxide	75-56-9		3.0E-02	2.4E-1	2.4E-1	3.7E-6	1.3E-2
Pyrene	129-00-0	3.0E-02					
Pyridine	110-86-1	1.0E-03					
Safrole	94-59-7						
Selenium	7782-49-2	5.0E-03					
Silver	7440-22-4	5.0E-03					
Strychnine and salts	57-24-9	3.0E-04					
Styrene	100-42-5	2.0E-01	1.0E+00				
Styrene-7,8-oxide	96-09-3						
Sulfide	18496-25-8						
TCDD, 2,3,7,8-	1746-01-6			1.5E+5	1.5E+5	3.3E+1	1.5E+5
Tetrachlorobenzene, 1,2,4,5-	95-94-3	3.0E-04					

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	Benchmarks Selected for Use in Deriving Phase 1A Screening Levels					
		Oral (RfD)	RfC (mg/m^3)	Oral CSF (food) (per mg/kg/d)	Oral CSF (H2O) (per mg/kg/d)	Inh URF (per ug/m^3)	Inh CSF (per mg/kg/d)
Tetrachlorodibenzodioxins	41903-57-5			0	0	0	0
Tetrachlorodibenzofurans	55722-27-5			0	0	0	0
Tetrachloroethane, 1,1,1,2-	630-20-6	3.0E-02		2.6E-2	2.6E-2	7.4E-6	2.6E-2
Tetrachloroethane, 1,1,2,2-	79-34-5			2.0E-1	2.0E-1	5.8E-5	2.0E-1
Tetrachloroethylene (perchloroethylene)	127-18-4	1.0E-02		5.2E-2	5.2E-2	5.8E-7	2.0E-3
Tetrachlorophenol, 2,3,4,6-	58-90-2	3.0E-02					
Tetraethyldithiopyrophosphate	3689-24-5	5.0E-04					
Thallium	7440-28-0						
Thallium (I) acetate	563-68-8	9.0E-05					
Thallium (I) carbonate	6533-73-9	8.0E-05					
Thallium (I) chloride	7791-12-0	8.0E-05					
Thallium (I) nitrate	10102-45-1	9.0E-05					
Thallium (I) sulfate	7446-18-6	8.0E-05					
Thiram	137-26-8	5.0E-03					
Toluene	108-88-3	2.0E-01	4.0E-01				
Toluene-2,4-diamine (2,4-diaminotoluene)	95-80-7			3.2E+0	3.2E+0		
Toluidine, p-	106-49-0			1.9E-1	1.9E-1		
Toxaphene	8001-35-2			1.1E+0	1.1E+0	3.2E-4	1.1E+0
trans-1,3-Dichloropropylene	10061-02-6						
Trichloro-1,2,2-trifluoroethane, 1,1,2- (Freon 113)	76-13-1	3.0E+01	3.0E+01				
Trichlorobenzene, 1,2,4-	120-82-1	1.0E-02	2.0E-01				
Trichloroethane, 1,1,1- (methyl chloroform)	71-55-6		1.0E+00				
Trichloroethane, 1,1,2- (vinyl trichloride)	79-00-5	4.0E-03		5.7E-2	5.7E-2	1.6E-5	5.7E-2
Trichloroethylene	79-01-6			1.1E-02	1.1E-02	1.7E-06	6.0E-03
Trichlorofluoromethane (CFC-11)	75-69-4	3.0E-01	7.0E-01				
Trichlorophenol, 2,4,5-	95-95-4	1.0E-01					
Trichlorophenol, 2,4,6-	88-06-2			1.1E-2	1.1E-2	3.1E-6	1.0E-2
Trichlorophenoxy) propionic acid, 2 (2,4,5-	93-72-1	8.0E-03					
Trichlorophenoxyacetic acid, 2,4,5-	93-76-5	1.0E-02					
Trichloropropane, 1,2,3-	96-18-4	6.0E-03		7.0E+0	7.0E+0		
Triethylamine	121-44-8		7.0E-03				
Trinitrobenzene, 1,3,5- (sym-)	99-35-4	3.0E-02					
tris(2,3-Dibromopropyl)phosphate	126-72-7						
Vanadium	7440-62-2	7.0E-03					
Vinyl acetate	108-05-4	1.0E+00	2.0E-01				
Vinyl chloride	75-01-4			1.9E+0	1.9E+0	8.4E-5	3.0E-1

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	Benchmarks Selected for Use in Deriving Phase 1A Screening Levels					
		Oral (RfD)	RfC (mg/m^3)	Oral CSF (food) (per mg/kg/d)	Oral CSF (H2O) (per mg/kg/d)	Inh URF (per ug/m^3)	Inh CSF (per mg/kg/d)
Warfarin	81-81-2	3.0E-04					
Xylene, m-	108-38-3	2.0E+00					
Xylene, o-	95-47-6	2.0E+00					
Xylene, p-	106-42-3						
Xylenes (total)	1330-20-7	2.0E+00					
Zinc	7440-66-6	3.0E-01					

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	EPA Benchmarks											
		RfD (mg/kg/d)	RfD Source	RfC (mg/m3)	RfC source	Oral CSF (mkd)-1	Oral CSF Source	Drinking H2O URF (per ug/L)	Oral URF Source	Inhal Unit Risk (ug/m3)-1	Inhal URF Source	HEAST inhal CSF (mkd)-1	Super-fund values
Acenaphthene	83329	6.0E-02	IRIS										
Acetaldehyde	75-07-0			9.0E-03	IRIS					2.2E-6	IRIS		
Acetone	67641	1.0E-01	IRIS										
Acetonitrile	75-05-8			6.0E-02	IRIS								
Acetophenone	98-86-2	1.0E-01	IRIS										
Acrolein	107-02-8	2.0E-02	HEAST	2.0E-05	IRIS								
Acrylamide	79-06-1	2.0E-04	IRIS			4.5E+0	IRIS	1.3E-04	IRIS	1.3E-3	IRIS	4.5E+0	
Acrylic acid	79-10-7	5.0E-01	IRIS	1.0E-03	IRIS								
Acrylonitrile	107-13-1	1.0E-03	HEAST	2.0E-03	IRIS	5.4E-1	IRIS	1.5E-05	IRIS	6.8E-5	IRIS	2.4E-1	
Aldicarb	116-06-3	1.0E-03	IRIS										
Aldrin	309-00-2	3.0E-05	IRIS			1.7E+1	IRIS	4.9E-04	IRIS	4.9E-3	IRIS	1.7E+1	
Allyl alcohol	107-18-6	5.0E-03	IRIS										
Allyl chloride (3-chloropropene)	107-05-1			1.0E-03	IRIS								
Ammonium vanadate	7803-55-6												
Amonium perchlorate	7790-98-9												
Aniline	62-53-3			1.0E-03	IRIS	5.7E-3	IRIS	1.6E-07	IRIS				
Anthracene	120-12-7	3.0E-01	IRIS										
Antimony	7440-36-0	4.0E-04	IRIS										
Antimony trioxide	1309-64-4	4.0E-04	HEAST	2.0E-04	IRIS								
Aramite	140-57-8	5.0E-02	HEAST			2.5E-2	IRIS	7.1E-07	IRIS	7.1E-6	IRIS	2.5E-2	
Arsenic, inorganic	7440-38-2	3.0E-04	IRIS			1.5E+0	IRIS	5.0E-05	IRIS	4.3E-3	IRIS		
Barium	7440-39-3	7.0E-02	IRIS	5.0E-04	HEAST2								
Benz(a)anthracene	56-55-3					7.3E-01	TEF	2.1E-05	TEF				
Benzene	71-43-2					2.9E-2[a]	IRIS	8.3E-07[a]	IRIS	8.3E-6[a]	IRIS	2.9E-2	6E-2 mg/m3 (subchronic RfC)

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	EPA Benchmarks											
		RfD (mg/kg/d)	RfD Source	RfC (mg/m3)	RfC source	Oral CSF (mkd)-1	Oral CSF Source	Drinking H2O URF (per ug/L)	Oral URF Source	Inhal Unit Risk (ug/m3)-1	Inhal URF Source	HEAST inhal CSF (mkd)-1	Super-fund values
Benzidine	92-87-5	3.0E-03	IRIS			2.3E+2	IRIS	6.7E-03	IRIS	6.7E-2	IRIS	2.3E+2	
Benzo(a)pyrene	50-32-8					7.3E+0	IRIS	2.1E-04	IRIS				
Benzo(b)fluoranthene	205-99-2					7.3E-01	TEF	2.1E-05	TEF				
Benzyl alcohol	100-51-6	3.0E-01	HEAST										
Benzyl chloride	100-44-7					1.7E-1	IRIS	4.9E-06	IRIS				
Beryllium	7440-41-7	2.0E-03	IRIS	2.0E-05	IRIS					2.4E-3	IRIS	8.4E+0	
Bis(2-chloroethyl)ether	111-44-4					1.1E+0	IRIS	3.3E-05	IRIS	3.3E-4	IRIS	1.1E+0	
Bis(2-chloroisopropyl)ether	39638-32-9	4.0E-02	IRIS			7.0E-2	HEAST	2.0E-06	HEAST	1.0E-5	HEAST	3.5E-2	
Bis(2-ethylhexyl)phthalate (DEHP; also di-)	117-81-7	2.0E-02	IRIS			1.4E-2	IRIS	4.0E-07	IRIS				subchronic RfC= 1E-2 mg/m3
Bis(chloromethyl)ether	542-88-1					2.2E+2	IRIS	6.2E-03	IRIS	6.2E-2	IRIS	2.2E+2	
Bromoform	75-25-2	2.0E-02	IRIS			7.9E-3	IRIS	2.3E-07	IRIS	1.1E-6	IRIS	3.9E-3	
Bromomethane (methyl bromide)	74-83-9	1.4E-03	IRIS	5.0E-03	IRIS								
Butadiene, 1,3-	106-99-0									2.8E-4	IRIS	1.8E+0	
Butanol, n- (n-butyl alcohol)	71-36-3	1.0E-01	IRIS										
Butyl benzyl phthalate	85-68-7	2.0E-01	IRIS										
Cadmium	7440-43-9	5.0E-04	IRIS							1.8E-3	IRIS		
Carbon disulfide	75-15-0	1.0E-01	IRIS	7.0E-01	IRIS								
Carbon tetrachloride (tetrachloromethane)	56-23-5	7.0E-04	IRIS			1.3E-1	IRIS	3.7E-06	IRIS	1.5E-5	IRIS	5.3E-2	subchronic RfC=2E-2 mg/m3
Chloral	75-87-6	2.0E-03	IRIS										
Chloral hydrate [trichloroacetaldehyde hydrate]	302-17-0												
Chlordane	57-74-9	5.0E-04	IRIS	7.0E-04	IRIS	3.5E-1	IRIS	1.0E-05	IRIS	1.0E-4	IRIS	1.3E+0	
Chlordecone	143-50-0												
Chlorine cyanide (cyanogen chloride)	506-77-4	5.0E-02	IRIS										

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	EPA Benchmarks											
		RfD (mg/kg/d)	RfD Source	RfC (mg/m3)	RfC source	Oral CSF (mkd)-1	Oral CSF Source	Drinking H2O URF (per ug/L)	Oral URF Source	Inhal Unit Risk (ug/m3)-1	Inhal URF Source	HEAST inhal CSF (mkd)-1	Super-fund values
Chloro-1,3-butadiene, 2- (chloroprene)	126-99-8	2.0E-02	HEAST2	7.0E-03	HEAST								
Chloroaniline, 4- (p-)	106-47-8	4.0E-03	IRIS										
Chlorobenzene	108-90-7	2.0E-02	IRIS	2.0E-02	HEAST2								subchronic RfC= 2E-1 mg/m3
Chlorobenzilate	510-15-6	2.0E-02	IRIS			2.7E-1	HEAST	7.8E-06	HEAST	7.8E-5	HEAST	2.7E-1	
Chlorodibromomethane (dibromochloromethane)	124-48-1	2.0E-02	IRIS			8.4E-2	IRIS	2.4E-06	IRIS				
Chloroform (trichloromethane)	67-66-3	1.0E-02	IRIS			6.1E-3	IRIS	1.7E-07	IRIS	2.3E-5	IRIS	8.1E-2	RfC not current
Chloromethane (methyl chloride)	74-87-3					1.3E-2	HEAST	3.7E-07	HEAST	1.8E-6	HEAST	6.3E-3	RfC=0.3 mg/m3
Chloromethyl methyl ether	107-30-2												
Chloronaphthalene, beta-	91-58-7	8.0E-02	IRIS										
Chlorophenol, 2-	95-57-8	5.0E-03	IRIS										
Chromium (III), insoluble salts	16065-83-1	1.5E+00	IRIS										
Chromium (VI)	18540-29-9	3.0E-03	IRIS	8E-6 or 1E-4	IRIS					1.2E-2	IRIS	4.1E+1	subchronic RfC= 4E-6 mg/m3
Chromium (VI) - chromic acid mists & dissolved Cr aerosols	18540-29-9			8.0E-06	IRIS								
Chromium (VI) - Cr particulates	18540-29-9			1.0E-04	IRIS								
Chrysene	218-01-9					7.3E-03	TEF	2.1E-07	TEF				
cis-1,3-Dichloropropylene	10061-01-5												
Cobalt (and cmpds)	7440-48-4												0.06 mkd (chronic RfD)
Copper	7440-50-8	*MCL only	HEAST										
Cresol mixtures	1319-77-3												
Cresol, m- (3-methylphenol)	108-39-4	5.0E-02	IRIS										
Cresol, o- (2-Methylphenol)	95-48-7	5.0E-02	IRIS										

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	EPA Benchmarks											
		RfD (mg/kg/d)	RfD Source	RfC (mg/m3)	RfC source	Oral CSF (mkd)-1	Oral CSF Source	Drinking H2O URF (per ug/L)	Oral URF Source	Inhal Unit Risk (ug/m3)-1	Inhal URF Source	HEAST inhal CSF (mkd)-1	Super-fund values
Cresol, p- (4-methylphenol)	106-44-5	5.0E-03	HEAST										
Cumene	98-82-8	1.0E-01	IRIS	4.0E-01	IRIS								
Cyanide (amenable)	57-12-5	2.0E-02	IRIS										
Cyanogen bromide	506-68-3	9.0E-02	IRIS										
Cyclohexanol	108-93-0												
Cyclohexanone	108-94-1	5.0E+00	IRIS										
DDD (p,p'-dichlorodiphenyldichloroethane)	72-54-8					2.4E-1	IRIS	6.9E-06	IRIS				
DDE (p,p'-dichlorodiphenyldichloroethylene)	72-55-9					3.4E-1	IRIS	9.7E-06	IRIS				
DDT (p,p'-dichlorodiphenyltrichloroethane)	50-29-3	5.0E-04	IRIS			3.4E-1	IRIS	9.7E-06	IRIS	9.7E-5	IRIS	3.4E-1	
Diallate	2303-16-4					6.1E-2	HEAST	1.7E-06	HEAST				
Dibenzo(a,h)anthracene	53-70-3					7.3E+0	TEF	2.1E-04	TEF				
Dibromo-3-chloropropane, 1,2- (DBCP)	96-12-8			2.0E-04	IRIS	1.4E+0	HEAST	4.0E-05	HEAST	6.9E-7	HEAST	2.4E-03	
Dibromoethane, 1,2- (ethylene dibromide)	106-93-4			2.0E-04	HEAST	8.5E+1	IRIS	2.5E-03	IRIS	2.2E-4	IRIS	7.6E-1	
Dichlorobenzene, 1,2- (o-)	95-50-1	9.0E-02	IRIS	2.0E-01	HEAST2								
Dichlorobenzene, 1,4-	106-46-7			8.0E-01	IRIS	2.4E-2	HEAST	6.8E-07	HEAST				
Dichlorobenzidine, 3,3'-	91-94-1					4.5E-1	IRIS	1.3E-05	IRIS				
Dichlorobromomethane (bromodichloromethane)	75-27-4	2.0E-02	IRIS			6.2E-2	IRIS	1.8E-06	IRIS				
Dichlorodifluoromethane [CFC-12]	75-71-8	2.0E-01	IRIS	2.0E-01	HEAST2								
Dichloroethane, 1,1-	75-34-3	1.0E-01	HEAST	5.0E-01	HEAST2								
Dichloroethane, 1,2- (ethylene dichloride)	107-06-2					9.1E-2	IRIS	2.6E-06	IRIS	2.6E-5	IRIS		
Dichloroethylene, 1,1-	75-35-4	9.0E-03	IRIS			6.0E-1	IRIS	1.7E-05	IRIS	5.0E-5	IRIS	2.0E-1	
Dichloroethylene, 1,2- (cis)	156-59-2	1.0E-02	HEAST										
Dichloroethylene, 1,2- (trans)	156-60-5	2.0E-02	IRIS										

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	EPA Benchmarks											
		RfD (mg/kg/d)	RfD Source	RfC (mg/m3)	RfC source	Oral CSF (mkd)-1	Oral CSF Source	Drinking H2O URF (per ug/L)	Oral URF Source	Inhal Unit Risk (ug/m3)-1	Inhal URF Source	HEAST inhal CSF (mkd)-1	Super-fund values
Dichlorophenol, 2,4-	120-83-2	3.0E-03	IRIS										
Dichlorophenoxyacetic acid, 2,4-(2,4-D)	94-75-7	1.0E-02	IRIS										
Dichloropropane, 1,2-	78-87-5			4.0E-03	IRIS	6.8E-2	HEAST	1.9E-06	HEAST				
Dieldrin	60-57-1	5.0E-05	IRIS			1.6E+1	IRIS	4.6E-04	IRIS	4.6E-3	IRIS	1.6E+1	
Diethyl phthalate	84-66-2	8.0E-01	IRIS										
Diethylstilbestrol	56-53-1					4.7E+3	HEAST	1.3E-01	HEAST				
Dimethoate	60-51-5	2.0E-04	IRIS										
Dimethoxybenzidine, 3,3'-	119-90-4					1.4E-2	HEAST	4.0E-07	HEAST				
Dimethylbenz[a]anthracene, 7,12-	57-97-6												
Dimethylbenzidine, 3,3'-	119-93-7					9.2E+0	HEAST	2.6E-04	HEAST				
Dimethylformamide, N,N-	68-12-2	1.0E-01	HEAST	3.0E-02	IRIS								
Dimethylphenol, 2,4-	105-67-9	2.0E-02	IRIS										
Dimethylphenol, 3,4-	95-65-8	1.0E-03	IRIS										
Dimethylphthalate	131-11-3												
Di-n-butyl phthalate	84-74-2	1.0E-01	IRIS										
Dinitrobenzene, 1,3- (m-)	99-65-0	1.0E-04	IRIS										
Dinitrophenol, 2,4-	51-28-5	2.0E-03	IRIS										
Dinitrotoluene, 2,4-	121-14-2	2.0E-03	IRIS										
Dinitrotoluene, 2,6-	606-20-2	1.0E-03	HEAST										
Di-N-octyl phthalate	117-84-0	2.0E-02	HEAST										
Dinoseb	88-85-7	1.0E-03	IRIS										
Dioxane, 1,4-	123-91-1					1.1E-2	IRIS	3.1E-07	IRIS				
Diphenylamine, N,N-	122-39-4	2.5E-02	IRIS										
Diphenylhydrazine, 1,2-	122-66-7					8.0E-1	IRIS	2.2E-05	IRIS	2.2E-4	IRIS	8.0E-1	
Direct Black 38	1937-37-7					8.6E+0	HEAST	2.4E-04	HEAST				
Direct Blue 6	2602-46-2					8.1E+0	HEAST	2.3E-04	HEAST				
Direct Brown 95	16071-86-6					9.3E+0	HEAST	2.6E-04	HEAST				

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	EPA Benchmarks											
		RfD (mg/kg/d)	RfD Source	RfC (mg/m3)	RfC source	Oral CSF (mkd)-1	Oral CSF Source	Drinking H2O URF (per ug/L)	Oral URF Source	Inhal Unit Risk (ug/m3)-1	Inhal URF Source	HEAST inhal CSF (mkd)-1	Super-fund values
Disulfoton	298-04-4	4.0E-05	IRIS										
Endosulfan	115-29-7	6.0E-03	IRIS										
Endothall	145-73-3	2.0E-02	IRIS										
Endrin	72-20-8	3.0E-04	IRIS										
Epichlorohydrin	106-89-8	2.0E-03	HEAST	1.0E-03	IRIS	9.9E-3	IRIS	2.8E-07	IRIS	1.2E-6	IRIS	4.2E-3	
Epoxybutane, 1,2-	106-88-7			2.0E-02	IRIS								
Ethoxyethanol acetate, 2-	111-15-9	3.0E-01	HEAST2										
Ethoxyethanol, 2- (ethylene glycol monoethyl ether)	110-80-5	4.0E-01	HEAST	2.0E-01	IRIS								
Ethyl acetate	141-78-6	9.0E-01	IRIS										
Ethyl chloride (chloroethane)	75-00-3			1.0E+01	IRIS								
Ethyl ether	60-29-7	2.0E-01	IRIS										
Ethyl methacrylate	97-63-2	9.0E-02	HEAST										
Ethyl methanesulfonate	62-50-0												
Ethylbenzene	100-41-4	1.0E-01	IRIS	1.0E+00	IRIS								
Ethylene glycol	107-21-1	2.0E+00	IRIS										
Ethylene oxide	75-21-8					1.0E+0	HEAST	2.9E-05	HEAST	1.0E-4	HEAST	3.5E-1	
Ethylene thiourea	96-45-7	8.0E-05	IRIS			1.1E-1	HEAST	3.4E-06	HEAST				
Fluoranthene	206-44-0	4.0E-02	IRIS										
Fluorene	86-73-7	4.0E-02	IRIS										
Fluoride	16984-48-8												
Formaldehyde	50-00-0	2.0E-01	IRIS							1.3E-5	IRIS	4.5E-2	
Formic acid	64-18-6	2.0E+00	HEAST										
Furan	110-00-9	1.0E-03	IRIS										
Furfural	98-01-1	3.0E-03	IRIS	5.0E-02	HEAST2								
Glycidaldehyde	765-34-4	4.0E-04	IRIS	1.0E-03	HEAST								
Heptachlor	76-44-8	5.0E-04	IRIS			4.5E+0	IRIS	1.3E-04	IRIS	1.3E-3	IRIS	4.5E+0	
Heptachlor epoxide	1024-57-3	1.3E-05	IRIS			9.1E+0	IRIS	2.6E-04	IRIS	2.6E-3	IRIS	9.1E+0	

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	EPA Benchmarks											
		RfD (mg/kg/d)	RfD Source	RfC (mg/m3)	RfC source	Oral CSF (mkd)-1	Oral CSF Source	Drinking H2O URF (per ug/L)	Oral URF Source	Inhal Unit Risk (ug/m3)-1	Inhal URF Source	HEAST inhal CSF (mkd)-1	Super-fund values
Hexachlorobenzene	118-74-1	8.0E-04	IRIS			1.6E+0	IRIS	4.6E-05	IRIS	4.6E-4	IRIS	1.6E+0	
Hexachlorobutadiene	87-68-3	2.0E-04	HEAST			7.8E-2	IRIS	2.2E-06	IRIS	2.2E-5	IRIS	7.8E-2	
Hexachlorocyclohexane, alpha-	319-84-6					6.3E+0	IRIS	1.8E-04	IRIS	1.8E-3	IRIS	6.3E+0	
Hexachlorocyclohexane, beta-	319-85-7					1.8E+0	IRIS	5.3E-05	IRIS	5.3E-4	IRIS	1.8E+0	
Hexachlorocyclohexane, gamma- (lindane)	58-89-9	3.0E-04	IRIS			1.3E+0	HEAST	3.7E-05	HEAST				
Hexachlorocyclopentadiene	77-47-4	7.0E-03	IRIS	7.0E-05	HEAST								
Hexachloroethane	67-72-1	1.0E-03	IRIS			1.4E-2	IRIS	4.0E-07	IRIS	4.0E-6	IRIS	1.4E-2	
Hexachlorophene	70-30-4	3.0E-04	IRIS										
Hexane, n-	110-54-3	6.0E-02	HEAST	2.0E-01	IRIS								
Hydrazine	302-01-2					3.0E+0	IRIS	8.5E-05	IRIS	4.9E-3	IRIS	1.7E+1	
Ideno[1,2,3-cd]pyrene	193-39-5					7.3E-1	TEF	2.1E-05	TEF				
Isobutyl alcohol	78-83-1	3.0E-01	IRIS										
Isophorone	78-59-1	2.0E-01	IRIS			9.5E-4	IRIS	2.7E-08	IRIS				
Lead and cmpds (inorganic)	7439-92-1												
Maleic anhydride	108-31-6	1.0E-01	IRIS										
Maleic hydrazide	123-33-1	5.0E-01	IRIS										
Manganese	7439-96-5	1.4E-01	IRIS	5.0E-05	IRIS								
Mercuric chloride	7487-94-7	3.0E-04	HEAST										
Mercury (elemental)	7439-97-6			3.0E-04	IRIS								
Methacrylonitrile	126-98-7	1.0E-04	IRIS	7.0E-04	HEAST2								
Methanol	67-56-1	5.0E-01	IRIS										
Methomyl	16752-77-5	2.5E-02	IRIS										
Methoxychlor	72-43-5	5.0E-03	IRIS										
Methoxyethanol acetate, 2-	110-49-6	2.0E-03	HEAST2										
Methoxyethanol, 2- (ethylene glycol methyl ether)	109-86-4	1.0E-03	HEAST2	2.0E-02	IRIS								
Methyl ethyl ketone	78-93-3	6.0E-01	IRIS	1.0E+00	IRIS								
Methyl isobutyl ketone	108-10-1	8.0E-02	HEAST	8.0E-02	HEAST2								

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	EPA Benchmarks											
		RfD (mg/kg/d)	RfD Source	RfC (mg/m3)	RfC source	Oral CSF (mkd)-1	Oral CSF Source	Drinking H2O URF (per ug/L)	Oral URF Source	Inhal Unit Risk (ug/m3)-1	Inhal URF Source	HEAST inhal CSF (mkd)-1	Super-fund values
Methyl mercury	22967-92-6	1.0E-04	IRIS										
Methyl methacrylate	80-62-6	1.4E+00	IRIS	7.0E-01	IRIS								
Methyl parathion	298-00-0	2.5E-04	IRIS										
Methyl tert-butyl ether	1634-04-4			3.0E+00	IRIS								
Methylaniline, 2- (o-toluidine)	95-53-4					2.4E-1	HEAST	6.9E-06	HEAST				
Methylcholanthrene, 3-	56-49-5												
Methylene bromide	74-95-3	1.0E-02	HEAST2										
Methylene chloride (dichloromethane)	75-09-2	6.0E-02	IRIS	3.0E+00	HEAST	7.5E-3	IRIS	2.1E-07	IRIS	4.7E-7	IRIS		
Methylene-bis(2-chloroaniline), 4,4'- (MBOCA)	101-14-4	7.0E-04	HEAST			1.3E-1	HEAST	3.7E-06	HEAST	3.7E-5	HEAST	1.3E-1	
Molybdenum	7439-98-7	5.0E-03	IRIS										
Naphthalene	91-20-3	2.0E-02	IRIS	3.0E-03	IRIS								RfD= 4E-2 mg/kg/d
Nickel subsulfide	12035-72-2									4.8E-4	IRIS	1.7E+0	
Nickel, soluble salts	7440-02-0	2.0E-02	IRIS										
Nitrobenzene	98-95-3	5.0E-04	IRIS	2.0E-03	HEAST2								
Nitropropane, 2-	79-46-9			2.0E-02	IRIS					2.7E-3	HEAST	9.4E+0	
N-Nitrosodiethylamine	55-18-5					1.5E+2	IRIS	4.3E-03	IRIS	4.3E-2	IRIS	1.5E+2	
N-Nitrosodimethylamine (N-methyl-N-nitroso-methanamine)	62-75-9					5.1E+1	IRIS	1.4E-03	IRIS	1.4E-2	IRIS	5.1E+1	
N-Nitroso-di-n-butylamine	924-16-3					5.4E+0	IRIS	1.6E-04	IRIS	1.6E-3	IRIS	5.4E+0	
N-Nitrosodi-n-propylamine	621-64-7					7.0E+0	IRIS	2.0E-04	IRIS				
N-Nitrosodiphenylamine	86-30-6					4.9E-3	IRIS	1.4E-07	IRIS				
N-Nitroso-N-methylethylamine	10595-95-6					2.2E+1	IRIS	6.3E-04	IRIS				
N-Nitrosopiperidine	100-75-4												
N-Nitrosopyrrolidine	930-55-2					2.1E+0	IRIS	6.1E-05	IRIS	6.1E-4	IRIS	2.1E+0	
Octamethylpyrophosphoamide	152-16-9	2.0E-03	HEAST										
Parathion	56-38-2	6.0E-03	HEAST										

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	EPA Benchmarks											
		RfD (mg/kg/d)	RfD Source	RfC (mg/m3)	RfC source	Oral CSF (mkd)-1	Oral CSF Source	Drinking H2O URF (per ug/L)	Oral URF Source	Inhal Unit Risk (ug/m3)-1	Inhal URF Source	HEAST inhal CSF (mkd)-1	Super-fund values
Pentachlorobenzene	608-93-5	8.0E-04	IRIS										
Pentachlorodibenzofuran, 1,2,3,7,8-	57117-41-6					7.5E+3	TEF	2.3E-01	TEF	1.7E+0	TEF	7.5E+3	
Pentachlorodibenzofuran, 2,3,4,7,8-	57117-31-4					7.5E+4	TEF	2.3E+00	TEF	1.7E+1	TEF	7.5E+4	
Pentachlorodibenzo-p-dioxin, 1,2,3,7,8-	40321-76-4					1.5E+5	TEF	4.5E+00	TEF	3.3E+1	TEF	1.5E+5	
Pentachloronitrobenzene	82-68-8	3.0E-03	IRIS			2.6E-1	HEAST	7.4E-06	HEAST				
Pentachlorophenol	87-86-5	3.0E-02	IRIS			1.2E-1	IRIS	3.0E-06	IRIS				
Perchlorate	14797-73-0												
Phenol	108-95-2	6.0E-01	IRIS										
Phenylenediamine , m-	108-45-2	6.0E-03	IRIS										
Phorate	298-02-2	2.0E-04	HEAST										
Phthalic anhydride	85-44-9	2.0E+00	IRIS	1.2E-01	HEAST								
Polychlorinated biphenyls	1336-36-3					2.0 (food), 0.4 (H2O)	IRIS			0.0001 (evap congenr)	IRIS	2.0 (dust, aerosol), 0.4 (evap c)	
Pronamide	23950-58-5	7.5E-02	IRIS										
Propylene oxide	75-56-9			3.0E-02	IRIS	2.4E-1	IRIS	6.8E-06	IRIS	3.7E-6	IRIS	1.3E-2	
Pyrene	129-00-0	3.0E-02	IRIS										
Pyridine	110-86-1	1.0E-03	IRIS										
Safrole	94-59-7												
Selenium	7782-49-2	5.0E-03	IRIS										
Silver	7440-22-4	5.0E-03	IRIS										
Strychnine and salts	57-24-9	3.0E-04	IRIS										
Styrene	100-42-5	2.0E-01	IRIS	1.0E+00	IRIS								
Styrene-7,8-oxide	96-09-3												
Sulfide	18496-25-8												
TCDD, 2,3,7,8-	1746-01-6					1.5E+5	HEAST	4.5E+00	HEAST	3.3E+1	HEAST	1.5E+5	

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	EPA Benchmarks											
		RfD (mg/kg/d)	RfD Source	RfC (mg/m3)	RfC source	Oral CSF (mkd)-1	Oral CSF Source	Drinking H2O URF (per ug/L)	Oral URF Source	Inhal Unit Risk (ug/m3)-1	Inhal URF Source	HEAST inhal CSF (mkd)-1	Super-fund values
Tetrachlorobenzene, 1,2,4,5-	95-94-3	3.0E-04	IRIS										
Tetrachlorodibenzodioxins	41903-57-5					0.0E+0	TEF	0.0E+00	TEF	0.0E+0	TEF	0.0E+0	
Tetrachlorodibenzofurans	55722-27-5					0.0E+0	TEF	0.0E+00	TEF	0.0E+0	TEF	0.0E+0	
Tetrachloroethane, 1,1,1,2-	630-20-6	3.0E-02	IRIS			2.6E-2	IRIS	7.4E-07	IRIS	7.4E-6	IRIS	2.6E-2	
Tetrachloroethane, 1,1,2,2-	79-34-5					2.0E-1	IRIS	5.8E-06	IRIS	5.8E-5	IRIS	2.0E-1	
Tetrachloroethylene (perchloroethylene)	127-18-4	1.0E-02	IRIS			5.2E-02	HAD	1.5E-06	HAD	5.8E-07	HAD		
Tetrachlorophenol, 2,3,4,6-	58-90-2	3.0E-02	IRIS										
Tetraethyldithiopyrophosphate	3689-24-5	5.0E-04	IRIS										
Thallium	7440-28-0												
Thallium (I) acetate	563-68-8	9.0E-05	IRIS										
Thallium (I) carbonate	6533-73-9	8.0E-05	IRIS										
Thallium (I) chloride	7791-12-0	8.0E-05	IRIS										
Thallium (I) nitrate	10102-45-1	9.0E-05	IRIS										
Thallium (I) sulfate	7446-18-6	8.0E-05	IRIS										
Thiram	137-26-8	5.0E-03	IRIS										
Toluene	108-88-3	2.0E-01	IRIS	4.0E-01	IRIS								
Toluene-2,4-diamine (2,4-diaminotoluene)	95-80-7					3.2E+0	HEAST	9.1E-05	HEAST				
Toluidine, p-	106-49-0					1.9E-1	HEAST	5.4E-06	HEAST				
Toxaphene	8001-35-2					1.1E+0	IRIS	3.2E-05	IRIS	3.2E-4	IRIS	1.1E+0	
trans-1,3-Dichloropropylene	10061-02-6												
Trichloro-1,2,2-trifluoroethane, 1,1,2- (Freon 113)	76-13-1	3.0E+01	IRIS	3.0E+01	HEAST								
Trichlorobenzene, 1,2,4-	120-82-1	1.0E-02	IRIS	2.0E-01	HEAST								
Trichloroethane, 1,1,1- (methyl chloroform)	71-55-6												RfC= 1.0 mg/m3
Trichloroethane, 1,1,2- (vinyl trichloride)	79-00-5	4.0E-03	IRIS			5.7E-2	IRIS	1.6E-06	IRIS	1.6E-5	IRIS	5.7E-2	

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	EPA Benchmarks											
		RfD (mg/kg/d)	RfD Source	RfC (mg/m3)	RfC source	Oral CSF (mkd)-1	Oral CSF Source	Drinking H2O URF (per ug/L)	Oral URF Source	Inhal Unit Risk (ug/m3)-1	Inhal URF Source	HEAST inhal CSF (mkd)-1	Super-fund values
Trichloroethylene	79-01-6												oral URF=3.2 E-7; oral CSF=1.1 E-2; inh URF=1.7 E-6; inh CSF=6E-3
Trichlorofluoromethane (CFC-11)	75-69-4	3.0E-01	IRIS	7.0E-01	HEAST2								
Trichlorophenol, 2,4,5-	95-95-4	1.0E-01	IRIS										
Trichlorophenol, 2,4,6-	88-06-2					1.1E-2	IRIS	3.1E-07	IRIS	3.1E-6	IRIS	1.0E-2	
Trichlorophenoxy) propionic acid, 2 (2,4,5-	93-72-1	8.0E-03	IRIS										
Trichlorophenoxyacetic acid, 2,4,5-	93-76-5	1.0E-02	IRIS										
Trichloropropane, 1,2,3-	96-18-4	6.0E-03	IRIS			7.0E+0	HEAST	2.0E-04	HEAST				
Triethylamine	121-44-8			7.0E-03	IRIS								
Trinitrobenzene, 1,3,5- (sym-)	99-35-4	3.0E-02	IRIS										
tris(2,3-Dibromopropyl)phosphate	126-72-7												
Vanadium	7440-62-2	7.0E-03	HEAST										
Vinyl acetate	108-05-4	1.0E+00	HEAST	2.0E-01	IRIS								
Vinyl chloride	75-01-4					1.9E+0	HEAST	5.4E-05	HEAST	8.4E-5	HEAST	3.0E-1	
Warfarin	81-81-2	3.0E-04	IRIS										
Xylene, m-	108-38-3	2.0E+00	HEAST										
Xylene, o-	95-47-6	2.0E+00	HEAST										
Xylene, p-	106-42-3												
Xylenes (total)	1330-20-7	2.0E+00	IRIS										
Zinc	7440-66-6	3.0E-01	IRIS										

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Table A-1. (continued)

Constituent Name	CAS No.	Additional Benchmarks (non-IRIS, non-HEAST, non-Superfund)								
		Other EPA values	Source(s)	ATSDR oral MRL - chronic (mg/kg/d)	ATSDR inhal MRL - chronic (ppm)	CalEPA97 chronic inhal REL (mg/m3)	CalEPA99 chronic inhal REL (mg/m3)	CalEPA99 inhal unit risk (ug/m3)-1	CalEPA99 inhal CSF (mkd)-1	CalEPA99 Oral CSF (mkd)-1
Acenaphthene	83329									
Acetaldehyde	75-07-0					9.0E-03	not updated	2.7E-06		1.0E-02
Acetone	67641				13					
Acetonitrile	75-05-8									
Acetophenone	98-86-2									
Acrolein	107-02-8			0.0005		2.0E-05	2.0E-05			
Acrylamide	79-06-1					7.0E-04	not updated	1.3E-03		4.5E+00
Acrylic acid	79-10-7					1.0E-03	not updated			
Acrylonitrile	107-13-1			0.04		2.0E-03	2.0E-03	2.9E-04		1.0E+00
Aldicarb	116-06-3									
Aldrin	309-00-2			0.00003						
Allyl alcohol	107-18-6									
Allyl chloride (3-chloropropene)	107-05-1					1.0E-03	not updated	6.0E-06		2.1E-02
Ammonium vanadate	7803-55-6									
Amonium perchlorate	7790-98-9									
Aniline	62-53-3					1.0E-03	not updated	1.6E-06		5.7E-03
Anthracene	120-12-7									
Antimony	7440-36-0									
Antimony trioxide	1309-64-4					2.0E-04	not updated			
Aramite	140-57-8									
Arsenic, inorganic	7440-38-2			0.0003		3.0E-05	3.0E-05	3.3E-03	1.2E+01	1.5E+00

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Table A-1. (continued)

Constituent Name	CAS No.	Additional Benchmarks (non-IRIS, non-HEAST, non-Superfund)								
		Other EPA values	Source(s)	ATSDR oral MRL - chronic (mg/kg/d)	ATSDR inhal MRL - chronic (ppm)	CalEPA97 chronic inhal REL (mg/m3)	CalEPA99 chronic inhal REL (mg/m3)	CalEPA99 inhal unit risk (ug/m3)-1	CalEPA99 inhal CSF (mkd)-1	CalEPA99 Oral CSF (mkd)-1
Barium	7440-39-3									
Benz(a)anthracene	56-55-3							1.1E-04	3.9E-01	1.2E+00
Benzene	71-43-2					6.0E-02	6.0E-02	2.9E-05		1.0E-01
Benzidine	92-87-5					1.0E-02	not updated	1.4E-01		5.0E+02
Benzo(a)pyrene	50-32-8							1.1E-03	3.9E+00	1.2E+01
Benzo(b)fluoranthene	205-99-2							1.1E-04	3.9E-01	1.2E+00
Benzyl alcohol	100-51-6									
Benzyl chloride	100-44-7							4.9E-05		1.7E-01
Beryllium	7440-41-7					1.0E-06	1.0E-06	2.4E-03		8.4E+00
Bis(2-chloroethyl)ether	111-44-4							7.1E-04		2.5E+00
Bis(2-chloroisopropyl)ether	39638-32-9									
Bis(2-ethylhexyl)phthalate (DEHP; also di-)	117-81-7					1.0E-02	1.0E-02	2.4E-06		8.4E-03
Bis(chloromethyl)ether	542-88-1							1.3E-02		4.6E+02
Bromoform	75-25-2			0.2						
Bromomethane (methyl bromide)	74-83-9				0.005	5.0E-03	5.0E-03			
Butadiene, 1,3-	106-99-0					8.0E-03	8.0E-03	1.7E-04		3.4E+00
Butanol, n- (n-butyl alcohol)	71-36-3									
Butyl benzyl phthalate	85-68-7									
Cadmium	7440-43-9			0.0002		1.0E-05	2.0E-05	4.2E-03		1.5E+01
Carbon disulfide	75-15-0				0.3	7.0E-01	7.0E-01			
Carbon tetrachloride (tetrachloromethane)	56-23-5					4.0E-02	4.0E-02	4.2E-05		1.5E-01
Chloral	75-87-6									

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	Additional Benchmarks (non-IRIS, non-HEAST, non-Superfund)								
		Other EPA values	Source(s)	ATSDR oral MRL - chronic (mg/kg/d)	ATSDR inhal MRL - chronic (ppm)	CalEPA97 chronic inhal REL (mg/m3)	CalEPA99 chronic inhal REL (mg/m3)	CalEPA99 inhal unit risk (ug/m3)-1	CalEPA99 inhal CSF (mkd)-1	CalEPA99 Oral CSF (mkd)-1
Chloral hydrate [trichloroacetaldehyde hydrate]	302-17-0									
Chlordane	57-74-9			0.0006	0.00002 mg/m3					
Chlordecone	143-50-0			0.0005						
Chlorine cyanide (cyanogen chloride)	506-77-4									
Chloro-1,3-butadiene, 2- (chloroprene)	126-99-8									
Chloroaniline, 4- (p-)	106-47-8									
Chlorobenzene	108-90-7					1.0E+00	1.0E+00			
Chlorobenzilate	510-15-6									
Chlorodibromomethane (dibromochloromethane)	124-48-1	Inh CSF = 8.4E-2 per mkd; URF=2.4E-5 per μµg/m^3	Air Char. Study0.03							
Chloroform (trichloromethane)	67-66-3			0.01	0.02	3.0E-01	3.0E-01	5.3E-06		1.9E-02
Chloromethane (methyl chloride)	74-87-3				0.05					
Chloromethyl methyl ether	107-30-2									
Chloronaphthalene, beta-	91-58-7									
Chlorophenol, 2-	95-57-8	RfC=0.0014 mg/m^3	Air Char. Study							
Chromium (III), insoluble salts	16065-83-1									
Chromium (VI)	18540-29-9					8.0E-07	8.0E-07	1.5E-01	5.1E+02	4.2E-01
Chromium (VI) - chromic acid mists & dissolved Cr aerosols	18540-29-9				1E-4 mg/3					
Chromium (VI) - Cr particulates	18540-29-9									
Chrysene	218-01-9							1.1E-05	3.9E-02	1.2E-01
cis-1,3-Dichloropropylene	10061-01-5									

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	Additional Benchmarks (non-IRIS, non-HEAST, non-Superfund)								
		Other EPA values	Source(s)	ATSDR oral MRL - chronic (mg/kg/d)	ATSDR inhal MRL - chronic (ppm)	CalEPA97 chronic inhal REL (mg/m3)	CalEPA99 chronic inhal REL (mg/m3)	CalEPA99 inhal unit risk (ug/m3)-1	CalEPA99 inhal CSF (mkd)-1	CalEPA99 Oral CSF (mkd)-1
Cobalt (and cmpds)	7440-48-4	RfC=1E-5 mg/m^3	Air Char. Study	5.0E-06	not updated					
Copper	7440-50-8					2.0E-05	not updated			
Cresol mixtures	1319-77-3	RfC=4E-4mg/m^3	Air Char. Study	4.0E-03	1.8E-01					
Cresol, m- (3-methylphenol)	108-39-4									
Cresol, o- (2-Methylphenol)	95-48-7									
Cresol, p- (4-methylphenol)	106-44-5									
Cumene	98-82-8									
Cyanide (amenable)	57-12-5									
Cyanogen bromide	506-68-3									
Cyclohexanol	108-93-0	prov RfD=1.7E-5 mkd; prov RfC=6.0E-5 or 2.0E-5 mg/m^3	61FR 42317-354; 63FR 64371-402							
Cyclohexanone	108-94-1									
DDD (p,p'-dichlorodiphenyldichloroethane)	72-54-8									
DDE (p,p'-dichlorodiphenyldichloroethylene)	72-55-9									
DDT (p,p'-dichlorodiphenyltrichloroethane)	50-29-3									
Diallate	2303-16-4									
Dibenzo(a,h)anthracene	53-70-3							1.2E-03		4.1E+00
Dibromo-3-chloropropane, 1,2- (DBCP)	96-12-8							2.0E-03		7.0E+00
Dibromoethane, 1,2- (ethylene dibromide)	106-93-4					8.0E-04	8.0E-04	7.1E-05		2.5E-01

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	Additional Benchmarks (non-IRIS, non-HEAST, non-Superfund)								
		Other EPA values	Source(s)	ATSDR oral MRL - chronic (mg/kg/d)	ATSDR inhal MRL - chronic (ppm)	CalEPA97 chronic inhal REL (mg/m3)	CalEPA99 chronic inhal REL (mg/m3)	CalEPA99 inhal unit risk (ug/m3)-1	CalEPA99 inhal CSF (mkd)-1	CalEPA99 Oral CSF (mkd)-1
Dichlorobenzene, 1,2- (o-)	95-50-1									
Dichlorobenzene, 1,4-	106-46-7				0.1	8.0E-01	8.0E-01	1.1E-05		4.0E-02
Dichlorobenzidine, 3,3'-	91-94-1							3.4E-04		1.2E+00
Dichlorobromomethane (bromodichloromethane)	75-27-4	inh CSF=6.2E-2 per mkd; URF=1.8E-5 per μµg/m^3	Air Char. Study0.02							
Dichlorodifluoromethane [CFC-12]	75-71-8					1.0E+00	not updated			
Dichloroethane, 1,1-	75-34-3							1.6E-06		5.7E-03
Dichloroethane, 1,2- (ethylene dichloride)	107-06-2					4.0E-01	4.0E-01	2.2E-05		7.0E-02
Dichloroethylene, 1,1-	75-35-4			0.009		2.0E-02	2.0E-02			
Dichloroethylene, 1,2- (cis)	156-59-2									
Dichloroethylene, 1,2- (trans)	156-60-5									
Dichlorophenol, 2,4-	120-83-2									
Dichlorophenoxyacetic acid, 2,4- (2,4-D)	94-75-7									
Dichloropropane, 1,2-	78-87-5			0.09						
Dieldrin	60-57-1			0.00005						
Diethyl phthalate	84-66-2									
Diethylstilbestrol	56-53-1									
Dimethoate	60-51-5									
Dimethoxybenzidine, 3,3'-	119-90-4									
Dimethylbenz[a]anthracene, 7,12-	57-97-6	inh CSF=84 per mkd; URF=2.4E-2 per μµg/m^3	Air Char. Study					7.1E-02		2.5E+02

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	Additional Benchmarks (non-IRIS, non-HEAST, non-Superfund)								
		Other EPA values	Source(s)	ATSDR oral MRL - chronic (mg/kg/d)	ATSDR inhal MRL - chronic (ppm)	CalEPA97 chronic inhal REL (mg/m3)	CalEPA99 chronic inhal REL (mg/m3)	CalEPA99 inhal unit risk (ug/m3)-1	CalEPA99 inhal CSF (mkd)-1	CalEPA99 Oral CSF (mkd)-1
Dimethylbenzidine, 3,3'-	119-93-7									
Dimethylformamide, N,N-	68-12-2					3.0E-02	3.0E-02			
Dimethylphenol, 2,4-	105-67-9									
Dimethylphenol, 3,4-	95-65-8									
Dimethylphthalate	131-11-3									
Di-n-butyl phthalate	84-74-2									
Dinitrobenzene, 1,3- (m-)	99-65-0									
Dinitrophenol, 2,4-	51-28-5									
Dinitrotoluene, 2,4-	121-14-2	inh CSF=6.8E-1 per mkd; URF=1.9E-4 per μµg/m^3	Air Char. Study	0.002		7.0E-03	not updated	8.9E-05		3.1E-01
Dinitrotoluene, 2,6-	606-20-2									
Di-N-octyl phthalate	117-84-0									
Dinoseb	88-85-7									
Dioxane, 1,4-	123-91-1	RfC=0.8 mg/m^3	Air Char. Study	3.0E+00	3.0E+00			7.7E-06		2.7E-02
Diphenylamine, N,N-	122-39-4									
Diphenylhydrazine, 1,2-	122-66-7									
Direct Black 38	1937-37-7									
Direct Blue 6	2602-46-2									
Direct Brown 95	16071-86-6									
Disulfoton	298-04-4			0.00006						
Endosulfan	115-29-7			0.002						
Endothall	145-73-3									
Endrin	72-20-8			0.0003						

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	Additional Benchmarks (non-IRIS, non-HEAST, non-Superfund)								
		Other EPA values	Source(s)	ATSDR oral MRL - chronic (mg/kg/d)	ATSDR inhal MRL - chronic (ppm)	CalEPA97 chronic inhal REL (mg/m3)	CalEPA99 chronic inhal REL (mg/m3)	CalEPA99 inhal unit risk (ug/m3)-1	CalEPA99 inhal CSF (mkd)-1	CalEPA99 Oral CSF (mkd)-1
Epichlorohydrin	106-89-8					1.0E-03	1.0E-03	2.3E-05		8.0E-02
Epoxybutane, 1,2-	106-88-7					2.0E-02	2.0E-02			
Ethoxyethanol acetate, 2-	111-15-9	RfC=0.3 mg/m^3	Air Char. Study			3.0E-01	3.0E-01			
Ethoxyethanol, 2- (ethylene glycol monoethyl ether)	110-80-5					2.0E-01	2.0E-01			
Ethyl acetate	141-78-6									
Ethyl chloride (chloroethane)	75-00-3					1.0E+01	1.0E+01			
Ethyl ether	60-29-7									
Ethyl methacrylate	97-63-2									
Ethyl methanesulfonate	62-50-0									
Ethylbenzene	100-41-4					1.0E+00	1.0E+00			
Ethylene glycol	107-21-1	RfC=0.6 mg/m^3	Air Char. Study2			4.0E-01	4.0E-01			
Ethylene oxide	75-21-8					5.0E-03	3.0E-02	8.8E-05		3.1E-01
Ethylene thiourea	96-45-7					3.0E-03	not updated	1.3E-05		4.5E-02
Fluoranthene	206-44-0									
Fluorene	86-73-7									
Fluoride	16984-48-8									
Formaldehyde	50-00-0			0.2	0.008	2.0E-03	3.0E-03	6.0E-06		2.1E-02
Formic acid	64-18-6									
Furan	110-00-9									
Furfural	98-01-1									
Glycidaldehyde	765-34-4									
Heptachlor	76-44-8									
Heptachlor epoxide	1024-57-3									

(continued)

Table A-1. (continued)

Constituent Name	CAS No.	Additional Benchmarks (non-IRIS, non-HEAST, non-Superfund)								
		Other EPA values	Source(s)	ATSDR oral MRL - chronic (mg/kg/d)	ATSDR inhal MRL - chronic (ppm)	CalEPA97 chronic inhal REL (mg/m3)	CalEPA99 chronic inhal REL (mg/m3)	CalEPA99 inhal unit risk (ug/m3)-1	CalEPA99 inhal CSF (mkd)-1	CalEPA99 Oral CSF (mkd)-1
Hexachlorobenzene	118-74-1			0.00002		3.0E-03	not updated	5.1E-04		1.8E+00
Hexachlorobutadiene	87-68-3					9.0E-02	not updated			
Hexachlorocyclohexane, alpha-	319-84-6			0.008		2.0E-02	not updated			
Hexachlorocyclohexane, beta-	319-85-7					2.0E-03	not updated			
Hexachlorocyclohexane, gamma-(lindane)	58-89-9					3.0E-04	not updated	3.1E-04		1.1E+00
Hexachlorocyclopentadiene	77-47-4				0.0002	7.0E-04	not updated			
Hexachloroethane	67-72-1					8.0E-02	not updated			
Hexachlorophene	70-30-4									
Hexane, n-	110-54-3				0.6	2.0E-01	2.0E-01			
Hydrazine	302-01-2					2.0E-04	2.0E-04	4.9E-03	1.7E+01	3.0E+00
Ideno[1,2,3-cd]pyrene	193-39-5							1.1E-04	3.9E-01	1.2E+00
Isobutyl alcohol	78-83-1									
Isophorone	78-59-1	RfC=0.012 or 0.0037 mg/m^3	63FR 64371 and 61FR 423170.2			2.0E+00	2.0E+00			
Lead and cmpds (inorganic)	7439-92-1							1.2E-05	4.2E-02	8.5E-03
Maleic anhydride	108-31-6					2.0E-04	1.0E-03			
Maleic hydrazide	123-33-1									
Manganese	7439-96-5				0.00004 mg/m3	5.0E-05	5.0E-05			
Mercuric chloride	7487-94-7									
Mercury (elemental)	7439-97-6				0.0002 mg/m3	3.0E-04	3.0E-04			

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Table A-1. (continued)

Constituent Name	CAS No.	Additional Benchmarks (non-IRIS, non-HEAST, non-Superfund)								
		Other EPA values	Source(s)	ATSDR oral MRL - chronic (mg/kg/d)	ATSDR inhal MRL - chronic (ppm)	CalEPA97 chronic inhal REL (mg/m3)	CalEPA99 chronic inhal REL (mg/m3)	CalEPA99 inhal unit risk (ug/m3)-1	CalEPA99 inhal CSF (mkd)-1	CalEPA99 Oral CSF (mkd)-1
Methacrylonitrile	126-98-7									
Methanol	67-56-1	RfC=13 mg/m^3	Air Char. Study1.0E+011.0E+01							
Methomyl	16752-77-5									
Methoxychlor	72-43-5									
Methoxyethanol acetate, 2-	110-49-6	prov RfD=0.0057 mkd; prov RfC=0.03 mg/m^3	61FR 42317 and Air Char. Study9.0E-029.0E-02							
Methoxyethanol, 2- (ethylene glycol methyl ether)	109-86-4	prov RfD=0.0057 mkd	61FR 42317 2.0E-022.0E-02							
Methyl ethyl ketone	78-93-3					1.0E+00	1.0E+01			
Methyl isobutyl ketone	108-10-1									
Methyl mercury	22967-92-6			0.5 ug/kg/d						
Methyl methacrylate	80-62-6					1.0E-01	not updated			
Methyl parathion	298-00-0			0.0003						
Methyl tert-butyl ether	1634-04-4				0.7	3.0E+00	3.0E+00			
Methylaniline, 2- (o-toluidine)	95-53-4	inh CSF=2.4E-1 per mkd; URF=6.9E-5 per μµg/m^3	Air Char. Study							
Methylcholanthrene, 3-	56-49-5	inh CSF=7.4 per mkd; URF=2.1E-3 per μµg/m^3	Air Char. Study					6.3E-03		2.2E+01
Methylene bromide	74-95-3									
Methylene chloride (dichloromethane)	75-09-2			0.2	0.3	3.0E-01	4.0E-01	1.0E-06	3.5E-03	

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Table A-1. (continued)

Constituent Name	CAS No.	Additional Benchmarks (non-IRIS, non-HEAST, non-Superfund)								
		Other EPA values	Source(s)	ATSDR oral MRL - chronic (mg/kg/d)	ATSDR inhal MRL - chronic (ppm)	CalEPA97 chronic inhal REL (mg/m3)	CalEPA99 chronic inhal REL (mg/m3)	CalEPA99 inhal unit risk (ug/m3)-1	CalEPA99 inhal CSF (mkd)-1	CalEPA99 Oral CSF (mkd)-1
Methylene-bis(2-chloroaniline), 4,4'- (MBOCA)	101-14-4			0.003				4.3E-04		1.5E+00
Molybdenum	7439-98-7									
Naphthalene	91-20-3				0.002	9.0E-03	9.0E-03			
Nickel subsulfide	12035-72-2									
Nickel, soluble salts	7440-02-0				0.0002 mg/m3	5.0E-05	5.0E-05	2.6E-04		9.1E-01
Nitrobenzene	98-95-3					3.0E-02	not updated			
Nitropropane, 2-	79-46-9					2.0E-02	not updated			
N-Nitrosodiethylamine	55-18-5							1.0E-02		3.6E+01
N-Nitrosodimethylamine (N-methyl-N-nitroso-methanamine)	62-75-9							4.6E-03		1.6E+01
N-Nitroso-di-n-butylamine	924-16-3							3.1E-03		1.1E+01
N-Nitrosodi-n-propylamine	621-64-7							2.0E-03		7.0E+00
N-Nitrosodiphenylamine	86-30-6							2.6E-06		9.0E-03
N-Nitroso-N-methylethylamine	10595-95-6							6.3E-03		3.7E+00
N-Nitrosopiperidine	100-75-4							2.7E-03		9.4E+00
N-Nitrosopyrrolidine	930-55-2							6.0E-04		2.1E+00
Octamethylpyrophosphoamide	152-16-9									
Parathion	56-38-2									
Pentachlorobenzene	608-93-5									
Pentachlorodibenzofuran, 1,2,3,7,8-	57117-41-6							1.9E+00		6.5E+03
Pentachlorodibenzofuran, 2,3,4,7,8-	57117-31-4							1.9E+01		6.5E+04

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Table A-1. (continued)

Constituent Name	CAS No.	Additional Benchmarks (non-IRIS, non-HEAST, non-Superfund)								
		Other EPA values	Source(s)	ATSDR oral MRL - chronic (mg/kg/d)	ATSDR inhal MRL - chronic (ppm)	CalEPA97 chronic inhal REL (mg/m3)	CalEPA99 chronic inhal REL (mg/m3)	CalEPA99 inhal unit risk (ug/m3)-1	CalEPA99 inhal CSF (mkd)-1	CalEPA99 Oral CSF (mkd)-1
Pentachlorodibenzo-p-dioxin, 1,2,3,7,8-	40321-76-4							1.9E+01		6.5E+04
Pentachloronitrobenzene	82-68-8									
Pentachlorophenol	87-86-5			0.001		1.0E-01	not updated	5.1E-06		1.8E-02
Perchlorate	14797-73-0									
Phenol	108-95-2	prov RfC=0.02 or 0.006 mg/m^3	61FR 42317 and 63FR 24596			6.0E-01	6.0E-01			
Phenylenediamine , m-	108-45-2									
Phorate	298-02-2									
Phthalic anhydride	85-44-9					1.0E-02	1.0E-02			
Polychlorinated biphenyls	1336-36-3							5.7E-4 (high) (low)	2.0E-5	2.0E+0 (high) 7.0E-2 (low)
Pronamide	23950-58-5									
Propylene oxide	75-56-9					3.0E+00	3.0E-02	3.7E-06	1.3E-02	2.4E-01
Pyrene	129-00-0									
Pyridine	110-86-1									
Safrole	94-59-7									
Selenium	7782-49-2			0.005		8.0E-05	2.0E-02			
Silver	7440-22-4					2.0E-02	not updated			
Strychnine and salts	57-24-9									
Styrene	100-42-5				0.06	1.0E+00	1.0E+00			

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Table A-1. (continued)

Constituent Name	CAS No.	Additional Benchmarks (non-IRIS, non-HEAST, non-Superfund)								
		Other EPA values	Source(s)	ATSDR oral MRL - chronic (mg/kg/d)	ATSDR inhal MRL - chronic (ppm)	CalEPA97 chronic inhal REL (mg/m3)	CalEPA99 chronic inhal REL (mg/m3)	CalEPA99 inhal unit risk (ug/m3)-1	CalEPA99 inhal CSF (mkd)-1	CalEPA99 Oral CSF (mkd)-1
Styrene-7,8-oxide	96-09-3					6.0E-03	not updated			
Sulfide	18496-25-8									
TCDD, 2,3,7,8-	1746-01-6			0.000001 ug/kg/d				3.8E+01		1.3E+05
Tetrachlorobenzene, 1,2,4,5-	95-94-3									
Tetrachlorodibenzodioxins	41903-57-5									
Tetrachlorodibenzofurans	55722-27-5									
Tetrachloroethane, 1,1,1,2-	630-20-6									
Tetrachloroethane, 1,1,2,2-	79-34-5			0.04				5.8E-05		2.0E-01
Tetrachloroethylene (perchloroethylene)	127-18-4	oral URF=1.5E-6; oral CSF =5.2E-2; inh URF=5.8E-7; inh CSF=2E-3	1985 HAD & 1987 addend		0.04	4.0E-02	not updated	5.9E-06	2.1E-02	5.1E-02
Tetrachlorophenol, 2,3,4,6-	58-90-2					9.0E-02	not updated			
Tetraethyldithiopyrophosphate	3689-24-5									
Thallium	7440-28-0									
Thallium (I) acetate	563-68-8									
Thallium (I) carbonate	6533-73-9									
Thallium (I) chloride	7791-12-0									
Thallium (I) nitrate	10102-45-1									
Thallium (I) sulfate	7446-18-6									
Thiram	137-26-8									
Toluene	108-88-3				0.4	4.0E-01	4.0E-01			
Toluene-2,4-diamine (2,4-diaminotoluene)	95-80-7							1.1E-03		4.0E+00
Toluidine, p-	106-49-0									

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Table A-1. (continued)

Constituent Name	CAS No.	Additional Benchmarks (non-IRIS, non-HEAST, non-Superfund)								
		Other EPA values	Source(s)	ATSDR oral MRL - chronic (mg/kg/d)	ATSDR inhal MRL - chronic (ppm)	CalEPA97 chronic inhal REL (mg/m3)	CalEPA99 chronic inhal REL (mg/m3)	CalEPA99 inhal unit risk (ug/m3)-1	CalEPA99 inhal CSF (mkd)-1	CalEPA99 Oral CSF (mkd)-1
Toxaphene	8001-35-2									
trans-1,3-Dichloropropylene	10061-02-6									
Trichloro-1,2,2-trifluoroethane, 1,1,2- (Freon 113)	76-13-1					9.0E+01	not updated			
Trichlorobenzene, 1,2,4-	120-82-1									
Trichloroethane, 1,1,1- (methyl chloroform)	71-55-6					1.0E+00	1.0E+00			
Trichloroethane, 1,1,2- (vinyl trichloride)	79-00-5					4.0E-01	not updated	1.6E-05		5.7E-02
Trichloroethylene	79-01-6					6.0E-01	6.0E-01	2.0E-06	1.0E-02	1.5E-02
Trichlorofluoromethane (CFC-11)	75-69-4					2.0E+01	not updated			
Trichlorophenol, 2,4,5-	95-95-4									
Trichlorophenol, 2,4,6-	88-06-2							2.0E-05		7.0E-02
Trichlorophenoxy) propionic acid, 2 (2,4,5-	93-72-1									
Trichlorophenoxyacetic acid, 2,4,5-	93-76-5									
Trichloropropane, 1,2,3-	96-18-4									
Triethylamine	121-44-8					7.0E-03	7.0E-03			
Trinitrobenzene, 1,3,5- (sym-)	99-35-4									
tris(2,3-Dibromopropyl)phosphate	126-72-7									
Vanadium	7440-62-2	RfC=7E-5 mg/m^3	Air Char. Study							
Vinyl acetate	108-05-4					2.0E-01	2.0E-01			

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Table A-1. (continued)

Constituent Name	CAS No.	Additional Benchmarks (non-IRIS, non-HEAST, non-Superfund)								
		Other EPA values	Source(s)	ATSDR oral MRL - chronic (mg/kg/d)	ATSDR inhal MRL - chronic (ppm)	CalEPA97 chronic inhal REL (mg/m3)	CalEPA99 chronic inhal REL (mg/m3)	CalEPA99 inhal unit risk (ug/m3)-1	CalEPA99 inhal CSF (mkd)-1	CalEPA99 Oral CSF (mkd)-1
Vinyl chloride	75-01-4			0.00002		5.0E-03	not updated	7.8E-05		2.7E-01
Warfarin	81-81-2									
Xylene, m-	108-38-3									
Xylene, o-	95-47-6									
Xylene, p-	106-42-3									
Xylenes (total)	1330-20-7				0.1	2.0E-01	7.0E-01			
Zinc	7440-66-6			0.3		9.0E-04	not updated			

References

References for TEFs:

EPA98= http://www.epa.gov/nceawww1/dchem.htm

EPA93=Provisional guidance for quantitative risk assessment of PAHs, EPA/600/R-93-089

[a] Benzene oral CSF (food, water) = 0.015 to 0.055 per mg/kg/day; inhalation URF = 2.2×10^{-6} to 7.8×10^{-6} per $\mu g/m^3$; inhalation CSF = 7.7×10^{-3} to 2.7×10^{-2} per mg/kg/day (revised on IRIS 1/00).

Appendix B

Statistical Analysis Weights and Variance Estimation for the Surface Impoundment Study Screening Survey

Appendix B

Statistical Analysis Weights and Variance Estimation for the Surface Impoundment Study Screening Survey

The statistical analysis weights for the observational units in any probability-based sample survey are the initial sampling weights adjusted to reduce the potential for bias due to survey nonresponse. The initial sampling weight for each unit is the reciprocal of the probability that the unit was selected into the sample. If each unit could have more than one linkage to the sampling frame (or list) from which the sample was selected, the initial sampling weights must be adjusted to compensate for this multiplicity. Finally, a model-based estimate of the probability of responding is usually used to reduce the potential for bias due to nonresponse. In the sections that follow, we discuss each of these steps for computing the statistical analysis weights for the Surface Impoundment Study screening survey. In the last section, we discuss estimation of sampling variances using the screening survey data.

B.1 Initial Sampling Weights

Because of major differences in the sources and availability of sampling frame data, three primary sampling strata were defined for selection of facilities for the screening survey based on the facility's regulatory status under the Clean Water Act:

1. **Direct discharge (Section 402) impoundments:** These impoundments treat waste in systems that ultimately discharge directly into surface waters. This subpopulation is regulated under CWA Section 402, which requires National Pollution Discharge Elimination System (NPDES) permits for all facilities that discharge to "waters of the United States."

2. **"Zero discharge" impoundments:** These impoundments are not designed to discharge waste into the environment except through infiltration into soil or evaporation. Facilities that use infiltration or evaporation ponds for waste treatment or disposal may be regulated under a variety of state laws addressing both waste handling and groundwater protection. Specific regulations regarding these impoundments vary by State.

3. **Indirect discharge (Section 307) impoundments:** These impoundments treat or hold waste prior to discharging to a publicly owned treatment works (POTW). Facilities that discharge significant waste flows to POTWs must comply with federal and local standards for pretreatment of waste in order to prevent adverse impacts on the public treatment plants. Local POTWs are the principal permitting authorities for CWA Section 307 facilities.

For direct discharge facilities, RTI constructed an essentially complete sampling frame of 43,050 facilities from the NPDES permits in the EPA's Permit Compliance System (PCS) database. We partitioned the sampling frame into three primary sampling strata, defined as follows:

1. Facilities in high-priority SICs (26, 2819, 2824, 2834, 2869, 2897, 2911, 30, 33, or 36).

2. All other facilities with in-scope SICs.

3. The six pilot study facilities.

Stratum 1, the high-priority SICs, were expected to contain a higher proportion of facilities that use surface impoundments to manage decharacterized waste waters. Hence, this stratum was sampled at a higher rate than Stratum 2, the remainder of the in-scope SICs, to ensure that the Phase 1 screening survey would include an adequate number of facilities using surface impoundments to manage decharacterized waste waters. Each of these strata was then partitioned into substrata based on SIC codes, and the substrata were all sampled at the same rate within each primary sampling stratum. Hence, a stratified simple random sample of 2,000 facilities was selected from 15 sampling strata, and the six pilot study facilities were retained with certainty.

For zero discharge facilities, IEc constructed a sampling frame of 5,807 facilities from available state data and two federal databases: EPA's Toxics Release Inventory (TRI) and the AIRS Facility Subsystem (AFS). We stratified the sampling frame according to the general categories of completeness for the different state and federal data sources, and according to high and low priority SIC codes. Table B-1 summarizes the sampling strata for the zero discharge facilities. A stratified random sample of 250 facilities was selected using the same sampling rate for all strata except for the Oklahoma database of private sewage treatment facilities. We expected this group of facilities to be mostly out-of-scope, and, if in-scope, to be relatively homogeneous. Hence, we sampled them at one-half the rate used for the other strata.

Because local POTWs are the principal permitting authorities for indirect discharge facilities, IEc used anecdotal information collected from EPA, state and local personnel, and database information from EPA Region 7 to construct a purposive sampling frame of 35 facilities. All 35 facilities were included in the screening sample.

Table B-1. Zero Discharge Sample Frame Stratification

Database Strata	Facilities in TRI/AFS	High Priority SIC Code Facilities	Low Priority SIC Code Facilities	Facilities with No SIC Code	Facilities in SIC Code 4952
Complete Databases: CA, KY, MI, NV, NH, NM, NC, OK(1), OK(2),[a] PA, TN, VT, WI	228	61	306	1155	886 facilities in OK(2)[a]
General Databases: FL, KS, MD, MN, MI, NJ, NY, OR, VA, WA	128	127	543	1592	95
Partial Databases: AR, HI, ME, MA, MT, RI, TX, UT	116	121		117	138
No State Information: AL, AK, AZ, CO, CT, DE, GA, ID, IL, IN, IO, LA, MO, NE, ND, OH, SC, SD, WY, WV, PR	194	N/A	N/A	N/A	N/A

Notes:

[a] The Oklahoma (2) database includes an unusually extensive listing of private sewage treatment facilities. We expect most of these facilities to be out of scope, and we therefore sampled only this database at a rate lower then the rest of the frame in order to avoid spending considerable project resources examining these facilities.

Subsequent to selection of this sample for the screening survey, EPA and IEc determined that some of the sample facilities were ineligible for Phase 2 of the study, and those facilities were removed from the sample before mailing the screening questionnaires. Hence, we have computed the initial sampling weight for each of the 2,019 facilities that were mailed the screening questionnaire. The sampling weight for each of the 35 indirect discharge facilities is undefined (missing) because these facilities were purposively selected. If the six pilot study facilities are included in any statistical analyses their analysis weight will unity (1.00) because they were included in the sample with certainty. For each of the other 1,984 facilities mailed a screener, the initial sampling weight was computed as

$$w_1(j) = N_1(j) / n_1(j),$$

where

$N_1(j)$ = Total number of facilities in stratum *j*, and
$n_1(j)$ = Number of facilities selected into the sample from stratum *j*.

The frame count, $N_1(j)$, sample size, $n_1(j)$, and initial sampling weight, $w_1(j)$, are shown for each stratum in B-Table 2.[1]

B.2 Multiplicity Adjustments

The PCS data used to construct the sampling frame for the direct discharger sample were outfall- or pipe-level records. We first collapsed the pipe-level records to the permit level by permit number (NPID). We then combined permits to the facility level, but there was no unique facility ID to guide this process. Hence, we conservatively merged permits to the facility level only when it was quite clear that there were multiple permits for the same facility. We merged up to three different permits into a single facility-level record. Any facilities that had multiple permits that did not get merged into a single facility-level record on the sampling frame had multiple chances to be selected into the sample.

Therefore, in the screening questionnaire we listed all permits that had been used to define the facility on the sampling frame, and we asked each facility to list any additional permits that had been active for the facility at any time since June 1, 1990. Partway through data collection, we discovered that some facilities did not understand that these additional permits should include stormwater permits. Hence, we set up a computer-assisted telephone interviewing (CATI) application to call the screener respondents and probe for any additional permits that had not been listed in their questionnaire responses. We used both the responses to the original question, Question 7, as well as the responses to the supplemental CATI question to make the weight adjustments for frame multiplicity.

We first cleaned the responses to the questions regarding the additional permits. NPDES permit numbers are all 9-digit ID numbers for which the first two digits are a U.S. State or Territory abbreviation. Of course, the permit numbers reported in the survey did not all conform to this format. The data cleaning consisted of removing extraneous characters (e.g., blank, dash, #, NPDES, etc.) as needed to produce ID numbers in the proper format for matching against the NPDES permit numbers on the sampling frame. Leading zeros and/or state abbreviations were inserted into other reported numbers when those edits produced ID numbers in the NPDES format. In addition, when two permits numbers had been keyed as a single response in the survey, those permit numbers were moved into separate variables, which resulted in one additional Question 7 response variable that was not in the raw survey responses. Permit numbers that clearly were not in the format of an NPDES permit number received only minimal editing.

[1] The sample of 250 facilities was selected as an initial sample of 150 facilities plus 10 independent supplemental samples of 10 facilities each, resulting in some unintended variation in the stratum sampling rates for the combined sample.

Table B-2. Initial Sampling Weights

Type of Facility	Sampling Stratum	Frame Count	Sample Size	Initial Weight
Direct Dischargers (DISCHARG=1)	126	927	142	6.528
	128	1019	156	6.532
	129	440	67	6.567
	130	1478	226	6.540
	133	1752	268	6.537
	136	919	141	6.518
	2A	5169	141	36.660
	2B	3442	95	36.232
	2C	3000	82	36.585
	2D	3212	88	36.500
	2E	2680	73	36.712
	2F	3642	100	36.420
	2G	2688	74	36.324
	2H	9276	254	36.520
	2I	3400	93	36.559
	3	6	6	1.000
Zero Dischargers (DISCHARG=2)	1	228	13	17.539
	2	128	6	21.333
	3	116	4	29.000
	4	194	6	32.333
	5	61	5	12.200
	6	127	6	21.167
	7	121	6	20.167
	8	301	13	23.154
	9	543	25	21.720
	10	1155	55	21.000
	11	1592	74	21.514
	12	117	4	29.250
	13	891	22	40.500

After having completed the cleaning of the permit numbers for all screeners, we determined if any facilities reported any of the preloaded permit numbers as additional permits. For this task, we can confined our attention to the completed screeners for direct discharge facilities (DISCHARG=1), including the screeners completed by former owners. For each sampled direct discharge facility, we first compared the permit numbers reported in the screeners as additional permit numbers against the up to three NPDES permit numbers that defined the facility on the sampling frame. If the facility incorrectly reported any of these permit numbers as *additional* permit numbers, they were deleted from the cleaned variables identifying the additional permit numbers reported in the survey.

The next step was to determine the sample multiplicity for each of the 1,603 direct discharge facilities for which the current or most recent owner was a respondent (P1RESP=1). The multiplicity, $m(j)$, of the j-th sample facility is the number of facilities on the full sampling frame of 43,050 facilities that were linked to the sample facility. We merged the additional permits numbers (not preloaded) that were reported by each facility against the facility-level sampling frame permit numbers to determine the number of *additional* facilities on the sampling frame that were linked to the sample facility. The facility's multiplicity, $m(j)$, is then this count plus one (i.e., the number of additional facilities plus the one originally selected). For most direct discharge facilities, the multiplicity is one (1.00) because there were no additional facilities on the sampling frame that were linked to the sample facility.

The nonresponse adjustments require that the frame multiplicity be known for every sample facility, not just the responding facilities. Therefore, for each direct discharger sampling stratum, we computed the average multiplicity among the facilities with known multiplicity (the respondents) and imputed the multiplicity for each nonresponding facility within each sampling stratum to be the average multiplicity for the stratum. After having computed or imputed the multiplicity, $m(j)$, for each direct discharge sample facility, we computed the multiplicity-adjustment to the sampling weight for the j-th facility as follows:

$w_2(j) = 1 / m(j)$ for direct discharge facilities
$w_2(j) = 1$ for zero discharge facilities.

Lessler and Kalsbeek (1992, Section 5.2.2) show how this using this multiplicity adjustment produces survey estimates that are design-unbiased.

B.3 Nonresponse Adjustments

Weight adjustments to reduce the potential bias due to survey nonresponse are based on models for the probability of responding, using data that are available for both the respondents and the nonrespondents. Since the sampling stratum was the only thing we knew about the nonresponding facilities, we used sample-based ratio adjustments based on the sampling strata (Kalton and Maligalig, 1991). The nonresponse adjustments were defined only for the direct and zero discharge facilities because the indirect discharger sample was not a probability-based sample.

The weight adjustment for nonresponse is simply the reciprocal of the weighted response rate. Therefore, strata for which the number of respondents is small (e.g., less than 20) must be collapsed with other strata to form weighting classes. Moreover, combining strata to form weighting classes reduces the variance inflation that results from variability in the analysis weights. Hence, in order to determine weighting classes for the screening survey, we reviewed the following statistics for each sampling stratum:

- number of sample facilities, n_s
- number of facilities with known eligibility status, n_k
- response rate for eligibility determination, $r_k = (n_k / n_s) * 100$
- number of eligible facilities, n_e
- number of responding facilities, n_r
- unweighted response rate, $r_u = (n_r / n_e) * 100$.

After reviewing the pattern of survey responses and eligibility by sampling strata, we decided that each of the 15 sampling strata for the direct discharger sample contained sufficient numbers of respondents to be a separate weighting class. These are the first 15 weighting classes. However, because of the smaller sample size for the zero discharger sample, we combined strata to form weighting classes as follows:

- Weighting class 16 consists of zero discharger strata 1 through 4: the facilities from the TRI or AFS portion of the sampling frame;

- Weighting class 17 consists of zero discharger strata 5, 6, and 9: the facilities with high-priority SICs; and

- Weighting class 18 consists of the remainder of the zero discharger facilities.

Having defined the weighting classes for nonresponse adjustment, we implemented the weight adjustments for nonresponse in two stages. We first made an adjustment for inability to determine whether or not a facility was eligible for the Phase 1 screening interview (i.e., was in operation at any time since June 1, 1990). The second stage of nonresponse adjustment was an adjustment for nonresponse among the facilities known to be eligible for the screening survey.

The weight adjustment factor for inability to determine eligibility for the screening interview was computed for the *c*-th weighting class follows:

$$w_3(c) = \frac{\sum_{j \in c} w_1(j)\, w_2(j)}{\sum_{j \in c} w_1(j)\, w_2(j)\, I_k(j)} \quad ,$$

where $I_k(j)$ is an indicator that the eligibility status or the *j*-th facility is known, i.e.,

$I_k(j) = 1$	if the eligibility status of the *j*-th facility is known (P1ELIG=1 or 2)
$I_r(j) = 0$	otherwise.

This adjustment is equivalent to assuming that the proportion of sample facilities that are eligible for the screening survey (i.e., in operation at any time since June 1, 1990) is the same among those with known and unknown eligibility status.

Similarly, the weight adjustment factor for survey nonresponse was defined for the *c*-th weighting class as follows:

where I_r and I_e are indicators of response and eligibility status, respectively, i.e.,

$I_r(j) = 1$	if the *j*-th facility was a screener respondent (P1RESP=1)
$I_r(j) = 0$	otherwise, and
$I_e(j) = 1$	if the *j*-th facility was eligible for Phase 1 (P1ELIG=1)
$I_e(j) = 0$	otherwise.

The final statistical analysis weight was then be defined for the *j*-th facility in the *c*-th weighting class as the product of the various weight components, as follows:

$$w_5(j) = w_1(j)\, w_2(j)\, w_3(c)\, w_4(c)\, I_r(j)\ .$$

One property of this analysis weight is that the sum of this weight for the respondents in each weighting class is identical to the sum of the multiplicity-adjusted weights of all eligible sample facilities in that weighting class, exactly as if all the facilities had responded.

After computing these analysis weights, we performed several weight checks to verify that each weight component had been computed correctly.

B.4 Variance Estimation

Since sample facilities were selected using a stratified simple random sampling design, standard textbook formulae for stratified random sampling designs can be used to compute sampling variances, except that the observations must be weighted by the statistical analysis weights to account for survey nonresponse. However, the number of responding facilities is as small as two in some of the sampling strata used for the zero discharger sample because of the small sample sizes and high rates of ineligibility for zero dischargers. Therefore, we recommend that the collapsed sampling strata used for the weighting classes (P1WTCLAS) be used as the analysis strata when computing sampling variances.

If one wishes to compute sample means and proportions, those estimates are ratio estimates. Ratio estimators are nonlinear statistics, which require special-purpose software. One option is to use RTI's SUDAAN® software package. If one uses SUDAAN to analyze the data, we recommend that the following design options be used to compute sampling variances.

DESIGN=STRWR
NEST=P1WTCLAS.

These options specify that the design is a stratified random sampling design in which units were selected with replacement and that the variable P1WTCLAS defines the analysis strata. The with-replacement option is recommended because the survey results will be used to make inferences regarding the super-population of all survey-eligible facilities, whether or not they were included on the sampling frame constructed for this study and because the zero discharger frame is known to be incomplete.

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Appendix C

Examples of Toxicity Benchmarks for Ecological Risk Assessment

Table C-1. Selected Sources of Toxicity Data.

DATABASES

- Hazardous Substances Data Bank (HSDB). National Library of Medicine, National Toxicology Information Program. Bethesda, MD.
- Integrated Risk Information System (IRIS). U.S. EPA, Office of Health and Environmental Assessment, Environmental Criteria and Assessment Office.
- PHYTOTOX. Chemical Information System (CIS) Database.
- Registry of Toxic Effects of Chemical Substances (RTECS). National Institute for Occupational Safety and Health (NIOSH), Washington, D.C.

COMPILATIONS

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- U.S. Environmental Protection Agency (U.S. EPA). 1995. Great Lake Water Quality Criteria Documents for the Protection of Wildlife. EPA 820/b-85/008. Office of Water. Washington, D.C.
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- Venugopal, B. and T.D. Luckey. 1978. *Metal Toxicity in Mammals. 2* . Plenum Press. New York, NY.
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PRIMARY LITERATURE

- Over 400 citations

Table C-2
Toxicity Benchmarks for Mammals

Chemical	Test Species	Age	Observed Effect	Effect Level	Exposure Duration	Food Conc. (mg/kg)	Water Conc. (mg/L)	% Chem.	Ingest. Rate (g/d)	Drink Rate (mL/d)	Conv. Factor	Body Weight (kg)	Toxicity Benchmark (mg/kg-d)	Reference	Uncertainty Factor: Subchronic-to-Chronic	Uncertainty Factor: Endpoint-to-NOAEL
Inorganics																
Antimony	Mouse	Not given	• No adverse effect on survivorship, and no histopathological changes and only minor reductions in growth at 540 days and median life	NOAEL	Lifetime		5	1		5	0.001	0.025	1.0	Schroeder *et al.* 1968	—	—
Arsenic	Mouse	Weanling	• No adverse effects on maternal survival, mean litter size, number of runts, and number of still • births	NOAEL	3 generations		5	1		5	0.001	0.025	1.0	Schroeder & Mitchener 1971	—	—
Barium	Rat	Weanling	• No adverse effect on growth or food and water consumption	NOAEL	16 months		100	1		22	0.001	0.435	5.1	Perry *et al*. 1983	—	—
Beryllium	Rat	Weanling	• No adverse effect on survival, growth, median life span, and longevity	NOAEL	Lifetime		5	1		25	0.001	0.25	0.5	Schroeder & Mitchener 1975	—	—
Cadmium	Rat	Adult	• No adverse effects on number of copulating females, number of pregnant females, total implants, live fetuses, average fetal weight, and	NOAEL	12 weeks							0.25	1.0	Sutou *et al*. 1980b	—	—
Chromium III	Rat	Adult and offspring	• No adverse effects on reproduction and longevity	NOAEL	2 years	50,000		0.68	15		0.001	0.25	2,000	Ivankovic & Preussmann 197	—	—
Chromium VI	Rat	Adult	• No adverse effect on growth and no adverse systemic pathologies	NOAEL	1 year		25	1		25	0.001	0.25	2.5	MacKenzie *et al*. 1985	—	—
Cobalt	Rat	Newborn	• Decreased growth in rat pups	LOAEL	30 days							0.25	12	Domingo *et al.* 1985	—	10
Copper	Mink	Kit	• No adverse effects on kit mortality, length of gestation, and kit weight	NOAEL	1 year	85.5		1	137		0.001	1	12	Aulerich *et al*. 1982	—	—
Lead, organo-	Rat	Adult	• Increased young deaths and number of runts; by the second generation (F_2), there were insufficient numbers to continue the investigation	Effects Level	3 generations							0.25	1.0	Azar *et al*. 1973 Schoreder & Mitchener 1971	—	—
Manganese	Rat	14-day-old pups to adult	• No effect on growth, percent pregnant, litter size, ovulations, fetal resorptions, pre-implantation deaths, or fetal weight	NOAEL	> 100 days	1100		1	15		0.001	0.25	88	Laskey *et al.* 1982	—	—
Mercury	Mink	Adult	• No adverse effects on fertility, kit weight, and kit survivorship	NOAEL	6 months	10		0.739	137		0.001	1	1.0	Aulerich *et al.* 1974	—	—
Mercury, Organo-	Rat	Adult	• No adverse effects on prenatal development	NOAEL	3 generations	0.5		0.7989	15		0.001	0.25	0.024	Verschuuren *et al.* 1976	—	—
Molybdenum	Mouse	Adult	• Reduced reproductive success and increased incidence of runts	LOAEL	3 generations	0.45	10	1	3	5	0.001	0.025	2.1	Schroeder & Mitchener 1971	—	10
Nickel	Rat	Adult	• No adverse effects on fertility, gestation, offspring viability, and lactation indices	NOAEL	3 generations	250		1	15		0.001	0.25	15	Ambrose *et al*. 1976	—	—
Selenium	Rat	Adult	• No adverse effects on fertility, number of young, juvenile growth, and juvenile survival	NOAEL	2 generations		1.5	1		25	0.001	0.25	0.15	Rosenfeld & Beath 1954	—	—
Silver	Rat	Adult	• "Excellent clinical condition" was reported and no adverse effect on behavior and fluid consumption	NOAEL	12 weeks		648	1		25	0.001	0.25	65	Walker 1971	—	—
Thallium	Rat	Adult	• No adverse effects on male reproductive tract morphology or function	NOAEL	60 days							0.365	0.74	Formigli et al. 1986	—	—
Vanadium	Rat	Adult	• No adverse effects on fertility, number of litters, number of dead offspring/litter, and average body	NOAEL	60 days (gestation)			0.4178				0.26	2.1	Domingo *et al.* 1986	—	—
Zinc	Rat	Adult	• No adverse effect on fetal development	NOAEL	16 days (gestation)	2,000		1	15		0.001	0.25	120	Schlicker & Cox 1968	—	—
Volatile Organic Compounds																
BTEX																
Benzene	Mouse	Adult	• Increased maternal mortality and embryonic resorption	EL	10 days (gestation)		0.26361				1,000	0.025	264	Nawrot & Staples 1979	—	10
Toluene	Rat	Adult	• Increased maternal mortality and embryonic resorption	EL	10 days (gestation)		0.2598				1,000	0.25	260	Nawrot & Staples 1979	—	10
Ethylbenzene	• No toxicity benchmark is proposed •															
Xylene	Rat	Adult	• No adverse histopathological changes in reproductive organs	NOAEL	10 days (gestation)							0.25	500	NTP 1986	—	—
Trichloroethene-Related VOCs																
Dichloroethene, 1,2-	Rat	Adult	• No adverse histopathological changes in reproductive organs	NOAEL	90 days							0.25	206	McCauley *et al*. 1990	10	—
Dichloroethane, 1,2-	Mouse	Adult	• No adverse effects on fertility, number of live fetuses, litter survival and growth, malformations, pathology, or adult mortality	NOAEL	2 generations (24 to 25 weeks each)		290	1		6	1,000	0.035	50	Lane *et al.* 1982	—	—

Table C-2
Toxicity Benchmarks for Mammals

Chemical	Test Species	Age	Observed Effect	Effect Level	Exposure Duration	Food Conc. (mg/kg)	Water Conc. (mg/L)	% Chem.	Ingest. Rate (g/d)	Drink Rate (mL/d)	Conv. Factor	Body Weight (kg)	Toxicity Benchmark (mg/kg-d)	Reference	Uncertainty Factor: Subchronic-to-Chronic	Uncertainty Factor: Endpoint-to-NOAEL
Tetrachloroethene	Rat	Adult	• Increased mortality, however, no adverse effects on testes and ovaries	LOAEL	78 weeks							0.25	385	NCI 1977	—	10
Trichloroethane	Mouse	Adult	• No effects on fertility, incidence of implants or resorptions, number of live fetuses, frequency of live litters, litter size, postnatal growth, postnatal survival, or incidence of congenital malformations	NOAEL	2 generations (24 to 25 weeks each)		5,830	0.97		6	1,000	0.035	1,000	Lane *et al*. 1982	—	—
Trichloroethene	Rat	Adult	• No adverse maternal toxicity, fetal mortality, and teratogenic effects	NOAEL	35 days (gestation)							0.25	100	Manson *et al*. 1984	—	—
Chlorobenzene-Related VOCs																
Chlorobenzene	Mouse	Adult	• No decrease in survival.	NOAEL	103 weeks							0.025	120	Kluwe *et al*. 1985	—	—
Dichlorobenzene	Rat	Fetus	• Decrease in maternal weight and an increase in the incidence of an extra rib in the fetuses of pregnant rats	LOAEL	10 days							0.25	500	Giavini et al. 1986	—	10
Other VOCs																
Acetone	Rat	Adult	• No adverse effect on sperm motility, incidence of abnormal sperm, and testicular histopathology	NOAEL	13 weeks							0.25	1,700	Dietz et al. 1991	10	—
Dichloropropane, 1,2-	• No toxicity benchmark is proposed •															
Polycyclic Aromatic Hydrocarbons and Semivolatile Organic Compounds																
Benzo[a]pyrene	Mouse	Adult	• Reduced F1 fertility, fewer and smaller F2 litters, and decreased weight of 42-day-old pups	LOAEL	10 days (gestation)							0.025	10	MacKenzie and Angevine 1981	—	10
Naphthalene	Rat	Adult	• No adverse effects on body weight and water consumption	NOAEL	10 days (gestation)							0.25	50	Navarro et al. 1991	—	—
Methylphenol, 2-	Mink	Adult	• No adverse effect on reproduction	NOAEL	6 months	1,600		1	120		1,000	1	200	Hornshaw *et al*. 1986	—	—
Pentachlorophenol	Rat	Adult	• No adverse effects on number of pups born alive or development	NOAEL	4 months	3		1	15		0.001	0.25	0.18	Schwetz *et al*. 1978	—	—
Chlorinated Pesticides																
Aldrin / Dieldrin	Rat	Adult	• No adverse effects on number of pregnancies, number of pups per litter, offspring mortality, and weight of young at weanling	NOAEL	3 generations							0.25	0.10	Treon and Cleveland 1954, 1955	—	—
BHC	Rat	Adult	• No adverse effects on survival, fertility, litter size, birth weights, and pup and weanling body weights	NOAEL	4 generations	40		1	15		0.001	0.25	2.4	Grant et al. 1977	—	—
Chlordane	Rat	Adult	• No adverse effects viability and abundance of	NOAEL	6 generations	25		1	3		0.001	0.025	3.0	Keplinger et al. 1968	—	—
DDT / DDD / DDE	Rat	Adult	• No adverse effects on number of young produced	NOAEL	2 years	10		1	28		0.001	0.35	0.80	Fitzhugh 1948	—	—
Endosulfan	Rat	Adult	• No adverse effect on development	NOAEL	84 days							0.25	0.20	Hoeschst 1984	—	—
Heptaclor	Mink	Adult	• No adverse effect on percentage of successful litters, percent of kits born alive, kit birth weight, kit survival, body weight of the parental generation, and central nervous system effects	NOAEL	181 days							1.0	1.0	Crum et al. 1993	—	—
Polychlorinated Biphenyls																
Total PCBs	Mink	Adult	• No adverse effects on maternal mortality, number of offspring, or offspring survival	NOAEL	4.5 months	1		1	140		0.001	1.0	0.14	Aulerich & Ringer 1977	—	—
Dioxins and Furans																
2,3,7,8-TCDD	Rat	Adult/ Fetus	• Decreased gestational survival index; decreased fetal weight	LOAEL	3 generations							0.25	0.000001	Murray *et al*. 1979	—	10

Definitions:

BHC	-	Benzene hexachloride.
% Chem.	-	Percent of chemical.
g/d	-	Grams per day.
kg	-	Kilogram.
mg/kg	-	Milligrams per kilogram.
mg/kg-d	-	Milligrams per kilogram per day.
mg/L	-	Milligrams per liter.
mL/d	-	Milliliters per day.
NOAEL	-	No observed adverse effect level.
LOAEL	-	Low observed adverse effect level.
PAHs	-	Polycyclic aromatic hydrocarbons.

Table C-2
Toxicity Benchmarks for Mammals

Chemical	Test Species	Age	Observed Effect	Effect Level	Exposure Duration	Food Conc. (mg/kg)	Water Conc. (mg/L)	% Chem.	Ingest. Rate (g/d)	Drink Rate (mL/d)	Conv. Factor	Body Weight (kg)	Toxicity Benchmark (mg/kg-d)	Reference	Uncertainty Factor: Subchronic-to-Chronic	Uncertainty Factor: Endpoint-to-NOAEL
PCBs	-	Polychlorinated biphenyls.														
RTV	-	Reference toxicity value.														
TCDD	-	Tetrachlorodibenzo-*p*-dioxin.														
VOCs	-	Volatile organic chemicals.														

Table C-3
Toxicity Benchmarks for Birds

Chemical	Test Species	Age	Observed Effect	Effect Level	Duration	Food Conc. (mg/kg)	Water Conc. (mg/L)	% Chem.	Ingest. Rate (g/d)	Drink Rate (ml/d)	Conv. Factor	Body Weight (kg)	Toxicity Benchmark (mg/kg-d)	Reference	Uncertainty Factor: Subchronic-to-Chronic	Uncertainty Factor: Endpoint-to-NOAEL
Inorganics																
Antimony	• No toxicity benchmark is proposed •															
Arsenic	Mallard	1 year	• No effect on egg weight, duckling production, duckling body weight, duckling growth, or number of days between pairing and 1st egg.	NOAEL	4 weeks prior to pairing through multiple hatchings							1	5.5	Stanley, Jr. *et al*. 1994	—	—
Barium	Chicken	1-day-old	• Well tolerated by the chicks	NOAEL	4 weeks	1,000		1	13		0.001	0.121	100	Johnson *et al*. 1960		
Beryllium	• No toxicity benchmark is proposed •															
Cadmium	Chicken	Adult	• No adverse effects on egg production	NOAEL	8 months	12		1	140		0.001	0.8	2.1	Leach *et al*. 1979	—	—
Chromium III	American black duck		• No adverse systemic pathologies and no adverse effect on growth	NOAEL	10 months	10		1	125		0.001	1.25	1.0	Haseltine *et al*. 1985	—	—
Chromium VI	• No toxicity benchmark is proposed •															
Cobalt	• No toxicity benchmark is proposed •															
Copper	Chicks	1 day	• No adverse effects on growth	NOAEL	10 weeks	403		1	44		0.001	0.534	33	Mehring *et al*. 1960	10	—
Lead, metallic	American	Adult	• No adverse effects on survival and	NOAEL	6 months	50		1	10		0.001	0.13	3.8	Patee 1984	—	—
Lead, organo-	Japanese quail	Adult	• No adverse effect on growth and hatching success, and minor reductions in number of	NOAEL	12 weeks	1		1	17		0.001	0.15	0.11	Edens *et al*. 1976	—	—
Manganese	Japanese quail	1 day	• No adverse effect on growth	NOAEL	75 days							0.072	980	Laskey & Edens 1985	—	—
Mercury	Japanese quail	Adult	• Reduced fertility and hatchability	NOAEL	1 year	4.0		1	17		0.001	0.15	0.45	Hill and Schaffner 1976	—	10
Mercury, Organo-	Mallard	Adult and 9-day-old	• Fewer eggs and ducklings	LOAEL	3 generations	0.5		1	128		0.001	1	0.06	Heinz 1979	—	10
Molybdenum	Chicken	7 months	• Fewer eggs were laid and embryo viability was reduced	LOAEL	21 days	500		1	140		0.001	0.8	88	Lepore & Miller 1965	—	10
Nickel	Mallard	1-day-old	• No adverse effects on survivorship and growth	NOAEL	90 days	176		1	78.2		0.001	0.782	18	Cain & Pafford 1981	—	—
Selenium	Mallard	Adult	• No adverse effects on growth, adult survival, duckling survival, and deformed embryos	NOAEL	78 days	5		1	100		0.001	1	0.5	Heinz et al. 1987	—	—
Silver	• No toxicity benchmark is proposed •															
Thallium	• No toxicity benchmark is proposed •															
Vanadium	Mallard	Adult	• No adverse effects on mortality, body weight, or blood chemistry	NOAEL	12 days	110		1	121		0.001	1.17	11	White & Dieter 1978	10	—
Zinc	Chicken	Adult	• No adverse effects on fertility, egg hatchability, and body weight of 3-week old	NOAEL	44 weeks	228		1	123		0.001	1.935	14	Stahl *et al*. 1990	—	—
Volatile Organic Compounds																
BTEX																
Benzene	• No toxicity benchmark is proposed •															
Toluene	• No toxicity benchmark is proposed •															
Ethylbenzene	• No toxicity benchmark is proposed •															
Xylene	• No toxicity benchmark is proposed •															
Trichloroethene-Related VOCs																
Dichloroethene, 1,2-	• No toxicity benchmark is proposed •															
Dichloroethane, 1,2-	Chicken	Chick to adult	• Reduced egg weight.	LAOEL	2 years	250		1	100		0.001	1.6	16	Alumot *et al*. 1976b	—	10
Tetrachloroethene	• No toxicity benchmark is proposed •															
Trichloroethane	• No toxicity benchmark is proposed •															
Trichloroethene	• No toxicity benchmark is proposed •															
Chlorobenzene-Related VOCs																
Chlorobenzene	• No toxicity benchmark is proposed •															
Dichlorobenzene	• No toxicity benchmark is proposed •															

Table C-3
Toxicity Benchmarks for Birds

Chemical	Test Species	Age	Observed Effect	Effect Level	Duration	Food Conc. (mg/kg)	Water Conc. (mg/L)	% Chem.	Ingest. Rate (g/d)	Drink Rate (ml/d)	Conv. Factor	Body Weight (kg)	Toxicity Benchmark (mg/kg-d)	Reference	Uncertainty Factor: Subchronic-to-Chronic	Uncertainty Factor: Endpoint-to-NOAEL
Other VOCs																
Acetone	Japanese quail	Adult	• No mortality	NOAEL	5 days	40000		1	17		0.001	0.15	4,500	Hill *et al.* 1975	10	—
Dichloropropane, 1,2-	• No toxicity benchmark is proposed •															
Polycyclic Aromatic Hydrocarbons and Semivolatile Organic Compounds																
Benzo[a]pyrene	• No toxicity benchmark is proposed •															
Naphthalene	• No toxicity benchmark is proposed •															
Methylphenol, 4-	• No toxicity benchmark is proposed •															
Pentachlorophenol	Japanese quail	14 days	• Mortality	NOAEL	5 days	3,100		1	14		0.001	0.1	440	Hill & Camardese 1986	10	—
Chlorinated Pesticides																
Aldrin / Dieldrin	Mallard	Adult	• Some mortality	LOAEL	30 days							1.0	5.0	Hudson *et al.* 1984	10	10
BHC	Mallard	Adult	• No adverse effects on food intake, water consumption, body weight, egg laying frequency, egg size and weight, eggshell thinning, and eggshell porosity	NOAEL	8 weeks							1.0	5.7	Chakravarty & Lahiri 1986	—	—
Chlordane	Red-winged blackbird	Adult	• No mortality	NOAEL	84 days	10			14		0.001	0.064	2.2	Stickel *et al.* 1983	10	—
DDT / DDD / DDE	Pelican	Adult	• Adverse effects on reproductive success	LOAEL	6 years	0.15		1	660		0.001	3.5	0.028	Anderson *et al.* 1975	—	3
Endosulfan	Gray partridge	Adult	• No reproductive effect	NOAEL	4 weeks	125		1	32		0.001	0.4	10	Abiola 1992	—	—
Heptachlor	Bobwhite quail	Adult	• Mortality	LD_{50}	5 days							0.15	11	Hill *et al.* 1975	—	100
Polychlorinated Biphenyls																
Total PCBs	Screech owl	Adult	• No adverse effects on fertility and	NOAEL	2 generations	3			25		0.001	0.2	0.42	McLane & Hughes 1980	—	—
Dioxins and Furans																
2,3,7,8-TCDD	Chicken	3-day-old	• No mortality or chick edema	Subchronic	21 days							0.203	0.0001	Schwetz *et al.* 1973	10	—
2,3,7,8-TCDF	Chicken	1-day-old	• No mortality or chick edema	Subchronic	21 days							0.178	0.001	McKinney *et al.* 1976	10	10

Definitions:

BHC	-	Benzene hexachloride.
% Chem.	-	Percent of chemical.
g/d	-	Grams per day.
kg	-	Kilogram.
LD50	-	Lethal dose (50%).
mg/kg	-	Milligrams per kilogram.
mg/kg-d	-	Milligrams per kilogram per day.
mg/L	-	Milligrams per liter.
mL/d	-	Milliliters per day.
NOAEL	-	No observed adverse effect level.
LOAEL	-	Low observed adverse effect level.
PAHs	-	Polycyclic aromatic hydrocarbons.
PCBs	-	Polychlorinated biphenyls.
RTV	-	Reference toxicity value.
TCDD	-	Tetrachlorodibenzo-*p*-dioxin.
TCDF	-	Tetrachlorodibenzofuran.
VOCs	-	Volatile organic chemicals.

Table C-4
Toxicity Benchmarks for Amphibians

Chemical	Test Species	Age	Observed Effect	Effect Level	Duration	Toxicity Benchmark (ug/L)	Reference	Duration-to-Chronic	Endpoint-to-NOAEL	Amphibian RTVs (ug/L)
Inorganics										
Antimony				• No toxicity benchmark is proposed •						
Arsenic				• No toxicity benchmark is proposed •						
Barium				• No toxicity benchmark is proposed •						
Beryllium	Spotted	Larva	• Mortality	LC_{50}	96 hours	3,100	Slonim and Ray 1975	—	100	31
Cadmium	Clawed Toad	3-4 weeks	• No inhibition of larval development	NOAEL	100 days	9	Canton and Sloof 1982	—	—	9.0
Chromium				• No toxicity benchmark is proposed •						
Cobalt				• No toxicity benchmark is proposed •						
Copper	Clawed Toad	3-4 weeks	• Mortality	LC_{50}	48 hours	1,700	de Zwart and Sloof 1987	—	100	17
Lead	Argentine Toad	Embryo	• Arrested development	EC_{50}	48 hours	470	Perez-Coll *et al*. 1988	—	100	4.7
Manganese				• No toxicity benchmark is proposed •						
Mercury	Eastern narrow-mouthed toad	Embryo	• Arrested development	EC_{50}	96 hours post-hatching	1.3	Birge *et al*. 1983	—	100	0.013
Molybdenum				• No toxicity benchmark is proposed •						
Nickel				• No toxicity benchmark is proposed •						
Selenium	Clawed Toad	Embryo	• Arrested development	EC_{50}	7 days	1,500	Browne *et al*. 1979	—	100	15
Silver				• No toxicity benchmark is proposed •						
Thallium				• No toxicity benchmark is proposed •						
Vanadium				• No toxicity benchmark is proposed •						
Zinc	Clawed Toad	Embryo	• Arrested development	EC_{50}	96 hours	3,600	Dawson *et al*. 1988	—	100	36
Volatile Organic Compounds										
BTEX										
Benzene	Leopard frog	3-4 weeks	• Mortality	LC_{50}	48 hours	3,700	Sloof *et al*. 1983	—	100	37
Toluene	Leopard frog	Embryo	• Arrested development	LC_{50}	> 4 days	390		—	100	3.9
Ethylbenzene				• No toxicity benchmark is proposed •						
Xylene				• No toxicity benchmark is proposed •						
Trichloroethene-Related VOCs										
Dichloroethene, 1,2-				• No toxicity benchmark is proposed •						
Dichloroethane, 1,2-				• No toxicity benchmark is proposed •						
Tetrachloroethene				• No toxicity benchmark is proposed •						
Trichloroethane				• No toxicity benchmark is proposed •						
Trichloroethene	Clawed Toad	3-4 weeks	• Mortality	NOAEL	48 hours	29,000	Sloof *et al*. 1983	10	—	2,900
Chlorobenzene-Related VOCs										
Chlorobenzene	Northern leopard frog	Tadpole	• Mortality	LC_{50}	Fertilization to 4 days post-hatching	1,200	Birge and Cassidy 1983	—	100	12
Dichlorobenzene				• No toxicity benchmark is proposed •						
Other VOCs										
Acetone	Axolotl	Larva	• Mortality	LC_{50}	48 hours	20,000	Sloof & Baerselman 1980	10	10	200
Dichloropropane, 1,2-				• No toxicity benchmark is proposed •						
Polycyclic Aromatic Hydrocarbons and Semivolatile Organic Compounds										
Benzo[a]pyrene	Ribbed salamander	Larva	• Clastogenic effect	EC_{50}	8 days	10	Siboulet *et al*. 1984	—	10	1.0
Naphthalene	Clawed toad	Larva	• Absence of swimming	EC_{50}	6 hours	1,700	Edmisten *et al*. 1982	—	100	17
Methylphenol, 2-	Clawed toad	Tadpole	• Mortality	NOAEL	48 hours	24,000	Sloof *et al.* 1983	10	—	2,400
Pentachlorophenol	Bullfrog	Tadpole	• Mortality	LC_{50}	96 hours	210	Thurston *et al.* 1985	10	10	2.1
Chlorinated Pesticides										
Aldrin / Dieldrin	Fowler's toad	Tadpole	• Mortality	LC_{50}	96 hours	68	Mayer & Ellersieck 1986	—	100	0.68
BHC	Chorus frog	Tadpole	• Mortality	LC_{50}	96 hours	2,600	Mayer & Ellersieck 1986	—	100	26

Table C-4
Toxicity Benchmarks for Amphibians

Chemical	Test Species	Age	Observed Effect	Effect Level	Duration	Toxicity Benchmark (ug/L)	Reference	Duration-to-Chronic	Endpoint-to-NOAEL	Amphibian RTVs (ug/L)
Chlordane	Northern leopard frog	Adult	• Mortality	LC_{50}	96 hours	500	Kaplan and Overpeck 1964	—	100	5.0
DDT / DDD / DDE	Fowler's toad	7 weeks	• Mortality	LC_{50}	96 hours	30	Mayer & Ellersieck 1986	—	100	0.3
Endosulfan				• No toxicity benchmark is proposed •						
Heptachlor				• No toxicity benchmark is proposed •						
Polychlorinated Biphenyls										
Total PCBs	American toad	Embyros	• Mortality	LC_{50}	Fertilization to 4 days post-hatching	2.0	Birge & Cassidy 1983	—	100	0.02
Dioxins and Furans										
PCDDs and PCDFs				• No toxicity benchmark is proposed •						

Definitions:

BHC	-	Benzene hexachloride.
EC_{50}	-	Effect concentration (50%).
LC_{50}	-	Lethal concentration (50%).
mg/L	-	Micrograms per liter.
NOAEL	-	No observed adverse effect level.
PAHs	-	Polycyclic aromatic hydrocarbons.
PCBs	-	Polychlorinated biphenyls.
PCDDs	-	Polychlorinated dibenzo-*p* -dioxins.
PCDFs	-	Polychlorinated dibenzofurans.
RTV	-	Reference toxicity value.
VOCs	-	Volatile organic chemicals.

Table C-5
Toxicity Benchmarks for Soil Invertebrates

Chemical	Toxicity Benchmark (mg/kg_{soil})	Reference
Inorganics		
Antimony	• No toxicity benchmark is proposed •	
Arsenic	40	van den Berg *et al.* 1993
Barium	620	van den Berg *et al.* 1993
Beryllium	• No toxicity benchmark is proposed •	
Cadmium	12	van den Berg *et al.* 1993
Chromium	230	van den Berg *et al.* 1993
Cobalt	240	van den Berg *et al.* 1993
Copper	190	van den Berg *et al.* 1993
Lead	290	van den Berg *et al.* 1993
Manganese	• No toxicity benchmark is proposed •	
Mercury	10	van den Berg *et al.* 1993
Molybdenum	480	van den Berg *et al.* 1993
Nickel	210	van den Berg *et al.* 1993
Selenium	• No toxicity benchmark is proposed •	
Silver	• No toxicity benchmark is proposed •	
Thallium	• No toxicity benchmark is proposed •	
Vanadium	• No toxicity benchmark is proposed •	
Zinc	720	van den Berg *et al.* 1993
Volatile Organic Compounds		
BTEX		
Benzene	• No toxicity benchmark is proposed •	
Toluene	• No toxicity benchmark is proposed •	
Ethylbenzene	• No toxicity benchmark is proposed •	
Xylene	• No toxicity benchmark is proposed •	
Trichloroethene-Related VOCs		
Dichloroethene, 1,2-	• No toxicity benchmark is proposed •	
Dichloroethane, 1,2-	• No toxicity benchmark is proposed •	
Tetrachloroethene	• No toxicity benchmark is proposed •	
Trichloroethane	• No toxicity benchmark is proposed •	
Trichloroethene	• No toxicity benchmark is proposed •	
Chlorobenzene-Related VOCs		
Chlorobenzene	30	van den Berg *et al.* 1993
Dichlorobenzene	• No toxicity benchmark is proposed •	
Other VOCs		
Acetone	• No toxicity benchmark is proposed •	
Dichloropropane, 1,2-	• No toxicity benchmark is proposed •	
Polycyclic Aromatic Hydrocarbons and Semivolatile Organic Compounds		
Benzo[a]pyrene	• No toxicity benchmark is proposed •	
Naphthalene	• No toxicity benchmark is proposed •	
Methylphenol, 4-	• No toxicity benchmark is proposed •	
Pentachlorophenol	5	van den Berg *et al.* 1993

Table C-5
Toxicity Benchmarks for Soil Invertebrates

Chemical	Toxicity Benchmark (mg/kg_{soil})	Reference
Chlorinated Pesticides		
Aldrin / Dieldrin	• No toxicity benchmark is proposed •	
BHC	• No toxicity benchmark is proposed •	
Chlordane	• No toxicity benchmark is proposed •	
DDT / DDD / DDE	• No toxicity benchmark is proposed •	
Endosulfan	• No toxicity benchmark is proposed •	
Heptachlor	• No toxicity benchmark is proposed •	
Polychlorinated Biphenyls		
Total PCBs	• No toxicity benchmark is proposed •	
Dioxins and Furans		
2,3,7,8-TCDD	5	Reinecke and Nash 1984

Definitions:

BHC	-	Benzene hexachloride.
mg/kg_{soil}	-	Milligrams per kilogram soil.
PAHs	-	Polycyclic aromatic hydrocarbons.
PCBs	-	Polychlorinated biphenyls.
TCDD	-	Tetrachlorodibenzo-*p* -dioxin.
VOCs	-	Volatile organic chemicals.

Table C-6
Toxicity Benchmarks for Plants

Chemical	Observed Effect	Effect Level	Conc. in leaf (mg/kg_{leaf})	BCF (kg_{soil}/kg_{leaf})	Toxicity Benchmark (mg/kg_{soil})	Reference	Endpoint-to-NOAEL	Plant RTV (mg/kg_{soil})
Inorganics								
Antimony	Normal concentration in leaves	NOAEL	50	0.2	250	Kabata-Pendias & Pendias 1984	—	250
Arsenic	Normal concentration in leaves	NOAEL	1.7	0.04	43	Kabata-Pendias & Pendias 1984	—	43
Barium	Excessive concentration in leaves	LOAEL	500	0.15	3,300	Kabata-Pendias & Pendias 1984	10	330
Beryllium	Normal concentration in leaves	NOAEL	7.0	0.01	700	Kabata-Pendias & Pendias 1984	—	700
Cadmium	Normal concentration in leaves	NOAEL	0.2	0.36	0.56	Kabata-Pendias & Pendias 1984	—	0.56
Chromium	Normal concentration in leaves	NOAEL	0.5	0.0075	67	Kabata-Pendias & Pendias 1984	—	67
Cobalt	Normal concentration in leaves	NOAEL	1.0	0.02	50	Kabata-Pendias & Pendias 1984	—	50
Copper	Normal concentration in leaves	NOAEL	30	0.40	75	Kabata-Pendias & Pendias 1984	—	75
Lead	Normal concentration in leaves	NOAEL	10	0.045	220	Kabata-Pendias & Pendias 1984	—	220
Manganese	Normal concentration in leaves	NOAEL	300	0.25	1,200	Kabata-Pendias & Pendias 1984	—	1,200
Mercury	Excessive concentration in leaves	LOAEL	1.0	0.9	1.1	Kabata-Pendias & Pendias 1984	10	0.11
Molybdenum	Normal concentration in leaves	NOAEL	1.0	0.25	4.0	Kabata-Pendias & Pendias 1984	—	4.0
Nickel	Normal concentration in leaves	NOAEL	5.0	0.06	83	Kabata-Pendias & Pendias 1984	—	83
Selenium	Normal concentration in leaves	NOAEL	2.0	0.025	80	Kabata-Pendias & Pendias 1984	—	80
Silver	Normal concentration in leaves	NOAEL	0.5	0.4	1.3	Kabata-Pendias & Pendias 1984	—	1.3
Thallium	Excessive concentration in leaves	LOAEL	20	0.004	5,000	Kabata-Pendias & Pendias 1984	10	500
Vanadium	Normal concentration in leaves	NOAEL	1.5	0.0055	270	Kabata-Pendias & Pendias 1984	—	270
Zinc	Normal concentration in leaves	NOAEL	150	1.5	100	Kabata-Pendias & Pendias 1984	—	100
Volatile Organic Compounds								
BTEX								
Benzene	• No phytotoxicity benchmark is proposed •							
Toluene	Reduced seed germination	LOAEL			2,000	Will & Suter 1995	10	200
Ethylbenzene	• No phytotoxicity benchmark is proposed •							
Xylene	Reduced root length	LOAEL			100	Hulzebos et al. 1993	10	10
Trichloroethene-Related VOCs								
Dichloroethene, 1,2-	• No phytotoxicity benchmark is proposed •							
Dichloroethane, 1,2-	• No phytotoxicity benchmark is proposed •							
Tetrachloroethene	• No phytotoxicity benchmark is proposed •							
Trichloroethane	• No phytotoxicity benchmark is proposed •							
Trichloroethene	• No phytotoxicity benchmark is proposed •							
Chlorobenzene-Related VOCs								
Chlorobenzene	• No phytotoxicity benchmark is proposed •							
Dichlorobenzene	• No phytotoxicity benchmark is proposed •							
Other VOCs								
Acetone	• No phytotoxicity benchmark is proposed •							
Dichloropropane, 1,2-	• No phytotoxicity benchmark is proposed •							
Polycyclic Aromatic Hydrocarbons and Semivolatile Organic Compounds								
Benzo[a]pyrene	• No phytotoxicity benchmark is proposed •							
Naphthalene	Reduced lettuce seed germination and growth	EC_{50}			100	Hulzebos et al. 1993	100	1.0
Methylphenol, 4-	• No phytotoxicity benchmark is proposed •							
Pentachlorophenol	• No phytotoxicity benchmark is proposed •							
Chlorinated Pesticides								
Aldrin / Dieldrin	• No phytotoxicity benchmark is proposed •							
BHC	• No phytotoxicity benchmark is proposed •							
Chlordane	• No phytotoxicity benchmark is proposed •							
DDT / DDD / DDE	• No phytotoxicity benchmark is proposed •							
Endosulfan	• No phytotoxicity benchmark is proposed •							
Heptachlor	• No phytotoxicity benchmark is proposed •							

Table C-6
Toxicity Benchmarks for Plants

Chemical	Observed Effect	Effect Level	Conc. in leaf (mg/kg_{leaf})	BCF (kg_{soil}/kg_{leaf})	Toxicity Benchmark (mg/kg_{soil})	Reference	Endpoint-to-NOAEL	Plant RTV (mg/kg_{soil})
Polychlorinated Biphenyls								
Total PCBs	No effect on growth	NOAEL			40	Strek & Weber 1980	—	40
Dioxins and Furans								
PCDDs	• No phytotoxicity benchmark is proposed •							
PCDFs	• No phytotoxicity benchmark is proposed •							

Definitions:

BHC	-	Benzene hexachloride.
EC_{50}	-	Effect concentration (50%).
kg_{soil}/kg_{leaf}	-	Kilograms in soil per kilograms in leaf.
mg/kg_{leaf}	-	Milligrams per kilogram leaf.
mg/kg_{soil}	-	Milligrams per kilogram soil.
NOAEL	-	No observed adverse effect level.
LOAEL	-	Low observed adverse effect level.
PAHs	-	Polycyclic aromatic hydrocarbons.
PCBs	-	Polychlorinated biphenyls.
PCDDs	-	Polychlorinated dibenzo-*p*-dioxins.
PCDFs	-	Polychlorinated dibenzofurans.
VOCs	-	Volatile organic chemicals.

Table C-7
Toxicity Benchmarks for Freshwater Aquatic Biota

Chemical	Toxicity Benchmark (mg/L)	Reference
Inorganics		
Antimony	30	U.S. EPA 1986
Arsenic	150	U.S. EPA 1999
Barium	4.0	U.S. EPA 1993b
Beryllium	0.66	U.S. EPA 1993b
Cadmium	TBC	U.S. EPA 1999
Chromium III	TBC	U.S. EPA 1999
Chromium VI	11	U.S. EPA 1999
Cobalt	23	U.S. EPA 1993b
Copper	TBC	U.S. EPA 1999
Lead	TBC	U.S. EPA 1999
Manganese	120	U.S. EPA 1993b
Mercury	0.77	U.S. EPA 1999
Molybdenum	370	U.S. EPA 1993b
Nickel	TBC	U.S. EPA 1999
Selenium	5.0	U.S. EPA 1999
Silver	3.4[a]	U.S. EPA 1999
Thallium	12	U.S. EPA 1993b
Vanadium	20	U.S. EPA 1993b
Zinc	TBC	U.S. EPA 1999
Volatile Organic Compounds		
BTEX		
Benzene	130	U.S. EPA 1993b
Toluene	9.8	U.S. EPA 1993b
Ethylbenzene	7.3	U.S. EPA 1993b
Xylene	13	U.S. EPA 1993b
Trichloroethene-Related VOCs		
Dichloroethene, 1,2-	590	U.S. EPA 1993b
Dichloroethane, 1,2-	910	U.S. EPA 1993b
Tetrachloroethene	98	U.S. EPA 1993b
Trichloroethane	11	U.S. EPA 1993b
Trichloroethene	47	U.S. EPA 1993b
Chlorobenzene-Related VOCs		
Chlorobenzene	64	U.S. EPA 1993b
Dichlorobenzene	15	U.S. EPA 1993b
Other VOCs		
Acetone	1,500	U.S. EPA 1993b
Dichloropropane, 1,2-	5,700[b]	U.S. EPA 1986

Table C-7
Toxicity Benchmarks for Freshwater Aquatic Biota

Chemical	Toxicity Benchmark (mg/L)	Reference
Polycyclic Aromatic Hydrocarbons and Semivolatile Organic Compounds		
Benzo[a]pyrene	0.014	U.S. EPA 1993b
Naphthalene	12	U.S. EPA 1993b
Methylphenol, 2-	13	U.S. EPA 1986
Pentachlorophenol	• No toxicity benchmark is proposed •	
Chlorinated Pesticides		
Aldrin / Dieldrin	0.056	U.S. EPA 1999
BHC	0.95[a]	U.S. EPA 1986
Chlordane	0.0043	U.S. EPA 1999
DDT / DDD / DDE	0.1	U.S. EPA 1993b
Endosulfan	0.051	U.S. EPA 1993b
Heptachlor	0.0038	U.S. EPA 1993b
Polychlorinated Biphenyls		
Total PCBs	0.14	U.S. EPA 1993b
Dioxins and Furans		
PCDDs	• No toxicity benchmark is proposed •	
PCDFs	• No toxicity benchmark is proposed •	

Definitions:

BHC	Benzene hexachloride.
PAHs	Polycyclic aromatic hydrocarbons.
PCBs	Polychlorinated biphenyls.
PCDDs	Polychlorinated dibenzo-*p*-dioxins.
PCDFs	Polychlorinated dibenzofurans.
TBC	To be calculated. (The toxicity benchmark for this metal is expres and will be calculated based on the hardness of impoundment wat
µg/L	Micrograms per liter.
VOCs	Volatile organic chemicals.

Notes:

a = Criterion maximum concentration (U.S. EPA 1999)

b = lowest chronic value

Table C-8
Toxicity Benchmarks for Sediment Associated Biota

Chemical	Toxicity Benchmark (mg/kg_{sed})	Reference
Inorganics		
Antimony	2.0	Long *et al.* 1995
Arsenic	8.2	Long *et al.* 1995
Barium	• No toxicity benchmark is proposed •	
Beryllium	• No toxicity benchmark is proposed •	
Cadmium	1.2	Long *et al*. 1995
Chromium	81	Long *et al*. 1995
Cobalt	• No toxicity benchmark is proposed •	
Copper	34	Long *et al*. 1995
Lead	47	Long *et al*. 1995
Manganese	• No toxicity benchmark is proposed •	
Mercury	0.15	Long *et al.* 1995
Molybdenum	• No toxicity benchmark is proposed •	
Nickel	21	Long *et al.* 1995
Selenium	• No toxicity benchmark is proposed •	
Silver	1.0	Long *et al*. 1995
Thallium	• No toxicity benchmark is proposed •	
Vanadium	• No toxicity benchmark is proposed •	
Zinc	150	Long *et al.* 1995
Volatile Organic Compounds		
BTEX		
Benzene	• No toxicity benchmark is proposed •	
Toluene	• No toxicity benchmark is proposed •	
Ethylbenzene	• No toxicity benchmark is proposed •	
Xylene	• No toxicity benchmark is proposed •	
Trichloroethene-Related VOCs		
Dichloroethene, 1,2-	• No toxicity benchmark is proposed •	
Dichloroethane, 1,2-	• No toxicity benchmark is proposed •	
Tetrachloroethene	• No toxicity benchmark is proposed •	
Trichloroethane	• No toxicity benchmark is proposed •	
Trichloroethene	• No toxicity benchmark is proposed •	
Chlorobenzene-Related VOCs		
Chlorobenzene	• No toxicity benchmark is proposed •	
Dichlorobenzene	• No toxicity benchmark is proposed •	
Other VOCs		
Acetone	• No toxicity benchmark is proposed •	
Dichloropropane, 1,2-	• No toxicity benchmark is proposed •	
Polycyclic Aromatic Hydrocarbons and Semivolatile Organic Compounds		
Benzo[a]pyrene	0.43	Long *et al.* 1995
Naphthalene	0.16	Long *et al.* 1995
Methylphenol, 4-	• No toxicity benchmark is proposed •	
Pentachlorophenol	• No toxicity benchmark is proposed •	

Table C-8
Toxicity Benchmarks for Sediment Associated Biota

Chemical	Toxicity Benchmark (mg/kg_{sed})	Reference
Chlorinated Pesticides		
Aldrin / Dieldrin	• No toxicity benchmark is proposed •	
BHC	• No toxicity benchmark is proposed •	
Chlordane	• No toxicity benchmark is proposed •	
DDT / DDD / DDE	0.0016	Long *et al.* 1995
Endosulfan	• No toxicity benchmark is proposed •	
Heptachlor	• No toxicity benchmark is proposed •	
Polychlorinated Biphenyls		
Total PCBs	0.023	Long *et al.* 1995
Dioxins and Furans		
PCDDs	• No toxicity benchmark is proposed •	
PCDFs	• No toxicity benchmark is proposed •	

Definitions:

BHC	-	Benzene hexachloride.
mg/kg_{sed}	-	Milligrams per kilogram sediment.
PAHs	-	Polycyclic aromatic hydrocarbons.
PCBs	-	Polychlorinated biphenyls.
PCDDs	-	Polychlorinated dibenzo-*p* -dioxins.
PCDFs	-	Polychlorinated dibenzofurans.
VOCs	-	Volatile organic chemicals.

Appendix D

3MRA Simulation Modules

Assumptions, Limitations, Inputs, and Outputs

Appendix D

3MRA Simulation Modules

Assumptions, Limitations, Inputs, and Outputs

The SI Study will utilize the HWIR 3MRA Model for the Phase II risk assessment. To address multiple exposure simultaneously, the 3MRA Model includes 17 functional modules. Fourteen of these component modules will be applied to the SI Study risk assessment[1]. The assumptions and limitations and detailed input and output requirements are provided for each module in this Appendix.

D.1 System Input/Output Specifications

Within the 3MRA system, data are passed to and between modules using prespecified formats and file structures.There are three types of sequence- independent, comma-separated value (CSV) files used by the 3MRA module: site simulation files (*.SSF), global result files (*.GRF), and dictionary files (*.DIC). Sequence-independence means that a parameter can be read from anywhere in a file without having to query the file line by line. Sequence independence also implies that the ordering of parameters within the file is inconsequential.

Using this convention, established by PNNL (PNNL 1998) for HWIR99, a parameter may be read directly from a file with the assistance of functions in 3MRA (PNNL 1998). These ASCII, comma-delimited files are accessed by the module using a specially-provided dynamic link library provided in the HWIRIO.DLL. Each file has a corresponding data dictionary file in the /SSF/ subdirectory (i.e., sl.dic, cp.dic, and sw.dic).

Figure 3-11 shows how data is passed between modules in the 3MRA model; these data are transferred via *.GRF files. Dictionary files (DIC) define the parameters found in corresponding *.SSFs and *.GRFs. The "*" represents a module abbreviation. For example, VZ.DIC defines all parameters which may appear in VZ.SSF and VZ.GRF. A detailed discussion of each file type follows.

[1] Three 3MRA source modules are not needed for the SI Study risk assessment: landfill, waste pile, and aerated tank.

- *.DIC files define what parameters are allowable as well as their specifications. These dictionary files list the variable names along with their dimensions, data type (i.e., character or “string”, real or “float,” or integer), minimum and maximum limits, units, and a brief description. For some arrays, the maximum number of entries are also given.

- Site simulation files (*.SSF) contain parameters for input only (e.g., read-only files) used by specific modules. Their access is limited to one module except for the site layout SSF (SL.SSF), which includes site layout and other variables needed by several simulation modules, and the chemical properties SSF (CP.SSF) that contains all chemical-specific properties and benchmarks.

- Global result files (*.GRF) are files generated by modules, which, in turn, may be used as input files for other modules (e.g., read and write files).

The file name (*.SSF or *.GRF) is provided for each of the inputs and outputs listed below by module.

D.2 Source Modules

The source module employed for the Surface Impoundment (SI) Study risk analysis must model multimedia releases both before and after closure of the impoundment. The SI module currently in the HWIR 3MRA Model only models releases up to closure. For the SI Study risk assessment, sludge from SI operation will be assumed to be left in place after closure, where it is subject to volatilization, wind and water erosion, and leaching. Currently, the best option to model these processes is the 3MRA land application unit (LAU) module, which includes all needed release mechanisms and can be adapted to the SI post-closure scenario simply by adjusting input variables.

The remainder of this section provides the assumptions and limitations of the 3MRA SI and LAU modules and details their input requirements and outputs. This information was extracted and adapted from the HWIR 3MRA background documents (U.S. EPA, 1999a, 1999b), which contain additional detail, including all assumptions, governing equations, boundary conditions, solution techniques, and supporting references.

D.2.1 Functionality - SI Operating Module

The SI operating module functionality may be summarized as follows:

- Models single unit (cannot model multiple impoundments at a site)
- Uses mass balance approach considering contaminant removal by volatilization, biodegradation, hydrolysis, leaching, and partitioning to solids
- Estimates volatilization rates for both aerated and quiescent surfaces
- Estimates infiltration rate and contaminant leachate flux rates
- Estimates suspended solids removal (settling) efficiency
- Estimates temperature effects on contaminant degradation and volatilization
- Cannot model catastrophic failures.

The SI module calculates volatile emissions flux from a simulated wastewater treatment tank. The unit has only volatile air emissions (no particulates) and is assumed to have a pervious bottom so that contaminant leaching to the subsurface can occur. There is no runoff and overland flow of contaminant. The module is a quasi-steady-state module, and the emissions occur only while the unit operates.

D.2.2 Assumptions and Limitations - SI Module

The general module construct used for the SI module includes losses due to volatilization from aerated and/or quiescent surfaces, biodegradation, hydrolysis, solids settling/accumulation,

and leaching. This general module construct can be useful for a wide variety of types of SIs. However, certain processes, such as chemical precipitation, however, may not be explicitly modeled with this module construct. However, with judicious selection of the input parameters, the general module construct can provide accurate fate estimates for most tank and SI waste applications. For example, if the precipitation rate for chemical precipitation is known, the input parameters used for "biomass" growth could be manipulated to simulate the solids generation rate caused by precipitation (rather than biomass growth).

The following assumptions are used in the development of the SI module solution:

- Two-compartment module: "mostly" well-mixed liquid compartment and a well-mixed sediment compartment, which includes a temporary accumulating solids compartment
- First-order kinetics for volatilization in liquid compartment
- First-order kinetics for hydrolysis in both liquid and sediment compartment
- First-order kinetics for biodegradation with respect to both contaminant concentration and biomass concentration in liquid compartment
- First-order kinetics for biodegradation in sediment compartment
- Darcy's law for calculating the infiltration rate
- First-order kinetics for solids settling
- First-order biomass growth rate with respect to total biological oxygen demand (BOD) loading
- First-order biomass decay rate within the accumulating sediment compartment
- No contaminant in precipitation/rainfall
- Linear contaminant partitioning among adsorbed solids, dissolved phases, and vapor phases
- Consideration of only one contaminant at a time (does not simulate fate and transport of reaction products or multiple chemicals).
- Limitation of the maximum infiltration rate to that which does not cause ground water "mounding" and to no more than 99 percent of the maximum influent rate.
- Limitation of the minimum effluent rate to no less than one percent of the influent rate..

Due to the simplicity of the biodegradation rate module employed and the use of Henry's law partitioning coefficients, the module is most applicable to dilute aqueous wastes. At higher contaminant concentrations, biodegradation of toxic constituents may be expected to exhibit zero-order or even inhibitory rate kinetics. For waste streams with high contaminant or high total organic concentrations, vapor phase contaminant partitioning may be better estimated using partial pressure (Raoult's law) rather than Henry's law. Also, because daughter products are not included in the module, any contaminant emissions or leachate generated as a reaction intermediate or end product from either biodegradation or hydrolysis are not included in the module output.

D.2.3 Functionality - LAU (SI Postclosure) Module

The source term module developed for LAUs estimates annual average surface soil constituent concentrations and constituent mass emission rates to air, surface water, and groundwater. The LAU source emission module includes a local watershed module to estimate constituent mass flux rates from runoff and erosion to a downslope waterbody, as well as surface soil constituent concentrations in buffer areas downslope of a land-based waste management unit (WMU). The LAU module also includes a Generic Soil Column Module (GSCM) that describes the dynamics of constituent mass fate and transport within nonwastewater WMUs and near-surface soils in watershed subareas.[2] The LAU module functionality may be summarized as follows:

- Performs constituent mass balance
- Can consider waste additions/removals to simulate active facilities
- Jointly estimates constituent mass losses due to a variety of first-order mechanisms, including:
  - Volatilization of gas-phase constituent mass from the surface to the air
  - Leaching of aqueous-phase constituent mass by advection or diffusion from the bottom of the WMU or vadose zone
  - Hydrolysis and biodegradation
  - Suspension of constituent mass adsorbed to surface particles due to wind action and vehicular activity
  - Suspension of constituent mass adsorbed to surface particles due to water erosion
  - Surface runoff of aqueous-phase constituent mass.

[2] The term "soil" is used loosely here to refer to a porous medium, whether it is sludge left in place after SI closure or near-surface soil in a watershed subarea downslope from the SI.

Governing equations for the LAU module are similar to those used by Jury et al. (1983, 1990) and Shan and Stevens (1995) modified to allow for the periodic addition of constituent mass and enhanced constituent mass loss rates in the surface soil (e.g., due to runoff, erosion, wind, and mechanical processes) (U.S. EPA, 1999b).

D.2.4 Assumptions and Limitations - LAU (SI Post-Closure) Module

The following assumptions were made in the development of the LAU module to be used to model the SI after closure:

- The contaminant partitions to three phases: adsorbed (solid), dissolved (liquid), and gaseous (as in Jury et al., 1983, 1990). The model is not applicable if nonaqueous phase liquid (NAPL) is present. Similarly, with metals, the presence of a precipitate is not allowed.

- The contaminant undergoes reversible, linear equilibrium partitioning between the adsorbed and dissolved phases (as in Jury et al., 1983, 1990). The sorptive capacity of the soil column solids is considered to be infinite with respect to the total mass of contaminant over the duration of the simulation (i.e., the soil column sorptive capacity does not become exhausted).
- Contaminant in the dissolved and gaseous phases is assumed to be in equilibrium and to follow Henry's law (as in Jury et al., 1983, 1990).

- The total water flux or infiltration rate (I, m/d) is constant in space and time (as in Jury et al., 1983, 1990) and greater than or equal to zero. It is specified as an annual average.

- Although some inputs are annual average, others (e.g., wind velocities) are long-term annual averages. Accordingly, the outputs are not strictly applicable to individual years (i.e., the module is designed to only support estimation of chronic, long-term average risk estimates).

- Material in the soil column (including waste) can be approximated as unconsolidated homogeneous porous media whose basic properties (density, organic carbon, water content, porosity) are average annual values, constant in space.

- Contaminant mass may be lost from the soil column due to one or more first-order loss processes.

- The total chemical flux is the sum of the vapor flux and the flux of the dissolved solute (as in Jury et al., 1983, 1990).

- The chemical is transported in one dimension (up or down) through the soil column (as in Jury et al., 1983, 1990).

- The vapor-phase and liquid-phase porosity and tortuosity factors obey the module of Millington and Quirk (1961) (as in Jury et al., 1983, 1990).

- The modeled spatial domain of the soil column remains constant in volume and fixed in space with respect to a vertical reference, e.g., the water table.

- The module allows consideration of only one contaminant at a time and does not simulate fate and transport of reaction products or multiple chemicals.

D.2.5 Inputs for the Source Modules

Table D-1 summarizes the input variables for the SI module and Table D-2 lists the values used by the LAU module. Both modules use data provided from the header file (hd.ssf), site layout file (sl.ssf), source module-specific file (i.e., si.ssf, la.sf), and the daily (LAU), monthly (SI), annual (LA), and long-term annual average (LAU) meteorological data files. All SSF files are expected to be in an SSF subdirectory; the meteorological data are expected to be in a MetData subdirectory. For the SI, because the operating temperature in the unit may vary as a function of the ambient temperature and hydraulic residence time, the module also uses chemical property information calculated as a function of the unit temperature. Much of these data are provided through calls to the chemical property dll functions (which use data files stored in a chemical properties subdirectory). Some temperature correction routines are embedded within the SI module program. The LAU receives chemical data corrected to the long-term annual average temperature at the site.

D.2.6 Outputs from the Source Modules

Table D-3 lists the outputs from the SI module. The primary outputs of the SI module include:

- *Outputs to Air Module* - the annual average volatilization rate, which provides input for calculations of air transport of contaminant using the air module.

- *Outputs to the Vadose Zone Module* - the average annual infiltration rate and the average annual leachate contaminant flux rate, which are inputs used by the vadose zone module to calculate contaminant flux to groundwater.

The volatilation rate is calculated for a number of years specified either as the total number of years of the simulation or the number of years the unit is operated. Infiltration to the vadose zone is assumed to be driven by the hydrostatic pressure head produced by the wastewater in the unit and when the unit ceases operation it is assumed that no additional contaminant leaches from the source. Annual liquid infiltration rates and contaminant leachate flux rates are both calculated at the base of the unit.

The SI module generates a results file (sr.grf) in the grf subdirectory containing all module outputs used as inputs for other modules. The program may also generate warning messages (e.g., if the calculated unit temperature is below freezing, a warning is generated).

Table D-4 lists the outputs from the LAU module. Time series outputs to the various other HWIR99 modules include:

- *Outputs to Air Module***.** All annual time series outputs to the Air Module are reported up to and including the last year that there is nonzero volatile or particulate emission flux. After this all emissions will be zero and are not reported. Thus, the annual time series outputs to the Air Module are all the same length.

- *Outputs to the Vadose Zone Module*. The annual time series of leachate flux for each local watershed is reported up to and including the last year that there is a nonzero flux in any local watershed. This results in the same time series length for all local watersheds. After this, all leachate flux values for all local watersheds will be zero and are not reported. Annual infiltration rate is reported from year one to the last year that meteorological data are available for the simulation.

- *Outputs to the Surface Water Module*. The annual time series of contaminant loading to the waterbody are reported up to and including the last year that there is nonzero loading from any local watershed. This results in the same reported time series length for all local watersheds. Solids loads and runoff from all local watershed(s) are reported up to the last year that meteorological data are available.

- *Outputs to Exposure Modules (Human and Ecological)*. The annual time series of depth-weighted average soil contaminant concentrations in the LAU and in the buffer area downslope from the LAU is reported to the the last year of nonzero concentrations in each local watershed and subarea. Thus, the length of the reported time series for soil concentrations in each local watershed and subarea may differ. The same is true for surface soil contaminant concentrations.

The LAU module generates a results file (sr.grf) in the grf subdirectory containing all module outputs used as inputs for other modules. The program may also generate warning messages (e.g., if constituent solubility is exceeded in the WMU a warning is generated).

Table D-1. Summary of Inputs for Surface Impoundment Source Module

File	Variable Name	Units	Data Type	Variable Name in Module Code	Description
HD.SSF	CPDirectory		String	m_pathname, pathname	Path for location of chemical properties files
	MetData		String	MetPath	Path for location of meteorological files
SL.SSF	SrcArea	m^2	Real	m_A_wmu, A_wmu, A_tot	Area of the waste management unit
	SiteLatitude	degrees	Real	m_Lat	Latitude of the site
	SiteLongitude	degrees	Real	m_Long	Longitude of the site
	MetSta		String	m_MetSta, MetSta	ID number for meteorological station associated with site
	NyrMax	years	Integer	m_NyrMax	Maximum module simulation time
	SrcPh	pH units	Real	m_pH, pH	Waste pH
	SrcTemp	degrees Celsius	Real	m_T_waste, T_waste	Temperature of the waste
	SrcType		String	m_WMUType, WMUType	Type of waste management unit (AT or SI)
	SrcNumLWS		Integer	m_SrcNumLWS, SrcNumLWS	Number of local watersheds (SI only)
	SrcLWSNumSubArea		Integer	m_SrcLWSNumSubArea[ ]	Number of subareas in the local watershed (SI only)
	SrcLWSSubAreaIndex	unitless	Integer	m_SrcLWSSubAreaIndex[ ]	Local watershed subarea containing WMU (SI only)
	SrcLWSSubAreaArea	m^2	Real	m_SrcLWSSubAreaArea[ ]	Area of a subarea in the local watershed (SI only)
	TermFrac	fraction	Real	m_TermFrac	Peak output fraction for simulation termination
	SrcDepth	m	Real	m_SrcDepth	Depth of source (0 for AT)
	NumVad		Integer	m_NumVad, NumVad	Number of vadose zones (SI only)

(continued)

Table D-1. (continued)

File	Variable Name	Units	Data Type	Variable Name in Module Code	Description
	N_stot[a]	unitless	Integer	m_N_stot, N_stot	Number of subsurface soil layers (currently hardwired to 1) (SI only)[a]
	VadSATK	cm/h	Real	m_hydc_s[ ], hydc_s[ ]	Saturated hydraulic conductivity in the subsurface soil layer (SI only)
	VadThick[a]	m	Real	m_d_s[ ][ ], d_s[ ]	Thickness of the subsurface soil layer (SI only)[a]
	VadALPHA	1/cm	Real	m_alpha_s[ ], alpha_s[ ]	Alpha soil parameter for subsurface soil (SI only)
	VadBETA	unitless	Real	m_beta_s[ ], beta_s[ ]	Beta soil parameter for subsurface soil (SI only)
SI.SSF	VadSATK	cm/h	Real	m_hydc_liner, hydc_liner	Hydraulic conductivity of the liner (SI only)
	d_liner	m	Real	m_d_liner, d_liner	Thickness of SI liner (currently hardwired to 0.5 m) (SI only)
	VadALPHA	1/cm	Real	m_alpha_liner, alpha_liner	Alpha soil parameter for SI liner (SI only)
	VadBETA	unitless	Real	m_beta_liner, beta_liner	Beta soil parameter for SI liner (SI only)
	hydc_sed	m/s	Real	m_hydc_sed, hydc_sed	Hydraulic conductivity of the sediment that accumulates in the unit (SI only)
	bio_yield	g/g	Real	m_bio_yield, bio_yield	Biomass yield in g dry wt biomass/g CBOD
	CBOD	g/cm^3	Real	m_CBOD, CBOD	Carbonaceous biochemical oxygen demand for the chemical
	C_in	mg/L	Real	m_C_in, C_in	Concentration of chemical in hazardous waste
	EconLife	year	Integer	m_EconLife, EconLife	Economic life of the unit

(continued)

Table D-1. (continued)

File	Variable Name	Units	Data Type	Variable Name in Module Code	Description
	NumEcon		Integer	m_NumEcon, NumEcon	Number of economic lifetimes that the unit operates
	d_imp	cm	Real	m_d_imp, d_imp	Diameter of the impeller used to aerate the unit
	dmeanTSS	cm	Real	m_m, m	Mean particle of an influent particle
	d_setpt	fraction	Real	m_d_setpt, d_setpt	Fraction full of sediment at which unit is dredged
	d_wmu	m	Real	m_d_wmu, d_wmu, d_tot	Depth of the waste management Unit
	F_aer	fraction	Real	m_F_aer, F_aer	Fraction of the unit surface area that is aerated
	focW	mass fraction	Real	m_foc, foc	Fraction of organic carbon in the waste
	fwmu	mass fraction	Real	m_fwmu, fwmu	Fraction of waste that is hazardous
	J	lb O_2/h-hp	Real	m_J, J	O_2 transfer rating of aerator
	kba1	unitless	Real	m_kba1, kba1	Ratio of biologically active solids to the total solids concentration
	k_dec	1/s	Real	m_k_dec, k_dec	Anaerobic digestion/decay constant of the organic sediment
	u_l	g/cm-s	Real	m_mu_H2O, mu_H2O	Viscosity of water
	MWt_H2O	g/mol	Real	m_MWt_H2O, MWt_H2O	Molecular weight of water
	n_imp	unitless	Integer	m_n_imp, n_imp	Number of impellers/aerators
	O2Eff	unitless	Real	m_O2eff, O2eff	O_2 transfer correction factor
	Powr	hp	Real	m_Powr, Powr	Total power to aerators/impellers

(continued)

Table D-1. (continued)

File	Variable Name	Units	Data Type	Variable Name in Module Code	Description
	Q_wmu	m^3/s	Real	m_Q_wmu, Q_wmu, Q_in	Total influent flow rate into the unit
	rho_l	g/cm^3	Real	m_rho_H2O, rho_H2O	Density of water
	rho_part	g/cm^3	Real	m_rho_part, rho_part	Density of particles in the influent waste
	TSS_in	g/cm^3	Real	m_TSS_in, TSS_in	Total suspended solids concentration in the influent
	w_imp	rad/s	Real	m_w_imp , w_imp	Rotational speed of impellers
CP.SSF	NumChem		Integer	m_NumChem,	Number of chemical species
	ChemType		String	m_ChemType, ChemType	Type of chemical
	ChemADiff	cm^2/s	Real	m_Da, Da	Diffusivity of chemical in air
	ChemWDiff	cm^2/s	Real	m_Dw, Dw	Diffusivity of chemical in water
	ChemHLC	(atm m^3) / mol	Real	m_HLC, HLC	Henry's law constant for the chemical
	ChemKoc	mL/g	Real	m_Koc, Koc	Soil-water partitioning coefficient for the chemical
	ChemAnaBioRate	1/day	Real	m_kbiou, kbs	Biodegradation / decay rate of contaminant in sediment compartment
	ChemAerBioRate[b]	1/day	Real	m_kbioa, kbm	Complex first-order biodegradation rate constant for the chemical[b]
	ChemHydRate	1/day	Real	m_k_hyd, k_hyd	Hydrolysis rate for the chemical
	ChemSol	mg/L	Real	m_Sol, Sol	Chemical solubility
	ChemCASID		String	m_CAS, CAS	Chemical CAS ID number
	ChemName		String	m_ChemName, ChemName	Chemical name

(continued)

Table D-1. (continued)

File	Variable Name	Units	Data Type	Variable Name in Module Code	Description
	ChemKd	L/kg	Real	m_Kds, Kds	Solid/water partition coefficient
Met data file	---	°C	Real	m_AvgTemp[ ][ ]	Average monthly temperature
	---	m/s	Real	m_um[y][z]	Monthly average windspeed
	---	m/d	Real	m_AvgPpt[ ][ ]	Average monthly precipitation
	---	m/d	Real	m_E[ ][ ]	Average monthly evaporation
	---		Integer	NyrMet	Number of years of meteorological data

[a] The module currently assumes there is one native soil layer and that the thickness of the underlying soil layer is assumed to be a minimum of 1 meter thick. If the regional vadose zone thickness is less than $1+d_{wmu}$, then the impoundment is assumed to be built up (via an earthen berm) so that there is 1 meter of soil between the bottom of the SI and the ground water.

[b] Note: If normalized biodegradation rate constants are unavailable, normalized biodegradation rates constants are estimated from first-order biodegradation rate constants developed for soil systems by assuming the effective biomass in the soil system is 2.0×10^{-6} Mg/m^3. This value was developed by RTI as an interim estimate until a more rigorously developed value for this parameter is available from EPA.

Table D-2. Summary of Inputs for Land Application Unit (LAU) Source Module

File	Variable Name	Units	Data Type	Description
HD.SSF	CPDirectory		String	Path for location of chemical properties files
	MetData		String	Path for location of meteorological files
SL.SSF	SrcArea	m^2	Real	Area of LAU
	SiteLatitude	degrees	Real	Latitude of the site
	MetSta		String	ID number for meteorological station associated with site
	NyrMax	years	Integer	Maximum module simulation time
	SrcNumLWS		Integer	Number of local watersheds
	SrcLWSNumSubArea		Integer	Number of subareas in the local watershed
	SrcLWSSubAreaIndex	unitless	Integer	Local watershed subarea containing LAU
	SrcLWSSubAreaArea	m^2	Real	Area of a subarea in the local watershed
	TermFrac	fraction	Real	Peak output fraction for simulation termination
	SrcDepth	m	Real	Depth of source (tilling depth)
LA.SSF	asdm	mm	Float	Mode of the aggregate size distribution (LAU surface)
	bcm	unitless	Float	Boundary condition multiplier (lower boundary)
	BDw	g/cm3	Float	Waste density (wet waste)
	C	unitless	Float	USLE cover factor (all local watershed subareas except LAU)
	CN	unitless	Float	SCS curve number (by local watershed subarea)
	CNwmu	unitless	Float	SCS curve number (LAU)
	ConVs	m/d	Float	Settling velocity (suspended solids)
	CTPwaste	ug/g	Float	Waste constituent concentration (LAU)
	CutOffYr	year	Integer	Operating life
	Cwmu	unitless	Float	USLE cover factor (LAU)
	deltDiv	unitless	Integer	Time step divider (for debugging)
	DRZ	cm	Float	Root zone depth (by local watershed subarea)
	effdust	unitless	Float	Dust suppression control efficiency
	fcult	unitless	Float	Number of cultivations per application

(continued)

Table D-2. (continued)

File	Variable Name	Units	Data Type	Description
	fd	1/mo	Float	Frequency of surface disturbance per month, active LAU
	focS	mass fraction	Float	Surface soil fraction organic carbon (by local watershed subarea)
	focW	mass fraction	Float	Fraction organic carbon (waste solids)
	fwmu	mass fraction	Float	Fraction hazardous waste applied to LAU
	Infild	m/d	Float	Input infiltration rate (for debugging)
	K	kg/m2	Float	USLE soil erodibility factor (by local watershed subarea)
	Ksat	cm/h	Float	Soil saturated hydraulic conductivity (by local watershed subarea)
	Kwmu	kg/m2	Float	USLE soil erodibility factor (LAU)
	Lc	unitless	Float	Roughness ratio (LAU)
	mt	m	Float	Distance vehicle travels on LAU surface
LA.SSF	Nappl	1/year	Integer	Waste applications per year
	nv	1/d	Float	Vehicles/day (mean annual)
	nw	unitless	Float	Wheels per vehicle (mean)
	P	unitless	Float	USLE soil erosion control factor (all local watershed subareas except LAU)
	Pwmu	unitless	Float	USLE soil erosion control factor (LAU)
	Rappl	Mg/m2-year	Float	wet waste application rate
	RunID		string	Run identification label (optional)
	SMb	unitless	Float	soil moisture coefficient b (by local watershed subarea)
	SMFC	volume %	Float	soil moisture field capacity (by layer and local watershed subarea)
	SMWP	volume %	Float	soil moisture wilting point (by layer and local watershed subarea)
	solid	mass percent	Float	percent solids (waste)

(continued)

Table D-2. (continued)

File	Variable Name	Units	Data Type	Description
	Ss	mass percent	Float	surface soil silt content
	Sw	mass percent	Float	waste solids silt content (as applied)
	Theta	degrees	Float	slope (by local watershed)
	thetawZ1d	volume fraction	Float	input volumetric water content in till zone (for debugging)
	thetawZ2d	volume fraction	Float	input volumetric water content in subsoil zone (for debugging)
	veg	fraction	Float	post-closure fraction vegetative cover
	vs	km/h	Float	vehicle speed (mean)
	vw	Mg	Float	vehicle weight (mean)
	WCS	volume fraction	Float	soil saturated water content or total porosity (by local watershed subarea)
	X	m	Float	flow length (by local watershed)
	zava	m	Float	averaging depth upper (depth averaged soil concentration)
	zavb	m	Float	averaging depth lower (depth averaged soil concentration)
	zruf	cm	Float	post-closure roughness height(LAU)
	zZ1sa	m	Float	modeled soil column depth (local watershed subareas other than LAU)
	zZ1WMU	m	Float	tilling depth (LAU)
	zZ2WMU	m	Float	subsoil layer thickness
CP.SSF	ChemCASID		String	CAS number of chemical
	ChemName		String	Chemical name
	ChemType		String	Type of chemical
	ChemTemp	degrees C	Real	Temperature for chemical properties
	ChemFracNeutral	Fraction	Real	Fraction of chemical in the neutral form
	ChemADiff	cm^2/s	Real	Diffusivity of chemical in air

(continued)

Table D-2. (continued)

File	Variable Name	Units	Data Type	Description
	ChemWDiff	cm^2/s	Real	Diffusivity of chemical in water
	ChemHLC	(atm m^3) / mol	Real	Henry's law constant for the chemical
	ChemKoc	mL/g	Real	Soil organic carbon - water partitioning coefficient (organic compounds)
	ChemAnaBioRate	1/day	Real	Biodegradation / decay rate of contaminant in sediment compartment
	ChemAerBioRate[b]	1/day	Real	Complex first-order biodegradation rate constant for the chemical[b]
	ChemHydRate	1/day	Real	Hydrolysis rate for the chemical
	ChemSol	mg/L	Real	Chemical solubility
	ChemKd	L/kg	Real	Solid/water partition coefficient (inorganic compounds; by media)
Met file	temp	degrees C	Real	Average daily air temperature
	jday		Integer	Julian day
	dailyR	1/t	Real	Daily USLE rainfall erosivity factor
	dailyppt	cm/d	Real	Total daily precipitation
	AvgTemp	degrees C	Real	Monthly mean temperature
	maxtemp	degrees C	Real	Maximum daily average temperature for month
	mintemp	degrees C	Real	Minimum daily average temperature for month
	PE		Real	Thornthwaite Precipitation Evaporation Index
	fw1	%	Real	Percent time wind speed is greater than 5.4 m/s
	up	m/s	Real	Long term mean annual windspeed
	Uplus	m/s	Real	Annual average fastest mile of wind
	p_days	d/yr	Real	Days per year with precipitation > 0.01 in
	pp	d/yr	Real	Mean number of days per year with ≥0.01 in precipitation
	Ed	m/d	Real	Average daily evaporation
	tsc	degrees C	Real	Long term average soil column temperature

(continued)

Table D-2. (continued)

File	Variable Name	Units	Data Type	Description
	---		Integer	Number of years of meteorological data

[a] The module currently assumes there is one native soil layer and that the thickness of the underlying soil layer is assumed to be a minimum of 1 meter thick. If the regional vadose zone thickness is less than $1+d_{wmu}$, then the impoundment is assumed to be built up (via an earthen berm) so that there is 1 meter of soil between the bottom of the SI and the ground water.

[b] Note: If normalized biodegradation rate constants are unavailable, normalized biodegradation rates constants are estimated from first-order biodegradation rate constants developed for soil systems by assuming the effective biomass in the soil system is 2.0×10^{-6} Mg/m^3. This value was developed by RTI as an interim estimate until a more rigorously developed value for this parameter is available from EPA.

Table D-3. Output Summary (SR.GRF) for Surface Impoundment Source Module

File	Code	Units	Data Type	Variable Name in Module Code	Description
SR.GRF	VENY		Integer	VENumOut	number of years in VE outputs
	VEYR	year	Integer	VEOutYear[ ]	Year associated with VE output
	VE	$g/m^2/d$	Real	E_wmu_t[ ]	Volatile emission rate
	LeachFluxNY		Integer	LeachFluxNumOut[ ]	Number of years in leach flux outputs (SI only)
	LeachFluxYR	year	Integer	LeachFluxOutYear[ ][ ]	Year associated with leach flux output (SI only)
	LeachFlux	$g/m^2/d$	Real	L_wmu_t[ ]	Leachate contaminant flux (SI only)
	NyrMet	year	Integer	nyrs	Number of years in the available met record (set equal to number of year unit operates)
	AnnInfil	m/d	Real	Infil_t[ ]	Annual average leachate infiltration rate (SI only)
	SrcOvl		Logic	l_SrcOvl	Flag for overland flow presence
	SrcSoil		Logic	l_SrcSoil	Flag for soil presence
	SrcLeachSrc		Logic	l_SrcLeachSrc	Flag for leachate presence when leachate is not met-driven (unit is active)
	SrcLeachMet		Logic	l_SrcLeachMet	Flag for leachate presence when leachate is met-driven
	SrcVE		Logic	l_SrcVE	Flag for volatile emissions presence
	SrcCE		Logic	l_SrcCE	Flag for chemical sorbed to particulates emissions presence
	SrcH2O		Logic	l_SrcH2O	Flag for surface water presence

Table D-4. Output Summary (SR.GRF) for the LAU Source Module (Post-Closure SI)

File	Variable Name[a] Module	Code	Definition	Units
SR.GRF	I	AnnInfil	Leachate infiltration rate (annual avg., WMU subarea(s) only)	m/d
	J_{vol}	VE	Volatile emission rate	$g/m^2/d$
		VEYR	Year associated with output	Year
		VENY	Number of years in outputs	Unitless
	CE30	CE	Constituent mass emission rate-PM30	$g/m^2/d$
		CEYR	Year associated with output	Year
		CENY	Number of years in outputs	Unitless
	E30	PE30	Eroded solids mass emission rate-PM30	$g/m^2/d$
		PE30YR	Year associated with output	Year
		PE30NY	Number of years in outputs	Unitless
	pmf	PMF	Particulate emission particle size distribution	Mass frac.
		PMFYR	Year associated with output	Year
		PMFNY	Number of years in outputs	Unitless
	Q	Runoff	Runoff flow to waterbody	m3/d
	J_{lch}	LeachFlux	Leachate contaminant flux	$g/m^2/d$
		LeachFluxYR	Year associated with output	Year
	LeachFlux NY	LeachFluxNY	Number of years in outputs	Unitless
		SWLoadChem	Chemical load to waterbody	g/d
		SWLoadChemYr	Year associated with output	year
		SWLoadChemNY	Number of years in outputs	Unitless
	CSL	SWLoadSolid	Total suspended solids load to waterbody	g/d
	C1	SWConcTot	Total chemical concentration in surface water runoff	mg/L
		SWConcTotYR	Year associated with output	Year
		SWConcTotNY	Number of years in outputs	Unitless
	C_T	CTss	Soil concentration in surface soil layer	µg/g
		CTssYR	Year associated with output	Year

(continued)

Table D-4. (continued)

File	Variable Name[a] Module	Code	Definition	Units
		CTssNY	Number of years in outputs	Unitless
	C_T	CTda	Depth-weighted average soil concentration (from zava to zavb)	µg/g
		CTdaYR	Year associated with output	Year
		CTdaNY	Number of years in outputs	Unitless
		SrcSoil	Flag for soil presence (true)	Logical
		SrcOvl	Flag for overland flow presence (true)	Logical
		SrcLeachMet	Flag for leachate presence when leachate is met-driven (true)	Logical
		SrcLeachSrc	Flag for leachate presence when leachate is not met-driven (false)	Logical
		SrcVE	Flag for volatile emissions presence (true)	Logical
		SrcCE	Flag for chemical sorbed to particulates emissions presence (true)	Logical
		SrcH2O	Flag for surface water presence for eco-exposure (false)	Logical
		NyrMet	Number of years in the available met record	Unitless

[a] Where the variable name is used in the code but not in the documentation, the first column is left blank.

D.3 Air Module

The HWIR 3MRA model air module is the Industrial Source Complex-Short Term (ISCST3) model, with pre- and postprocessors incorporated to adapt it to the 3MRA system,. The air module provides estimates of contaminant concentration, dry deposition (particles only), and wet deposition (particles and gases) for user-specified averaging periods (i.e., annually for HWIR99).

ISCST3 is used as legacy code in the 3MRA framework. That is, the model is left intact and system interfacing is handled using the pre- and postprocessors. The pre- and postprocessing code also provides additional functionality to support other 3MRA framework requirements. This section provides an overview of the assumptions, limitations, inputs, and outputs of the 3MRA air module as applied in HWIR; additional detail can be found in U.S. EPA (1999c and 1999d).

D.3.1 Functionality

ISCST3 is a steady-state Gaussian plume model. The model provides point estimates of ambient air concentration, dry deposition (particles only), and wet deposition (particles and gases) for user-specified averaging periods (e.g., annual). The regulatory version of the model has been modified to sample from a file of hourly meteorological data at regular intervals (SCIM function) and thus will only model a fraction of the hours for the period of record (e.g., 20 years). Sampling intervals of every 8 hours for wet deposition and every 8 days for dry deposition have been tested and are currently being used in HWIR. Sampling enables the model to execute more quickly while producing long-term annual averages comparable to those obtained from the full data set.

Because of computational time burden, the air model component is run outside of the FRAMES-HWIR system. The air concentrations and deposition rates are saved into a database that the FRAMES-HWIR system accesses. During 3MRA implementation, normalized emission rates (from the 3MRA source modules) are used as inputs along with the sampled meteorological data. Chemical-specific and temporal-specific concentrations and deposition rates are calculated in the ISCST3 postprocessor by multiplying the normalized concentration and deposition predictions by these chemical-specific annual emission rates.

For the outside 3MRA runs, ISCST3 predicts normalized concentrations and depositions at a set of grid points within the 2-km area of interest surrounding an impoundment, locations that are optimized by 3MRA to represent concentrations at human receptor points and deposition rates for watersheds, waterbodies, farms, and ecological habitats. Although a spline interpolation routine is available in the 3MRA postprocessor ISC3, this feature is not being used.

The major functionality provided by the pre- and postprocessing code is the following:

- **Decision to execute ISCST3.** If a given site/WMU combination has already been run by the Air Module in a set of model runs, the preexisting (saved) ISCST3 output file is used to calculate parameters for the Air Module output file, ar.grf. If not, ISCST3 is executed with pre- and postprocessing, which saves the ISC output files for future use in the grf\lfo directory and calculates parameters for the Air Module output file.

- **MASSFRAX calculation.** The preprocessor can calculate a source-specific, long-term average particulate mass fraction distribution (ISCST3 input variable, *MASSFRAX*) from the land-based source modules (landfill, wastepile, or land application unit) output time series *PMF* (the particle size distribution) and *PE30* (the mass flux of 30 µm or smaller particles). If the internal calculation of *MASSFRAX* is not exercised, then *MASSFRAX* is read as a fixed distribution (not WMU-specific) from the ar.ssf file.

- **Spline interpolation decision.** The preprocessor determines whether to execute ISCST3 to model **directly** ("ISCST3-model") to all site-specific output x-y coordinates requested by the 3MRA framework or, alternatively, to model to a prespecified (fixed) set of polar coordinates and then use a two-dimensional cubic spline method to interpolate from this polar set to the (larger) 3MRA-requested set of interest. The spline option was not used for HWIR99.

Other new features added to ISCST3 include a revised plume depletion scheme that replaces the computationally intensive Horst (1983) plume depletion algorithm with a faster, more robust plume depletion and settling algorithm developed by Venkatram (1988). This algorithm depletes material in a surface-based internal boundary layer that grows with distance from the source. In conjunction with this change, the deposition velocity algorithm was also modified by removing the inertial impaction term, which overestimates deposition velocity for some particle sizes. Also, a new output option was required to allow examination of concentration and deposition by particle size so that inhalation risks can be determined for pollutants with particle sizes $\leq$10 µm.

D.3.2 Assumptions and Limitations

- The ISCST3 modeling does not simulate chemical-specific fate processes such as photolysis and degradation.

- To conserve mass in the 3MRA framework, ISCST3 includes a source depletion algorithm that adjusts for the mass lost to deposition. However, module simulations showed that less than 1 percent of emitted mass is deposited within a 2-km radius with source depletion on. Therefore, to reduce computational burden, source depletion for deposition loss was not implemented in HWIR.

- One of the largest areas of uncertainty in the 3MRA air modeling is related to gas deposition. Although previous modeling exercises used a transfer coefficient to model the dry deposition of gases it is a challenge to preserve conservation of mass. Therefore, dry deposition of gases is not considered in HWIR

- Although chemical-specific scavenging coefficients should be used to calculate the wet deposition of gases, these values are not readily available. Instead, HWIR uses a single scavenging coefficient for all gases that approximates gases as very small particles. This approach may underpredict wet deposition for some gases and overpredict for others.

D.3.3 Inputs for the Air Module

Table D-5 summarizes the inputs passed by the 3MRA model system and read by the air module preprocessor. The input file for ISCST3-HWIR is generated by the Air Module preprocessor based on the module-specific input file, ar.ssf, the generic site layout file, sl.ssf, modeled inputs from the generic source output file, sr.grf, and certain "hard-wired" options set by certain variables in the ar.ssf file. The following options used by ISCST3-HWIR are identical for each model run:

- Calms processing routine is used

- Missing data processing routine is used

- SCIM is not used

- Plume depletion due to dry (particles only) and wet (vapors and particles) deposition is considered.

The use of rural or urban dispersion parameters is selected on a site-by-site basis. The type of model output depends on the facility, with concentration, dry deposition, and wet deposition being calculated for land application units, waste piles, and landfills. Only concentration and wet deposition were calculated for the surface impoundments and aerated tanks because the pollutants are only in the gaseous phase.

Source Parameters. Surface impoundments and land application units are modeled as ground-level area sources by ISCST3-HWIR. The air model receives inputs that are output by these source module(s) in the SR.GRF model file. These inputs include volatile constituent emission rates (*VE*) from both unit types and, from the LAU, particulate mass emission rates (*PE30*), and constituent mass emission rates for particulates (*CE*). Becaue a variable mass fraction distribution for particulates (MASSFRAXOption on) would make it necessary to rerun ISCST3 with each Monte Carlo sampling, a fixed MASSFRAX distribution for all sources was used to enable complete reuse of ISCST3 outputs from sample to sample. ISCST3 requires scavenging coefficients by particle size category for liquid precipitation one for frozen precipitation. Scavenging coefficients are assigned based on the size of the particles. Frozen and liquid precipitation were assumed to scavenge particles at the same rate.

Receptor Locations. Air modeling points (*AirLocX, AirLocY*) depend on the layout of the waterbodies, watersheds, human receptors, farms, and habitats around a site. For HWIR, ISCST3 model directly to all site-specific output x-y coordinates requested by the 3MRA framework.

Meteorological Inputs. Meteorological data are collected regionally by meteorological station, with a modeled site assigned to the nearest station with similar weather conditions and adequate weather data for the analysis. Hourly meteorological data are sent to the air module in separate ASCII files prepared by PCRAMMET and read directly by the model. These files were created for the meteorological surface stations and associated upper air stations necessary to cover meteorlogical condtions for the facilities being modeled. The hourly files are designated as #######h.dat, where ####### is the surface meteorological station number, and are formatted as follows.

Header Record
Sfc Station # Sfc Sta. Year Mixing Ht. Station # Mixing Ht. Sta. Year

Data Records (in each row, with each row corresponding to one hour)

Variable	*Description*	*Units*
001	Year	
002	Month	
003	Day	
004	Hour	
005	Random flow vector (wind dir)	(degrees)
006	Wind Speed	(m/s)
007	Ambient Temperature	(K)
008	Stability Category	
009	Rural Mixing Height	(m)
010	Urban Mixing Height	(m)
011	Friction Velocity at Application Site	(m/s)
012	Monin-Obukhov Length at app. Site	(m)
013	Roughness length at application site	(m)
014	Precipitation Code	
015	Precipitation Amount	(mm)

The length of the hourly meteorological files varies based on availability of data with a minimum file length of 10 years.

Most meteorological data were extracted from Solar and Meteorological Surface Observation Network (SAMSON; U.S. DOC and U.S. DOE, 1993) hourly data files and converted as necessary to daily time series, monthly time series, annual time series, and long-term averages for use with the various media modules. Because SAMSON precipitation data were inadequate, precipitation data were obtained from cooperative station daily summaries (NCDC et al., 1995), with SAMSON data used to help allocate these daily data to hourly time series. Mixing heights were obtained from upper air station data. Programs were used to fill in data where it was missing in SAMSON or NCDC datasets. Land use data also were required in

the vicinity of each meteorological station to derive air model inputs such as Bowen ratio, surface roughness height, minimum Monin-Obukhov length, noontime albedo, and the fraction of net radiation absorbed by the ground. Additional details on meteorological data collection and processing using PCRAMMET can be found in U.S. EPA (1999e).

D.3.4 Outputs from the Air Module

The air model output file (ar.grf) includes the following output variables, along with variables necessary to define the time series /receptor location arrays for each:

- PM10 concentrations
- Volatile concentrations (CVap)
- Vapor wet deposition (VapWDep)
- Particulate dry deposition (ParDDep)
- Particulate wet deposition (ParWDep).

Table D-6 summarizes the ouputs from the air module post processor.

Table D-5. Air Module Input Parameters

Input Parameter	Units	Description
Module-Specific Parameters (AR.SSF)		
NumAirSplineDist	unitless	Number of distances used to construct the polar mesh used to construct the spline
NumAirSplineAngle	unitless	Number of angles used to construct the polar mesh used to construct the spline
AirSplineDistance	m	Array of radial distances of polar mesh
AirSplineAngle	degrees	Array of angles used in polar mesh
SplineOption	unitless	Whether or not splining is an option. 0=no spline, 1=spline
StartYr		Required by ISCST3. Starting year of Met. file
ScimStr		Required by ISCST3. SCIM option
RuralStr		Required by ISCST3. Rural or Urban
DryDpStr		Required by ISCST3. Dry Depletion Option
WetDpStr		Required by ISCST3. Wet Depletion Option.
AirData		Required by ISCST3. Upper Air (Met.) Station number
SurfData		Required by ISCST3. Surface (Met.) Station number
AnemHght	m	Required by ISCST3. Anemometer height
SHight	m	Required by ISCST3. Source height
ArrayLen	unitless	Required by ISCST3. Length of array
MASSFRAXOption	unitless	Logical flag for whether to internally calculate *MASSFRAX* distribution (false) or read a fixed *MASSFRAX* (true) from AR.SSF.
MASSFRAX	fraction	Required by ISCST3. Fraction of particle size (1 dim. array for each particle-emitting source type, i.e. LAU, LF, and WP in that order)
PARTDIAM	μm	Required by ISCST3. Particle diameter (1 dim. array)
PARTSLIQ	h/s-mm	Required by ISCST3. Particle scavenging coefficient by liquid precipitation (1 dim. array)
PARTSICE	h/s-mm	Required by ISCST3. Particle scavenging coefficient by frozen precipitation (1 dim. array)
LiqScav	h/s-mm	Required by ISCST3. Gas scavenging coefficient by liquid precipitation (1 dim. array)
IceScav	h/s-mm	Required by ISCST3. Gas scavenging coefficient by frozen precipitation (1 dim. array)

(continued)

Table D-5. (continued)

Input Parameter	Units	Description
SCIMBYHR	unitless	Required by ISCST3. Sets model to skim through Metfile, picking certain hours according to array specifications
Site Layout Inputs (SL.SSF)		
AirLocX	m	Array for easting in site coordinate system (for each receptor location)
AirLocY	m	Array for northing in site coordinate system (for each receptor location)
MetSta		Met. Station identifier (<MetSta>L.dat (L: long-term), <MetSta>A.dat (A: annual time series), <MetSta>M.dat (M: monthly time series), <MetSta>D.dat (D: daily time series), <MetSta>H.dat (H: hourly time series))
NumAir		Number of air points
SettingID		Srctype (*One of LAU, LF, WP, AT, SI) + SiteID
SrcArea	m^2	Area of source
SrcLocX	m	Easting in site coordinate system (Source location). 0 at source centroid
SrcLocY	m	Northing in site coordinate system (Source location). 0 at source centroid
SrcType		One of {LAU, LF, WP, AT, SI}
Inputs from Source Module (SR.GRF)		
CE	float	$g/m^2/d$
PE30	float	$g/m^2/d$
PE30NY	integer	
PMF	float	
VE	float	$g/m^2/d$
VENY	integer	
SrcVE	logical	
SrcCE	logical	

Table D-6. AR.GRF Output Variables (Air Module Outputs)

Variable Name	Unit	Description
PM10	$\mu g/m^3$	2-dimensional array that provides information on total number of years of activity for PM10 at each receptor location and PM10 concentration in each year.
PM10YR	Year	Time series of years corresponding to this variable.
PM10NY	unitless	Number of years in the time series corresponding to this variable.
CVap	$\mu g/m^3$	2-dimensional array that provides information on total number of years of activity for volatiles at each receptor location and volatile concentration in each year.
CVapYR	Year	Time series of years corresponding to this variable.
CVapNY	unitless	Number of years in the time series corresponding to this variable.
VapWDep	$g/m^2/d$	2-dimensional array that provides information on total number of years of activity for vapor wet deposition at each receptor location and wet deposition flux for each year.
VapWDepYR	Year	Time series of years corresponding to this variable.
VapWDepNY	unitless	Number of years in the time series corresponding to this variable.
ParDDep	$g/m^2/d$	2-dimensional array that provides information on total number of years of activity for particulate dry deposition at each receptor location and dry deposition flux for each year.
ParDDepYR	Year	Time series of years corresponding to this variable.
ParDDepNY	unitless	Number of years in the time series corresponding to this variable.
ParWDep	$g/m^2/d$	2-dimensional array that provides information on total number of years of activity for particulate wet deposition at each receptor location and particulate wet deposition flux for each year.
ParWDepYR	Year	Time series of years corresponding to this variable.
ParWDepNY	unitless	Number of years in the time series corresponding to this variable.
SrcVE		Flag to tell if vapor
SrcCE		Flag to tell if particulate

D.4 Watershed Module

The watershed module models chemical fate and transport processes within a watershed subbasin, including erosion, runoff, leaching, volatilization, and degradation. It also estimates runoff and solids loads to surface waterbodies and recharge as an input for the aquifer module. This section summarizes the assumptions, limitations, inputs, and outputs. Additional detail, including all governing equations, can be found in U.S. EPA (1999f).

D.4.1 Functionality

The watershed module estimates soil chemical concentrations for each subbasin; streamflow and chemical and solids loading estimates for the surface water module (Section 3.3.5); and regional infiltration (recharge) estimates for the vadose zone module (Section 3.3.4). In summary, the watershed module addresses the following specific objectives:

- Simulate the time series of annual average chemical concentrations in surficial soil (top 1 cm) resulting from aerial deposition throughout the area of interest surrounding the WMU. (Note that, although chemical mass losses due to volatilization and leaching from the soil column are evaluated, these losses are simulated only for the purpose of estimating soil concentrations and waterbody loads; that is, these losses are not subsequently received as inputs by the Air or Vadose modules because they are secondary sources.)

- Simulate the time series of annual average chemical loadings in surface runoff and erosion that will enter individual waterbody reaches throughout the AOI.

- Simulate the time series of annual average runoff that will enter waterbodies throughout the AOI.

- Simulate the time series of annual average stream baseflow (dry weather streamflow) in waterbodies throughout the AOI. (Runoff plus baseflow represents total streamflow.)

- Simulate the time series of annual average eroded solids loads that will enter waterbodies throughout the AOI.

- Simulate the time series of annual average infiltration (recharge) rates for each watershed in the AOI.

Note that the watershed module simulates only **indirect** chemical loads to the waterbody; that is, the sole source of chemical to the watershed soils is aerial deposition. Chemical loads to the waterbody resulting from **direct** runoff and erosion from a closed surface impoundment are simulated by the LAU source module. Similarly, if a receptor is located in a buffer area between the closed impoundment and the downslope waterbody (i.e., in the local watershed), the **total** surficial soil concentration to which the receptor is exposed includes the aerial deposition-related

concentration simulated by the watershed module (for the subbasin containing the local watershed) **plus** the runoff/erosion-related concentration simulated by the LAU module.

D.4.2 Assumptions and Limitations

The watershed module's conceptual and mathematical models are very similar to those already described for the LAU module — the combined "local watershed/soil column". This algorithm is a dynamic, two-dimensional, fate and transport model that also includes hydrological functionality; assumptions and limitations associated with its application in either module are listed in Section D.2.1. However, the watershed module differs in that algorithm is applied to each watershed subbasin as a whole and subbasins are not disaggregated into "subareas" as are the local watersheds. Hence, the watershed module is a one-dimensional [vertical], lumped model that simulates each watershed individually. In the watershed module, although the depth of the soil column is a user-specified input, set at a default of 5 cm. Each soil column layer is 1 cm thick.

Another difference with the LAU module involves the size of the computational time step used to determine contaminant concentrations in runoff water. Because **indirect** soil concentrations resulting from aerial deposition are likely to be significantly less than soil concentrations resulting from **direct** runoff/erosion from a source, and aerial because deposition rates in 3MRA are known only on an average annual basis (not daily) the watershed module includes the following features.

- Soil erosion and runoff models are executed on a daily time step, with daily results rolled up to annual average soil erosion (CSL) and runoff volume (Q), which are used to estimate chemical losses in erosion and runoff as well as runoff flow and suspended solids loading to waterbodies.

- The computational time step used by the watershed/soil column algorithm is based on numerical considerations but does not exceed 1 year.

- Annual average runoff-related parameters and the annual average aerial deposition rates are used in applying the watershed/soil column algorithm at each computational time step.

In summary, annual average soil erosion and runoff are estimated on a daily time step, while the remainder of the model (contaminant mass fate and transport simulation) is executed on a computational time step that is typically much larger than one day and can vary each year of the simulation. All outputs are ultimately reported as annual averages, regardless of their individual computational time steps.

The watershed module uses the identical hydrology submodel used in the LAU model to estimate stormwater runoff and ground water infiltration. Streamflows are assumed to be made up of both stormwater runoff and baseflow. Baseflow is streamflow occurring during nonrunoff periods and is derived from ground water discharge to streams or interflow (shallow infiltration flowing parallel to the ground surface). Although baseflow can vary seasonally, or even near

continuously, as ground water levels and/or interflow varies, it was considered unnecessary (and computationally impractical) to attempt to estimate within-year variability in baseflows. Rather, a single estimate was derived based on 30Q2 low flow data, i.e., the minimum 30-day average flow occurring, on average, at least once every other year. A descriptions of how this flow statistic was derived can be found in U.S. EPA (1999f).

Like the LAU module, the watershed module also uses the (modified) Universal Soil Loss Equation (MUSLE), as described in U.S. EPA (1999a, 1999f), to predict soil erosion from watersheds considered in their entirety. In applying this model, watersheds are assumed to be homogeneous in terms of erosion characteristics, including sheet flow length and slope, as described in U.S. EPA (1999a, 1999f).

D.4.3 Inputs for the Watershed Module

Because of its similar design and construction, the watershed module inputs are similar to those previously shown in Table D-2 for the LAU module, except without the waste and WMU-related parameters. Table D-7 summarizes the watershed inputs. Note that like other modules, the watershed module receives inputs from the site layout and header files (sl.ssf, hd.ssf), as well as a module-specific input file (ws.ssf) containing inputs specific to the watershed module, and separate meteorological data files for daily and long term average meteorological data. In addition, the watershed module reads the ar.grf output file for dry and wet deposition rates.

D.4.4 Outputs from the Watershed Module

Table D-8 summarizes the outputs of the watershed module. These include, for each watershed subbasin, soil concentrations, infiltration rates, runoff to the downslope waterbodies, and chemical and solids loadings in this runoff. In addition the module provides stream baseflow estimates for each watershed subbasin. Note that time series reporting is subbasin-specific; that is, all outputs for a given subbasin are reported, including zeros, up to the year that the subbasin simulation is terminated.

Table D-7. Summary of Inputs for Watershed Module

File	Variable Name	Units	Data Type	Description
HD.SSF	CPDirectory		String	Path for location of chemical properties files
	MetData		String	Path for location of meteorological files
AR.GRF	SrcCE		Integer	Flag to tell if particulate
	VapWDep	$g/m^2/d$		Array of number of years of activity for vapor wet deposition and wet deposition flux for each year (by air point)
	VapWDepYR	Year		Time series of years for VapWDep
	VapWDepNY	unitless		Number of years in VapWDep time series
	ParDDep	$g/m^2/d$		Array of number of years of activity for particulate dry deposition by dry deposition flux for each year (by air point)
	ParDDepYR	Year		Time series of years for ParDDep
	ParDDepNY	unitless		Number of years in the ParDDep time series
	ParWDep	$g/m^2/d$		Array of total number of years of activity for particulate wet deposition by particulate wet deposition flux for each year (by air point)
	ParWDepYR	Year		Time series of years for ParWDep
	ParWDepNY	unitless		Number of years in the ParWDep time series
SL.SSF	SiteLatitude	degrees	Float	Latitude of the site
	MetSta		String	ID number for meteorological station associated with site
	NyrMax	years	Integer	Maximum module simulation time
	TermFrac	fraction	Float	Peak output fraction for simulation termination
	AirTemp	degrees C	Float	Long term annual air temperature for site
	NumAir		Integer	Number of air points at site
	WSSubAirFrac	fraction	Float	Fraction of watershed subbasin represented by air points
	WSSubAirIndex		Integer	Index of air points representing subbasin (by subbasin)
	WSSubNumAir		Integer	Number of air points that represent subbasin (by subbasin)
	NumWSSub		Integer	Number of watershed subbasins

(continued)

Table D-7. (continued)

File	Variable Name	Units	Data Type	Description
	WSSubArea	m2	Float	Area of subbasin (by watershed subbasin)
	WSSubNumSubArea		Integer	Number of subbasin subareas (= 1; by WS subbasin)
	WSTemp	degrees C	Float	Average watershed temperature (by site)
	focS	fraction	Float	soil fraction organic carbon (by WS subbasin)
WS.SSF	a_BF	m/day	Float	regression coefficient a for baseflow model
	b_BF	m/day	Float	regression coefficient b for baseflow model
	bcm	unitless	Float	Boundary condition multiplier (lower boundary)
	C	unitless	Float	USLE cover factor (by watershed subbasin)
	CN	unitless	Float	SCS curve number (by watershed subbasin)
	ConVs	m/d	Float	Settling velocity (suspended solids)
	deltDiv	unitless	Integer	Time step divider (for debugging only)
	DRZ	cm	Float	Root zone depth (by watershed subbasin)
	Infild	m/d	Float	Input infiltration rate (for debugging only)
	K	kg/m2	Float	USLE soil erodibility factor (by watershed subbasin)
	Ksat	cm/h	Float	Soil saturated hydraulic conductivity (by watershed subbasin)
	P	unitless	Float	USLE soil erosion control factor (by watershed subbasin)
	RunID		string	Run identification label (optional)
	SMb	unitless	Float	soil moisture coefficient b (by watershed subbasin)
	SMFC	volume %	Float	soil moisture field capacity (by layer and watershed subbasin)
	SMWP	volume %	Float	soil moisture wilting point (by layer and watershed subbasin)
	Theta	degrees	Float	slope (by local watershed)
	thetawZ1d	volume fraction	Float	input volumetric water content in till zone (for debugging)
	WCS	volume fraction	Float	soil saturated water content or total porosity (by watershed subbasin)
	X	m	Float	flow length (by watershed subbasin)

(continued)

Table D-7. (continued)

File	Variable Name	Units	Data Type	Description
	zava	m	Float	averaging depth upper (depth-averaged soil concentration)
	zavb	m	Float	averaging depth lower (depth-averaged soil concentration)
	zZ1sa	m	Float	modeled soil column depth (by watershed subbasin)
CP.SSF	ChemName		String	Name of chemical
	ChemCASID		String	Chemical CAS number
	ChemType		String	Type of chemical
	ChemTemp	degrees C	Real	Temperature for chemical properties
	ChemFracNeutral	fraction	Real	Fraction of chemical in neutral form
	ChemADiff	cm^2/s	Float	Diffusivity of chemical in air
	ChemWDiff	cm^2/s	Float	Diffusivity of chemical in water
	ChemHLC	(atm m^3) / mol	Float	Henry's law constant for the chemical
	ChemKoc	mL/g	Float	Soil organic carbon - water partitioning coefficient (organic compounds)
	ChemAnaBioRate	1/day	Float	Biodegradation / decay rate of contaminant in sediment compartment
	ChemAerBioRate[b]	1/day	Float	Complex first-order biodegradation rate constant for the chemical[b]
	ChemHydRate	1/day	Float	Hydrolysis rate for the chemical
	ChemSol	mg/L	Float	Chemical solubility
	ChemKd	L/kg	Float	Solid/water partition coefficient (inorganic compounds; by media)
Met file	temp	degrees C	Float	Average daily air temperature
	jday		Integer	Julian day
	dailyR	1/t	Float	Daily USLE rainfall erosivity factor (daily)
	dailyppt	cm/d	Float	Total daily precipitation
	AvgTemp	degrees C	Float	Mean monthly temperature
	maxtemp	degrees C	Float	Maximum daily average temperature for month
	mintemp	degrees C	Float	Minimum daily average temperature for month

(continued)

Table D-7. (continued)

File	Variable Name	Units	Data Type	Description
	PE		Float	Thornthwaite Precipitation Evaporation Index
	Ed	m/d	Float	Average daily evaporation
	tsc	degrees C	Float	Long term average soil column temperature
	---		Integer	Number of years of meteorological data

[a] The module currently assumes there is one native soil layer and that the thickness of the underlying soil layer is assumed to be a minimum of 1 meter thick. If the regional vadose zone thickness is less than $1+d_{wmu}$, then the impoundment is assumed to be built up (via an earthen berm) so that there is 1 meter of soil between the bottom of the SI and the ground water.

[b] Note: If normalized biodegradation rate constants are unavailable, normalized biodegradation rates constants are estimated from first-order biodegradation rate constants developed for soil systems by assuming the effective biomass in the soil system is 2.0×10^{-6} Mg/m^3. This value was developed by RTI as an interim estimate until a more rigorously developed value for this parameter is available from EPA.

Table D-8. Summary of Outputs (WS.GRF) for the Watershed Module

Output Variable	Description	Units
NyrMet	Number of years in the available meteorological record	Year
CTdaR	Depth-averaged soil concentration (from zava to zavb)	µg/g
CTdaRYR	Year associated with output	Year
CTdaRNY	Number of years in outputs	Unitless
CTssR	Surface soil concentration	µg/g
CTssRYR	Year associated with output	Year
CTssRNY	Number of years in outputs	Unitless
RunoffR	Annual average runoff flow to waterbody	m^3/d
BFann	Long-term annual average baseflow to waterbody	m^3/d
AnnInfil	Annual average recharge rate	m/d
SWLoadChemR	Chemical load (resulting from deposition only) to waterbody	g/d
SWLoadChemRYR	Year associated with output	year
SWLoadChemRNY	Number of years in outputs	Unitless
SWLoadSolidR	Total suspended solids in runoff	g/d

D.5 Vadose and Aquifer Modules

The HWIR 3MRA vadose and aquifer modules are a modified version of EPA's Composite Model for leachate migration with Transformation Products (EPACMTP) (US EPA, 1996a,b,c). This code simulates the fate and transport of contaminants released from land-based waste management units through the underlying unsaturated or vadose zone (soil) and saturated zone (surficial aquifer). EPACMTP replaced EPACML (US EPA, 1993) as the best available tool to predict potential exposure at a downstream receptor well. EPACMTP offers improvements to EPACML by considering: 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.

Detailed descriptions of both modules, including their purpose and scope of application, mathematical formulations, and use in HWIR99 may be found in U.S. EPA (1999g). Additional information relating to the EPACMTP and its verification is provided in the background documents for EPACMTP (US EPA, 1996a,b,c, 1997).

D.5.1 Functionality

EPACMTP comprises three major simulation components:

- A module that performs one-dimensional analytical and numerical solutions for water flow and contaminant transport in the vadose zone underlying a waste management unit.

- A numerical module that simulates steady-state groundwater flow subject to recharge from the vadose zone.

- A module comprising analytical and numerical solutions for contaminant transport in the saturated zone.

For 3MRA, portions of the EPACMTP code pertaining to the vadose zone make up the vadose zone module (VZM), and portions pertaining to the saturated zone make up the saturated zone module (SZM).

The VZM simulates infiltration and contaminant transport between the top of the vadose zone and the water table (see Figure 3-17). Flow in the vadose zone is modeled as steady-state, one-dimensional (vertical) flow from underneath the source (the WMU). Recharge occurs from the soil outside the WMU toward the water table. The lower boundary of the vadose zone is the water table. The flow in the vadose zone is predominantly gravity-driven, and therefore the vertical flow component accounts for most of the fluid flux between the source and the water table. The flow rate is determined by the long-term average infiltration rate through the waste management unit and recharge downgradient from the WMU.

Contaminant is transported in the vadose zone by advection and dispersion. The vadose zone is assumed to be initially contaminant-free, and it is assumed that contaminants migrate

vertically downward. The VZM can simulate both steady-state and transient transport, with single or multiple species chain decay reactions and linear or nonlinear sorption. The VZM consists of two submodules: one for flow calculations and one for transport.

The SZM simulates groundwater flow using either a three- or one-dimensional steady-state solution for predicting hydraulic head and Darcy velocities. The saturated groundwater system is assumed to be of constant thickness, subject to recharge along the top of the aquifer and a regional gradient defined by upstream and downstream head boundary conditions. The saturated zone transport module describes the advective-dispersive transport of dissolved contaminants in a three-dimensional, constant thickness aquifer. The initial contaminant concentration is set to zero. The concentration gradient along the downstream boundary is zero, and the lower aquifer boundary is taken to be impermeable. A zero concentration condition is used for the upstream aquifer boundary. Contaminants enter the saturated zone through a patch source on the upper aquifer boundary directly beneath the source. Recharge of contaminant-free infiltration water occurs along the upper aquifer boundary outside the patch source. Transport mechanisms considered are advection, dispersion, linear or nonlinear equilibrium adsorption, and first-order decay with daughter product formation. As in the unsaturated zone, the saturated zone transport module can simulate multispecies transport involving chain decay reactions. The saturated zone module performs a fully three-dimensional transport simulation.

The VZM and SZM, derived from the EPACMTP code, are, together, capable of simulating the fate and transport of dissolved contaminants from a point of release at the base of a waste disposal unit, through the unsaturated zone and underlying aquifer, to one or more receptor wells at arbitrary downstream locations in the groundwater system. The modules account for the major mechanisms affecting contaminant migration, including: transport by advection and hydrodynamic dispersion, retardation due to reversible linear or nonlinear equilibrium adsorption onto the soil and aquifer solid phase, and biochemical degradation processes. The latter may involve chain decay reactions if the contaminant(s) of concern form a decay chain.

D.5.2 Assumptions and Limitations

As is true of any model, EPACMTP and, its modules are based on a number of simplifying assumptions which make the code easier to use and ensure its computational efficiency. These assumptions, however, may cause application of the model to be inappropriate in certain situations. The inherent assumptions and limitations of the vadose zone module (VZM) and saturated zone module (SZM) are summarized below:

1) <u>Soil and Aquifer Medium Properties</u>. Soil and aquifer are uniform porous media, and flow and transport are governed by Darcy's law (Bear, 1972) and the advection-dispersion equation, respectively. The model does not account for the presence of preferential pathways such as fractures and macro-pores. Although the aquifer properties are assumed to be uniform, the model does allow for anisotropy in the hydraulic conductivity. Also, in the saturated zone module, effects due to the presence of fractures and heterogeneity are superimposed onto the base homogeneous model.

2) Flow in the Unsaturated Zone. Flow in the unsaturated zone is steady-state, one-dimensional vertical flow from underneath the source toward the lower boundary of the unsaturated zone, that is, toward the water table. The flow in the unsaturated zone is predominantly gravity-driven, and, therefore, the vertical flow component accounts for most of the fluid flux between the source and the water table. The flow rate is determined by the long-term average infiltration rate through the waste management unit. The long-term average infiltration rate is calculated from a series of annual average infiltration rates.

3) Flow in the Saturated Zone. The SZM is designed to simulate flow in an unconfined aquifer with constant saturated thickness. The concept employed is that of regional flow in the horizontal direction, with vertical disturbance due to recharge and infiltration from the overlying unsaturated zone and waste disposal facility. The lower boundary of the aquifer is assumed to be impermeable. Flow in the saturated zone is assumed to be steady-state.

   The SZM accounts for different recharge rates underneath and outside the source area. Groundwater mounding beneath the source is represented in the flow system by increased hydraulic head values at the top of the aquifer. This approach is reasonable as long as the height of the mound is small relative to the thickness of the saturated zone.

4) Transport in the Unsaturated Zone. Contaminant transport in the unsaturated zone is by advection and dispersion. The unsaturated zone is assumed to be initially contaminant-free and contaminants are assumed to migrate vertically downward from the disposal facility. The VZM simulates transient transport in the unsaturated zone, with single species or multiple species chain decay reactions, and linear or nonlinear sorption.

5) Transport in the Saturated Zone. Contaminant transport in the saturated zone is due to advection and dispersion. The aquifer is assumed to be initially contaminant-free and contaminants enter the aquifer only from the unsaturated zone immediately underneath the waste disposal facility, which is modeled as a rectangular horizontal plane source. The SZM simulates transient transport in a fully three-dimensional mode in order to obtain a scientifically rigorous analysis. The concentration at the water table must be specified as a function of time. The SZM is capable of simulating transient transport in a quasi-three dimensional mode when computational efficiency is desired (e.g., Monte Carlo simulations). The SZM can consider linear sorption and the transport of a single species or multiple species chain decay reactions.

6) Contaminant Phases. The VZM and SZM simulate constituent transport in the aqueous phase only, and disregard interphase mass transfer processes other than adsorption onto immobile solids. The modules do not account for volatilization in the unsaturated zone; this is a conservative approach for volatile chemicals in the aqueous phase. The modules also do not account for the presence of a NAPL (e.g.

oil) or transport in gas phase. When a mobile oil phase is present, significant migration may occur within it, so that the VZM and SZM may under predict the movement of hydrophobic chemicals.

7) Chemical Reactions. The groundwater pathway (VZM and SZM) modules take into account chemical reactions by adsorption and decay processes. The VZM allows sorption of organic compounds in the unsaturated zone to be represented by linear or nonlinear adsorption isotherms, while sorption in the saturated zone is always linear. It is assumed that the adsorption of contaminants onto the soil or aquifer solid phase occurs instantaneously and is entirely reversible.

The effect of geochemical interactions is especially important in the fate and transport analyses of metals. For the simulation of metals with non-linear adsorption, both modules utilize sorption isotherms generated by MINTEQA2 (Allison et al., 1991, a metal speciation model). MINTEQA2 generates concentration-dependent effective partition coefficients for various combinations of geochemical conditions. This procedure is described in the background document for the modeling of metals transport (EPA, 1996b).

The VZM and SZM also account for chemical and biological transformation processes. All transformation reactions are represented by first-order decay processes. An overall decay rate is determined within the modules, so that the modules cannot explicitly consider the separate effects of multiple degradation processes such as oxidation, hydrolysis and biodegradation. In order to increase their flexibility, both modules have the capability to determine the overall decay rate from chemical-specific hydrolysis constants and soil and aquifer temperature and pH values, and from biodegradation rates selected from a database. It is assumed that biodegradation is aerobic in the unsaturated zone and anaerobic in the saturated zone.

Both modules assume that the reaction stoichiometry is prescribed for scenarios involving chain decay reactions and applys to all transformation processes. The speciation factors are specified as constants by the user (see the EPACMTP Background Document, EPA, 1996a). In reality, these coefficients may change as functions of aquifer conditions (e.g., temperature and pH) and/or concentration levels of other chemical components.

D.5.3 Inputs for the Vadose and Saturated Zone Modules

A list of vadose zone-specific input parameters is provided in Table D-9, showing variables by file name. The VZM requires input about the site from the site layout SSF (sl.ssf), inputs specific to the vadose zone (e.g.,control parameters, soil characteristics, etc.) from the vadose zone module SSF (vz.ssf), chemical-specific data from the chemical properties SSF (cp.ssf), and outputs from the source module (i.e., chemical and water fluxes) from the source GRF (sr.grf).

A list of saturated zone-specific input parameters is provided in Table D-10. The SZM requires input about the site (sl.ssf), information specific to the aquifer (aq.ssf), and chemical-specific data from the chemical properties SSF (cp.ssf), as well as outputs from the source (sr.grf), watershed (ws.grf), and vadose zone (vz.grf) modules. Tables D-9 through D-12 specify source and destination files for all parameters in the VZM and SZM (SZM is also referred to as the aquifer module).

Table D-9. Vadose Zone Module Input Parameters

File	Code	Units	Data Type	Description
SL.SSF	AquFEOX	fraction	Float	Hydrous ferric oxide (HFO) adsorbent content
	AquLOM	mg/L	Float	Leachate organic matter
	NumVad		Integer	Number of vadose zones = number of local watersheds
	NyrMax	years	Integer	Maximum model simulation time
	SrcArea	m^2	Float	Area of source
	SrcLWSSubAreaArea	m2	Float	Area of local watershed subarea
	SrcLWSSubAreaIndex	unitless	Integer	Local watershed subarea containing WMU
	SrcNumLWS		Integer	Number of local watersheds
	TermFrac	fraction	Float	Termination peak fraction criteria
	VadALPHA	1/cm	Float	Soil retention paramter alpha
	VadBETA	unitless	Float	Soil retention paramter beta
	VadID		String	Setting ID for vadose zone
	VadPh	pH units	Float	Average vadose zone pH
	VadSATK	cm/hr	Float	Saturated hydraulic conductivity
	VadTemp	degrees C	Float	Average vadose zone temperature
	VadThick	m	Float	Vadose zone thickness
	VadWCR	L/L	Float	Residual water content
	VadWCS	L/L	Float	Saturated water content
VZ.SSF	DISPR	m	Float	Longitudinal dispersivity
	POM	g/g	Float	Percent organic matter
	RHOB	g/cm3	Float	Bulk density of soil
CP.SSF	ChemCASID		String	CASID
	ChemHydNumProd		Integer	Number of products
	ChemHydProdCASID		String	Product CASID
	ChemHydProdYield	moles/moles	Float	Product yield coefficient
	ChemHydRate	1/day	Float	Hydrolysis rate
	ChemKoc	mL/g	Float	Koc
	ChemMolWt	g/mole	Float	Molecular weight
	NumChem		Integer	Number of chemicals assc. W/parent
	ChemAerBioRate	1/day	Float	Aerobic biodegradation rate
SR.GRF	AnnInfil	m/d	Float	Leachate infiltration rate (annual avg. WMU only)
	LeachFlux	g/m2/d	float	Leachate contaminant flux
	LeachFluxNY		integer	Number of years in outputs
	LeachFluxYR	year	integer	Year associated with output
	NyrMet	year	Integer	Number of years in the available met record
	SrcLeachMet		Logical	Flag for leachate presence when leachate is met-driven
	SrcLeachSrc		Logical	Flag for leachate presence when leachate is not met-driven (active surface impoundments)
	TWT	yr	Float	Times for CWT

Table D-10. Aquifer Module Input Parameters

File	Code	Units	Data Type	Description
SL.SSF	AquDir	degrees	Float	Groundwater flow direction in degrees from North
	AquFEOX	fraction	Float	Hydrous ferric oxide (HFO) adsorbent content
	AquGrad		Float	Regional groundwater gradient
	AquId		String	Environmental setting ID for aquifer
	AquLOM	mg/L	Float	Leachate organic matter concentration
	AquPh	pH units	Float	Average aquifer pH
	AquSatk	m/yr	Float	Saturated hydraulic conductivity (aquifer)
	AquTemp	degrees C	Float	Average Aquifer Temperature
	AquThick	m	Float	Saturated zone thickness
	AquVadIndex		Integer	Index of vadose zone per aquifer
	AquWellFracZ	fraction	Float	Fractional depth of well in aquifer measured from watertable
	AquWellLocX	m	Float	Easting in UTM
	AquWellLocY	m	Float	Northing in UTM
	NumAqu		Integer	Number of aquifers
	NumAquWell		Integer	Number of drinking water wells
	NumWBN		Integer	Number of waterbody networks
	NumWSSub		Integer	Number of watershed sub basins
	NyrMax	years	Integer	Maximum model simulation time
	SrcArea	m^2	Float	Area of source
	SrcLocX	m	Float	Easting in site coordinate system (0)
	SrcLocY	m	Float	Northing in site coordinate system (0)
	TermFrac	fraction	Float	Termination peak fraction criteria
	VadID		String	Environmental setting ID for aquifer
	WBNNumRch		Integer	Number of reaches for this network
	WBNRchAquIndex		Integer	Index of aquifer that impacts this reach
	WBNRchLength	m	Float	Reach length
	WBNRchLocX	m	Float	Easting in UTM
	WBNRchLocY	m	Float	Northing in UTM
	WBNRchNumAqu		Integer	Number of aquifer that impact this reach
	WBNRchNumLoc	unitless	Integer	Number of x,y points associated with watershed
	WSSubArea	m^2	float	Area of watershed subbasin
AQ.SSF	AL	m	Float	Longitudinal dispersivity
	ALATRatio	m	Float	Horizontal transverse dispersivity
	ALAVRatio	m	Float	Vertical transverse dispersivity
	ANIST		Float	Anisotropy ratio

(continued)

Table D-10. (continued)

File	Code	Units	Data Type	Description
	AquAnaBioRandUnif		Integer	Uniformly distributed random number used to choose the anaerobic biodegradation regime: 0=methanogenic; 1= sulfate reducing
	AquDoFracture		Logical	Logical flag to turn fractures on or off
	AquDoHetero		Logical	Logical flag to turn heterogeneity on or off
	AquFractureID		Integer	Indicator for degree of fracturing of saturated porous media
	AquRandFractUnif		Float	Uniformly distributed random number-used when AquDoFracture==TRUE
	AquRandHeteroNorm		Float	Normally distributed random numbers with 0 mean and std of 1-used when AquDoHetero==TRUE
	AquRandHeteroUnif		Float	Uniformly distributed random number-used when AquDoHetero==TRUE
	BDENS	g/cm3	Float	Bulk density of soil
	FOC	fraction	Float	Fraction organic carbon
	POR		Float	Effective porosity
CP.SSF	ChemCASID		String	CASID
	ChemHydNumProd		Integer	Number of products
	ChemHydProdCASID		String	Product CASID
	ChemHydProdYield	moles/mole	Float	Product yield coefficient
	ChemHydRate	1/day	Float	Hydrolysis Rate
	ChemKoc	mL/g	Float	Koc
	ChemMetBioRate	1/day	Float	Anaerobic biodegradation under methanogenic red.
	ChemMolWt	g/mole	Float	Molecular weight
	ChemSO4BioRate	1/day	Float	Anaerobic biodegradation under SO4 reduction
	NumChem		Integer	Number of chemicals assc. w/parent
SR.GRF	SrcLeachMet		Logical	Flag for leachate presence when leachate is met-driven
	SrcLeachSrc		Logical	Flag for leachate presence when leachate is not met-driven (active surface impoundment)
WS.GRF	AnnInfil	m/d	Float	Annual average recharge rate (time series by watershed subbasin)
	NyrMet	year	Integer	Number of years in the available met record
VZ.GRF	CWT	mg/L	Float	Concentration at water table
	NTS	yr	Integer	Number of time-conc/flux pairs in TWT and CWT
	SINFIL	m/yr	Float	Long term average waterflux beneath source
	TSOURC	yr	Float	Duration of source boundary condition
	TWT	yr	Float	Times for CWT

Table D-11. Vadose Zone Module Outputs

File	Code	Units	Data Type	Description
VZ.GRF	CWT	mg/L	Float	Concentrations at water table
	NTS	yr	Integer	Number of time-conc/flux pairs in TWT and CWT
	SINFIL	m/yr	Float	Longterm average waterflux beneath source
	TSOURC	yr	Float	Duration of source boundary condition

Table D-12. Aquifer Module Outputs

File	Code	Units	Data Type	Description
AQ.SSF	AquRchMassFlux	g/yr	Float	Mass flux from aquifer to reach (time series by reach)
	AquRchMassFluxNY		Integer	Number of time - mass-flux-to-reach pairs
	AquRchMassFluxYR	year	Float	Time of mass flux from aquifer to reach
	AquRchWaterFlux	m3/day	Float	Total GW flux to reach
	AquWellConc	mg/L	Float	Observed well concentration
	AquWellConcFlag		Logical	Flag indicating well is within plume: T - yes, F - no (by well)
	AquWellConcNY		Integer	Number of time - observed well conc pairs
	AquWellConcYr	year	Integer	Time of observed well concentration

D.6 Surface Water Module

The HWIR 3MRA surface water module models streams, lakes, ponds, and wetlands and consists of the core model EXAMS II (Burns, 1997, Burns et al., 1982) and the interface module ExamsIO. This section describes the assumptions, limitations, inputs, and outputs of this module. Detailed documentation can be found in U.S. EPA (1999u), from which the following material was extracted.

D.6.1 Functionality

The 3MRA surface water module takes the loadings calculated by the source, atmospheric, watershed, and groundwater modules, along with data on meteorology, hydrology, environmental conditions, and chemical reactivity, and calculates the chemical concentrations throughout the waterbody network over time. The 3MRA surface water module contains the core model EXAMS II (Burns, 1997; Burns et al., 1982), which is a general surface water fate model for organic chemicals. This compartment model has been used routinely by both EPA and industry analysts for the analysis of expected pesticide concentrations in generically defined environments, such as farm ponds. It has also been used for site-specific analysis of pesticide concentrations in various waterbodies around the world. The interface module ExamsIO was developed specifically for this 3MRA project. It reads data from other 3MRA modules and databases and builds EXAMS input files describing the waterbody environment and chemical properties, along with the command file that specifies the chemical loading history and controls the EXAMS simulation. ExamsIO passes control to EXAMS, which conducts the simulation and produces intermediate results files. ExamsIO then processes the intermediate files and passes the output data back to the proper 3MRA database.

EXAMS II is an interactive modeling system that allows a user to specify and store the properties of chemicals and ecosystems, modify either via simple commands, and conduct rapid evaluations and sensitivity analyses of the probable aquatic fate of synthetic organic chemicals. EXAMS combines chemical loadings, transport, and transformation into a set of differential equations using the law of conservation of mass as an accounting principle. It accounts for all the chemical mass entering and leaving a system as the algebraic sum of external loadings, transport processes that export the compound from the system, and transformation processes within the system that convert the chemical to daughter products. The program produces output tables and simple graphics describing chemical exposure, fate, and persistence.

EXAMS represents each waterbody via a set of segments or distinct zones in the system. The program is based on a series of mass balances for the segments that give rise to a single differential equation for each segment. Working from the individual transport and transformation process equations, EXAMS compiles an overall equation for the net rate of change of chemical concentration in each segment. The resulting system of differential equations describes the mass balance for the entire system, which is then solved by the method of lines. EXAMS includes a descriptor language that simplifies the specification of system geometry and connectedness.

EXAMS includes process models of the physical, chemical, and biological phenomena governing the transport and fate of compounds. Each of the unit process equations used to

compute the kinetics of chemicals accounts for the interactions between the chemistry of a compound and the environmental forces that shape its behavior in aquatic systems. This "second-order" or "system-independent" approach lets one study the fundamental chemistry of compounds in the laboratory and then, based on independent studies of the levels of driving forces in aquatic systems, evaluate the probable behavior of the compound in systems that have never been exposed to it. Most of the process equations are based on standard theoretical constructs or accepted empirical relationships. The user can specify reaction pathways for the production of transformation products of concern, whose further fate and transport can then be simultaneously simulated by EXAMS.

EXAMS contains process modules for several chemical reactions. Equilibrium reactions are used for sorption and ionization. Kinetic reactions are used for volatilization, hydrolysis (acid, base, and neutral), biodegradation (water column and sediments), photolysis, oxidation, and reduction. EXAMS uses these modules as determined by the input chemical properties. EXAMS has been designed to accept standard water quality parameters and system characteristics that are commonly measured by limnologists throughout the world and chemical datasets conventionally measured or required by EPA regulatory procedures.

The contaminant fate algorithms in EXAMS include sorption to suspended solids, biotic solids, and sediment solids, but EXAMS does not simulate a solids balance. Solids concentrations are specified as input data. The effects of settling and resuspension on chemical fate are accounted for in a bulk sediment-water exchange term.

EXAMS can be run in three modes: steady-state, quasi-dynamic with steady environmental data, and quasi-dynamic with monthly environmental data. H-Exams implements mode 2, in which the model integrates the equations over specified time periods with given environmental and loading conditions. Pulse loadings are allowed by EXAMS in mode 2 simulations, but this capability is not implemented by H-Exams. The EXAMS simulation proceeds in yearly increments using yearly-average loadings and environmental conditions.

While EXAMS can be run interactively or as a batch program, H-Exams is implemented solely as a batch process. H-Exams does not consider transformations due to photolysis or oxidation. Transformation rate constants for hydrolysis, biodegradation, and reduction are calculated by the HWIR chemical processor and passed through the batch chemical database to EXAMS. Internal EXAMS algorithms for calculating rate constants are bypassed.

D.6.2 Assumptions and Limitations

EXAMS incorporates a few major assumptions. The model was designed to evaluate the consequences of longer-term, primarily time-averaged chemical loadings that ultimately result in trace-level contamination of aquatic systems. EXAMS generates a steady-state, average flow field (long-term or monthly) for the ecosystem. The program cannot then fully evaluate the transient, high concentrations that arise from chemical spills, although spills under average hydrological conditions can be studied. An assumption of trace-level chemical concentrations was used to design the process equations. The chemical is assumed not to radically change the environmental variables that drive its transformations. EXAMS uses linear sorption isotherms, and second-order

(rather than Michaelis-Menten-Monod) expressions for biotransformation kinetics, which is known to be valid for low concentrations of pollutants. Sorption is treated as a thermodynamic or constitutive property of each compartment in the system, that is, sorption-desorption kinetics are assumed to be rapid compared to other processes. While this assumption may be violated by extensively-sorbed chemicals, they tend to be captured by benthic sediments, where their release to the water column is controlled by benthic exchange processes.

In addition to the assumptions incorporated by EXAMS, the 3MRA implementation of Exams (H-Exams) employs several simplifications in order to meet requirements and constraints associated with the 3MRA system . The project design calls for repeated long simulations (200 to 10,000 years) executed quickly (seconds to minutes). This requirement limits the temporal resolution at which simulations can be conducted. Another important constraint is limited site-specific data. This constraint limits the accuracy with which a particular site can be described. The major model simplifications made in response to these project constraints include the use of average-yearly hydrological and loading inputs, the use of national distributions to specify some site-specific environmental conditions, and the use of a simple solids balance with no settling and burial. For sites that experience periodic drying, a small positive flow equivalent to 5 mm/year of direct precipitation onto the water body surface is maintained in order to keep the model functioning.

These simplifications lead to a degree of model error in the calculated concentrations. Using annual-average loadings and flows rather than daily loadings and flows will lead to calculated annual-average concentrations that are biased somewhat high, depending on the correlation between flow and loading at a particular site. This bias is somewhat mitigated for reactive and volatile chemicals where the loss rate is proportional to the concentration. The use of national distributions rather than site-specific environmental data could cause calculated concentrations to be low or high at a given location, with no known general bias. The simple solids balance will overestimate suspended solids concentrations slightly in streams and more significantly in ponds, wetlands, and lakes. Calculated total water column chemical concentrations will be high, while the dissolved chemical fraction will be low. The net result for dissolved water column chemical concentrations, which are used for fish exposure, is not expected to be biased significantly high or low.

The procedure for preventing drying of surface water reaches is more difficult to evaluate. This procedure conducts chemical loads downstream within a remnant aquatic reach rather than within runoff over a dry bed or subsurface flow within the bed. While the mass balance is maintained, the chemical and solids concentrations will tend to be elevated within the remnant reach. These elevated concentrations are probably realistic for years in which evaporation exceeds all hydrologic inflows.

D.6.3 Inputs for the Surface Water Module

Three site simulation files are generated for each execution of the surface water module – the site layout file sl.ssf, the chemical property file cpstream.ssf, and the surface water body file(s) sw*.ssf (where * stands for the water body number at a site). Table D-13 lists the input parameters contained in the various SSF and GRF files read by the surface water module. The

site layout SSF contains 35 variables used by the surface water module. The surface water SSF files contain 25 variables that are relevant only to the surface water module. The chemical SSF file contains 44 variables reead by the surface water module.

In addition the surface water model reads several global results files (GRFs) containing water, solids, contaminant loadings from other modules: 9 variables from the air module (ar.ssf), 7 variables from the source module (sr.grf), 7 variables from the watershed module (ws.grf), and 4 variables from the groundwater module (aq.grf).

The groundwater (aquifer) results file contains 9 variables, 4 of which are used by the surface water module.

D.6.4 Outputs from the Surface Water Module

The surface water model produces water and sediment chemical concentrations (dissolved and total) that are used by the aquatic foodweb, farm food chain, ecological exposure, and ecological risk modules, along with the number of values and output years. These variables are contained in the sw.grf and are listed in Table D-14.

Table D-13. Surface Water Module Inputs

File	Code	Units	Data Type	Description
sw.ssf	ahyd_d	m	FLOAT	hydraulic coefficient depth multiplier
sw.ssf	bhyd_d		FLOAT	hydraulic coefficient depth exponent
sw.ssf	ahyd_W	m	FLOAT	hydraulic coefficient width multiplier
sw.ssf	bhyd_W		FLOAT	hydraulic coefficient width exponent
sw.ssf	DepthSedRes	cm	float	underlying sediment layer depth
sw.ssf	DepthBenthos	cm	float	surficial sediment layer depth
sw.ssf	d_pond	m	float	depth of pond
sw.ssf	d_wtlnd	m	float	depth of wetland
sw.ssf	d_epil	m	FLOAT	depth of epilimnion
sw.ssf	d_hypol	m	FLOAT	depth of hypolimnion
sw.ssf	E_sw	cm2/sec	float	sediment-water column diffusion coefficient
sw.ssf	E_thermocline	cm2/sec	FLOAT	thermocline diffusion coefficient
sw.ssf	rhoDSedRes	g/mL	FLOAT	underlying sediment layer dry bulk density
sw.ssf	rhoDBenthos	g/mL	FLOAT	surficial sediment layer dry bulk density
sw.ssf	porSedRes	Lw/L	FLOAT	underlying sediment layer porosity
sw.ssf	porBenthos	Lw/L	FLOAT	surficial sediment layer porosity
sw.ssf	k_PlankCMin	yr^-1	FLOAT	Plankton carbon mineralization rate constant; not used in this HWIR application.
sw.ssf	k_SedG2	yr^-1	FLOAT	Sediment mineralization rate constant, G2 fraction; not used in this HWIR application.
sw.ssf	k_SedG3	yr^-1	FLOAT	Sediment mineralization rate constant, G3 fraction; not used in this HWIR application.
sw.ssf	v_bury	mm/yr	FLOAT	underlying sediment layer burial rate
sw.ssf	TrophicIndex		INTEGER	trophic index
sw.ssf	S_upstream	mg/L	FLOAT	[upstream suspended solids concentration]
sw.ssf	C_upstream	mg/L	FLOAT	upstream chemical concentration
sw.ssf	Q_upstream	m3/day	FLOAT	upstream flow
sl.ssf	WBNDOC	mg/L	Float	DOC of stream, lake, and wetland reaches in waterbody network
sl.ssf	WBNfocAbS	fraction	Float	fraction organic carbon of abiotic solids in water column
sl.ssf	WBNfocBioS	fraction	Float	fraction organic carbon of biotic solids in water column
sl.ssf	WBNfocSed	fraction	Float	fraction organic carbon in sediments of stream, lake, and wetland reaches
sl.ssf	WBNId		Integer	Environmental Setting Id for WBN
sl.ssf	WBNNumRch		Integer	Number of reaches for this network
sl.ssf	WBNpH	pH units	Float	pH of stream, lake, and wetland reaches in the waterbody network

(continued)

Table D-13. (continued)

File	Code	Units	Data Type	Description
sl.ssf	WBNRchAirFrac	fraction	Float	Fraction of this reach impacted by air point
sl.ssf	WBNRchAirIndex		Integer	Index of air point that impacts this reach
sl.ssf	WBNRchAquFrac	fraction	Float	Fraction of this reach impacted by the aquifer
sl.ssf	WBNRchAquIndex		Integer	Index of aquifer that impacts this reach
sl.ssf	WBNRchArea	m2	Float	reach surface area (nonstream reaches)
sl.ssf	WBNRchBodyType		String	Type of waterbody (Stream, Lake, Wetland)
sl.ssf	WBNRchHypoAreaFrac	fraction	Float	fraction of total surface area for hypolimnion
sl.ssf	WBNRchLength	m	Float	Reach Length
sl.ssf	WBNRchNumAir		Integer	Number of points that impact this reach
sl.ssf	WBNRchNumAqu		Integer	Number of aquifer that impact this reach
sl.ssf	WBNRchNumLoc	unitless	Integer	number of x,y points associated with watershed
sl.ssf	WBNRchNumRch		Integer	Number of reaches that impact this reach
sl.ssf	WBNRchNumWSSub		Integer	Number of watersheds that impacts this reach
sl.ssf	WBNRchOrder	unitless	Integer	stream order
sl.ssf	WBNRchRchFrac	fraction	Float	Fraction of this reach impacted by another reach
sl.ssf	WBNRchRchIndex		Integer	Index of reach that impacts this reach
sl.ssf	WBNRchSrcLWSFrac	fraction	Float	fraction of waterbody network reach impacted by the source local watershed
sl.ssf	WBNRchSrcLWSIndex		Integer	index of local watershed from source
sl.ssf	WBNRchType		String	Type of reach (Headwater, exiting, other)
sl.ssf	WBNRchWSSubFrac	fraction	Float	Fraction of this reach impacted by watershed
sl.ssf	WBNRchWSSubIndex		Integer	Index of watershed that impacts this reach
sl.ssf	WBNTemp	degrees Celsius	Float	median temperature of stream, lake, and wetland reaches in waterbody network
sl.ssf	WBNTOC	mg/L	Float	TOC of stream, lake, and wetland reaches in waterbody network
sl.ssf	WBNTSS	mg/L	Float	TSS of stream, lake, and wetland reaches in waterbody network
cp.ssf	ChemName		String	Chemical Name
cp.ssf	ChemActBioNumProd		Integer	Number of products
cp.ssf	ChemActBioProdCASID		String	Product CASID
cp.ssf	ChemActBioProdName		String	Product Name
cp.ssf	ChemActBioProdYield	moles/moles	Float	Product Yield Coefficient
cp.ssf	ChemActBioRate	1/day	Float	Activated Biodegradation
cp.ssf	ChemADiff	cm^2/s	Float	Air Diffusion Coefficient
cp.ssf	ChemAerBioNumProd		Integer	Number of products
cp.ssf	ChemAerBioProdCASID		String	Product CASID
cp.ssf	ChemAerBioProdName		String	Product Name

(continued)

Table D-13. (continued)

File	Code	Units	Data Type	Description
cp.ssf	ChemAerBioProdYield	moles/moles	Float	Product Yield Coefficient
cp.ssf	ChemAerBioRate	1/day	Float	Aerobic Biodegradation rate
cp.ssf	ChemAnaBioNumProd		Integer	Number of products
cp.ssf	ChemAnaBioProdCASID		String	Product CASID
cp.ssf	ChemAnaBioProdName		String	Product Name
cp.ssf	ChemAnaBioProdYield	moles/moles	Float	Product Yield Coefficient
cp.ssf	ChemAnaBioRate	1/day	Float	Anaerobic Biodegradation
cp.ssf	ChemAnaRedNumProd		Integer	Number of products
cp.ssf	ChemAnaRedProdCASID		String	Product CASID
cp.ssf	ChemAnaRedProdName		String	Product Name
cp.ssf	ChemAnaRedProdYield	moles/moles	Float	Product Yield Coefficient
cp.ssf	ChemAnaRedRate	1/day	Float	Anaerobic Reduction
cp.ssf	ChemDen	g/mL	Float	Density
cp.ssf	Chemfoc	fraction	Float	Fraction Organic Content of Medium
cp.ssf	ChemHLC	(atm m^3)/mol	Float	Henry's Law Constant
cp.ssf	ChemHydNumProd		Integer	Number of products
cp.ssf	ChemHydProdCASID		String	Product CASID
cp.ssf	ChemHydProdName		String	Product Name
cp.ssf	ChemHydProdYield	moles/moles	Float	Product Yield Coefficient
cp.ssf	ChemHydRate	1/day	Float	Catalyzed Hydrolysis
cp.ssf	ChemKd	L/kg	Float	Partition Coefficient for Med
cp.ssf	ChemKoc	mL/g	Float	Koc
cp.ssf	ChemKow		Float	Kow
cp.ssf	ChemMed		String	Solubility Media (Soil, Sediment,Surface Water, Waste)
cp.ssf	ChemMolWt	g/mole	Float	Molecular weight for the chemical
cp.ssf	ChemName		String	Name
cp.ssf	ChemPh	pH units	Float	[pH assumed for these properties]
cp.ssf	ChemSol	mg/L	Float	Solubility for each media
cp.ssf	ChemTemp	degrees Celsius	Float	Temperature assumed for these properties
cp.ssf	ChemType		string	Chemical Type (O, M, Hg, S, D)
cp.ssf	ChemVol	mL	Float	Volume
cp.ssf	ChemVp	torr	Float	Vapor Pressure
cp.ssf	ChemWDiff	cm^2/s	Float	Water Diffusion Coefficient
cp.ssf	NumChem		Integer	Number of chemicals described
sr.grf	Runoff	m3/d	float	runoff

(continued)

Table D-13. (continued)

File	Code	Units	Data Type	Description
sr.grf	SWLoadChem	g/d	float	chemical load to waterbody
sr.grf	SWLoadChemYR	year	integer	year associated with output
sr.grf	SWLoadChemNY		integer	number of years in outputs
sr.grf	SrcOvl		logical	flag for overland flow presence
sr.grf	SrcH2O		logical	flag for surface water presence
sr.grf	NyrMet	year	integer	number of years in the available met record
ar.grf	VapWDep	g/m2/d	FLOAT	vapor wet deposition flux
ar.grf	VapWDepYR	Year	Integer	year corresponding to vapor wet deposition flux value
ar.grf	VapWDepNY		Integer	number of annual vapor wet deposition flux values
ar.grf	ParDDep	g/m2/d	FLOAT	particle dry deposition flux
ar.grf	ParDDepYR	Year	Integer	year corresponding to particle dry deposition flux value
ar.grf	ParDDepNY		Integer	number of particle dry deposition flux values
ar.grf	ParWDep	g/m2/d	FLOAT	particle wet deposition flux
ar.grf	ParWDepYR	Year	Integer	year corresponding to particle dry deposition flux value
ar.grf	ParWDepNY		Integer	number of particle dry deposition flux values
ws.grf	NyrMet	year	integer	number of years in the available met record
ws.grf	RunoffR	m3/d	float	runoff flow to waterbody
ws.grf	BFann	m3/d	float	long-term avg baseflow to waterbody
ws.grf	SWLoadChemR	g/d	float	chemical load (deposition only) to waterbody
ws.grf	SWLoadChemRYR	year	integer	year associated with output
ws.grf	SWLoadChemRNY		integer	number of years in outputs
ws.grf	SWLoadSolidR	g/d	float	total suspended solids (runoff)
aq.grf	AquRchMassFlux	g/yr	Float	Mass Flux from Aquifer to Reach
aq.grf	AquRchMassFluxNY		Integer	Number of Time - Mass-Flux-to-Reach Pairs
aq.grf	AquRchMassFluxYR	year	Integer	Time of Mass Flux from Aquifer to Reach
aq.grf	AquRchWaterFlux	m3/day	Float	Total GW Flux to Reach

Table D-14. Surface Water Module Outputs (SW.GRF)

Code	Units	Data Type	Description
WBNConcBenthDiss	mg/L	Float	Dissolved chemical concentration in the surficial benthic layer
WBNConcBenthDissNY		Integer	Number of dissolved chemical concentration values in the surficial benthic layer
WBNConcBenthDissYr	year	Integer	Year corresponding to dissolved chemical concentration in benthic layer
WBNConcBenthTot	ug/g	Float	Total chemical concentration in the surficial benthic layer
WBNConcBenthTotNY		Integer	Number of total chemical concentration values in the surficial benthic layer
WBNConcBenthTotYr	year	Integer	Year corresponding to total chemical concentration in benthic layer
WBNConcWaterDiss	mg/L	Float	Dissolved chemical concentration in the water column
WBNConcWaterDissNY		Integer	Number of dissolved chemical concentration values in the water column
WBNConcWaterDissYr	year	Integer	Year corresponding to dissolved chemical concentration in the water column
WBNConcWaterTot	mg/L	Float	Total chemical concentration in the water column
WBNConcWaterTotNY		Integer	Number of total chemical concentration values in the water column
WBNConcWaterTotYr	year	Integer	Year corresponding to dissolved chemical concentration in the water column
WBNfocBenth	fraction	Float	Organic carbon content of benthic sediments
WBNfocBenthNY		Integer	Number of organic carbon content values
WBNfocBenthYr	year	Integer	Year corresponding to organic content values
WBNNumChem		Integer	Number of chemicals in output file
WBNTSSWater	mg/L	Float	Total suspended solids concentration in the water column
WBNTSSWaterNY		Integer	Number of suspended solids concentration values
WBNTSSWaterYr	year	Integer	Year corresponding to suspended solids values

D.7 Farm Food Chain Module

The farm food chain (FFC) 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 module is designed to predict the accumulation of a contaminant in the edible parts of a plant from uptake of contaminants in soil and through transpiration and direct deposition of the contaminant in air. 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 modeling construct for the FFC module is based on recent and ongoing research conducted by the U.S. Environmental Protection Agency (EPA) Office of Research and Development (ORD) and presented in *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (U.S. EPA, in press). Additional detail about the background and implementation of the model is available in U.S. EPA (1999i).

D.7.1 Functionality

The major computational functions performed by the Farm Food Chain Module are the following:

- *Concentrations of contaminants in homegrown produce.* The concentrations of contaminants in fruits and vegetables are calculated for home gardens and for farms.

- *Concentrations of contaminants in cattle feed*. The concentrations of contaminants in pasture grass (i.e., forage), silage, and grain are calculated for beef and dairy farms.

- *Concentrations of contaminants in locally grown beef and milk.* The concentrations of contaminants in beef and milk produced on local farms are calculated.

D.7.2 Assumptions and Limitations

The contaminant concentration calculations used in the Farm Food Chain Module reflect a number of assumptions and/or limitations:

- *Study area is bounded at 2 km.* It is assumed that all significant contaminant concentrations occur within 2 km of the source. Concentrations are not determined outside the 2-km study area.

- *Homogeneous concentrations in fruits and vegetables are assumed.* For unprotected fruits and vegetables, the exposure methodology makes no provision for the possible chemical concentration gradients within the produce that might result in different concentrations in edible portions.

- *Resuspension and redeposition on plants are not considered.* Plant concentrations are a function of the deposition of the contaminants that have been emitted from the waste management unit (WMU). Plant concentrations do not consider resuspension and redeposition. These processes can occur due to tillage, wind erosion, vehicular resuspension, and rainsplash, but will not be examined by this model.

- *Inhalation and dermal exposure are not considered in cattle.* Beef and dairy cattle calculations consider only contaminant pathways of food, soil, and water ingestion. Other pathways such as inhalation or dermal exposure are not considered in this module.

D.7.3 Inputs for the Farm Food Chain Module

The farm food chain module receives inputs from its module-specific input file (ff.ssf), the generic site layout file (Sl.ssf), the generic chemical properties file (cp.ssf), and modeled inputs from the following other modules: aquifer module (aq.grf), air module (ar.grf), surface water module (sw.grf), watershed module (ws.grf), and those source modules outputting (to a common grf file, sr.grf) a “true” for the soil-presence logical flag, srcsoil. These sources are the land application unit, landfill, wastepile, and surface impoundment. Input variables are listed and described in Table D-15.

D.7.4 Outputs from the Farm Food Chain Module

The farm food chain module outputs are written to the ff.grf file. The soil, plant, beef and milk outputs are 2-dimensional arrays indexed on time and space. Output variables are listed and described in Tables D-16.

Table D-15. Summary of Inputs for Farm Food Chain Module

File	Input Parameters	Units	Description
ff.ssf	*Fforage_<cattle type>*	Fraction	Fraction of forage grown in contaminated soil. (Note: "<cattle type>" is replaced with beef and milk.)
ff.ssf	*Fgrain_<cattle type>*	Fraction	Fraction of grain grown in contaminated soil. (Note: "<cattle type>" is replaced with beef and milk.)
ff.ssf	*Fsilage_<cattle type>*	Fraction	Fraction of silage grown in contaminated soil. (Note: "<cattle type>" is replaced with beef and milk.)
ff.ssf	*Fw_<plant type>*	Unitless	Fraction of wet deposition that adheres to the plant. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
ff.ssf	*MAF<plant type>*	Percent	Moisture adjustment factor to convert DW into WW. (Note: "<plant type>" is replaced with exfruit, exveg, leaf, profruit, proveg, and root.)
ff.ssf	*MAFleaf*	Percent	Moisture content in leaf.
ff.ssf	*Qp_forage_<cattle type>*	kg DW/d	Consumption rate of forage by cattle. (Note: "<cattle type>" is replaced with beef and milk.)
ff.ssf	*Qp_grain_<cattle type>*	kg DW/d	Consumption rate of grain by cattle. (Note: "<cattle type>" is replaced with beef and milk.)
ff.ssf	*Qp_silage_<cattle type>*	kg DW/d	Consumption rate of silage by cattle. (Note: "<cattle type>" is replaced with beef and milk.)
ff.ssf	*Qs_<cattle type>*	kg/d	Consumption rate of contaminated soil. (Note: "<cattle type>" is replaced with beef and milk.)
ff.ssf	*Qw_<cattle type>*	L/d	Consumption rate of water. (Note: "<cattle type>" is replaced with beef and milk.)
ff.ssf	*rho_leaf*	g/L	Density of the leaf.
ff.ssf	*Rp_<plant type>*	Unitless	Interception fraction. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
ff.ssf	*tp_<plant type>*	Year	Length of plant exposure to deposition. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
ff.ssf	*VapDdv*	cm/s	Vapor-phase dry deposition velocity.
ff.ssf	*VGag_<plant type>*	Unitless	Empirical correction factor. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
ff.ssf	*VGbg_root*	Unitless	Empirical correction factor for roots.
ff.ssf	*Yp_<plant type>*	kg DW/m^2	Yield or standing crop biomass. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
sl.ssf	*FarmAirFrac*	Fraction	Fraction of farm or crop area impacted by air points.

(continued)

Table D-15. (continued)

File	Input Parameters	Units	Description
sl.ssf	*FarmAirIndex*	NA	Index of points that impacts farm or crop area.
sl.ssf	*FarmAquIndex*	NA	Index of aquifer that impacts farm or crop area.
sl.ssf	*FarmAquWellFrac*	Fraction	Fraction farm uses aquifer well as animal DW source.
sl.ssf	*FarmAquWellIndex*	NA	Index of contributing subarea in local watershed indices associated with each farm.
sl.ssf	*FarmLWSIndex*	NA	Local watershed indices associated with each farm.
sl.ssf	*FarmLWSSubAreaFrac*	Fraction	Fraction of contribution of subarea in local watershed indices associated with each farm.
sl.ssf	*FarmNumAir*	Unitless	Number of air points that impact farm or crop area.
sl.ssf	*FarmNumAquWell*	Unitless	Number of wells in each aquifer impacting farm.
sl.ssf	*FarmNumLWS*	Unitless	Number of local watersheds impacting farm or crop area.
sl.ssf	*FarmNumWBNRch*	Unitless	Number of WBN reach that impact farm or crop area.
sl.ssf	*FarmNumWSSub*	Unitless	Number of watersheds that impact farm or crop area.
sl.ssf	*FarmWBNIndex*	NA	Index of WBN that impacts farm or crop area.
sl.ssf	*FarmWBNRchFrac*	Fraction	Fraction of farm or crop area impacted by WBN reach.
sl.ssf	*FarmWBNRchIndex*	NA	Index of WBN reach that impacts farm or crop area.
sl.ssf	*FarmWSSubFrac*	Fraction	Fraction of each watershed on farm.
sl.ssf	*FarmWSSubIndex*	NA	Index of watershed on farm.
sl.ssf	*focS*	Mass fraction	Fraction organic carbon (soil).
sl.ssf	*HumRcpAirIndex*	NA	Index of air points that impact receptor.
sl.ssf	*HumRcpLWSAreaIndex*	NA	Local watershed index for each human receptor.
sl.ssf	*HumRcpLWSSubAreaIndex*	NA	Local watershed subarea index for each human receptor.
sl.ssf	*HumRcpWSSubIndex*	NA	Index of watershed that impacts receptor.
sl.ssf	*NumFarm*	Unitless	Number of farm or crop areas.
cp.ssf	*ChemBa_<#>*	d/g	Biotransfer factor. (Note: “<plant type>” is replaced with beef and milk.)
cp.ssf	*ChemBa_water*	d/g	Biotransfer factor for dissolved contaminant in surface water.

(continued)

Table D-15. (continued)

File	Input Parameters	Units	Description
cp.ssf	*ChemBr_<plant type>*	(μg/g DW plant) / (μg/g soil)	Soil-to-plant bioconcentration factor. (Note: "<plant type>" is replaced with exfruit, exveg, forage, grain, profruit, proveg, root, and silage.)
cp.ssf	*ChemBs*	Fraction	Bioavailability fraction of contaminant in soil relative to vegetation.
cp.ssf	*ChemBv_ecf_plant*	Unitless	Empirical correction factor for Bv.
cp.ssf	*ChemBv_<plant type>*	(μg/g DW plant) / (μg/g air)	Mass-based air-to-plant biotransfer factor. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
cp.ssf	*ChemHLC*	(atm-m^3)/mol	Henry's law constant.
cp.ssf	*ChemKoc*	mL/g	Organic carbon partition coefficient
cp.ssf	*ChemKow*	Unitless	Octanol/water partition coefficient
cp.ssf	*ChemkpPar_<plant type>*	1/ yr	Plant surface loss of particle-bound constituent. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
cp.ssf	*ChemkpVap_<plant type>*	1/ yr	Degradation loss of vapor-phase constituents. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
cp.ssf	*ChemRCF*	(μg/g WW plant) / (μg/mL soil water)	Root concentration factor.
cp.ssf	*ChemType*	NA	Chemical type (O, M, Hg, S, or D)
aq.grf	*AquWellConc*	mg/L	Concentration of contaminant in the water of an aquifer well.
aq.grf	*AquWellConcNY*	Year	Number of years in the time series corresponding to this variable.
aq.grf	*AquWellConcYR*	Unitless	Time series of years corresponding to this variable.
ar.grf	*CVap*	μg/m^3	Concentration of chemical in air vapor.
ar.grf	*CVapNY*	Unitless	Number of years in the time series corresponding to this variable.
ar.grf	*CVapYR*	Year	Time series of years corresponding to this variable.
ar.grf	*ParDDep*	g/m2/d	Particle dry deposition rate.
ar.grf	*ParDDepNY*	Unitless	Number of years in the time series corresponding to this variable.
ar.grf	*ParDDepYR*	Year	Time series of years corresponding to this variable.

(continued)

Table D-15. (continued)

File	Input Parameters	Units	Description
ar.grf	*ParWDep*	$g/m^2/d$	Particle wet deposition rate.
ar.grf	*ParWDepNY*	Unitless	Number of years in the time series corresponding to this variable.
ar.grf	*ParWDepYR*	Year	Time series of years corresponding to this variable.
ar.grf	*VapWDep*	$g/m^2/d$	Vapor wet deposition rate.
ar.grf	*VapWDepNY*	Unitless	Number of years in the time series corresponding to this variable.
ar.grf	*VapWDepYR*	Year	Time series of years corresponding to this variable.
sr.grf	*CTda*	$\mu g/g$	Depth-averaged soil concentration across farm area.
sr.grf	*CTdaNY*	Year	Number of years in the time series corresponding to this variable.
sr.grf	*CTdaYR*	Unitless	Time series of years corresponding to this variable.
sr.grf	*CTss*	$\mu g/g$	Surficial soil concentration across farm area.
sr.grf	*CTssNY*	Year	Number of years in the time series corresponding to this variable.
sr .grf	*CTssYR*	Unitless	Time series of years corresponding to this variable.
sw.grf	*CTdaR*	$\mu g/g$	Depth-averaged soil concentration for the regional watershed area.
sw.grf	*CTdaRNY*	Year	Number of years in the time series corresponding to this variable.
sw.grf	*CTdaRYR*	Unitless	Time series of years corresponding to this variable.
sw.grf	*CTssR*	$\mu g/g$	Surface soil concentration for the regional watershed area.
swrf	*CTssRNY*	Year	Number of years in the time series corresponding to this variable.
sw.grf	*CTssRYR*	Unitless	Time series of years corresponding to this variable.

NA = Not applicable

Table D-16. Summary of Outputs Parameters for the Farm Food Chain Module

File	Code	Units	Description
ff.grf	*Abeef_farm*	mg/kg WW	Concentration of contaminant in beef.
ff.grf	*Abeef_farmNY*	Year	Number of years in the time series corresponding to this variable.
ff.grf	*Abeef_farmYR*	Unitless	Time series of years corresponding to this variable.
ff.grf	*Amilk_farm*	mg/kg WW	Concentration of contaminant in milk.
ff.grf	*Amilk_farmNY*	Year	Number of years in the time series corresponding to this variable.
ff.grf	*Amilk_farmYR*	Unitless	Time series of years corresponding to this variable.
ff.grf	*CTssAve_farm*	μg/g	Chemical concentration in surficial soil averaged over farm area.
ff.grf	*CTssAve_farmNY*	Year	Number of years in the time series corresponding to this variable.
ff.grf	*CTssAve_farmYR*	Unitless	Time series of years corresponding to this variable.
ff.grf	*P<plant type>_farmYR*	Unitless	Time series of years corresponding to this variable.
ff.grf	*P<plant type>_farm*	mg/kg WW	Concentration of contaminant for specific fruit and vegetable categories grown on a farm. (Note: “<plant type>” is replaced with exfruit, exveg, profruit, proveg, and root.)
ff.grf	*P<plant type>_farmNY*	Year	Number of years in the time series corresponding to this variable.
ff.grf	*P<plant type>_garden*	mg/kg WW	Concentration of contaminant for specific fruit and vegetable categories grown in a garden. (Note: “<plant type>” is replaced with exfruit, exveg, profruit, proveg, and root.)
ff.grf	*P<plant type>_gardenYR*	Unitless	Time series of years corresponding to this variable.
ff.grf	*P<plant type>_gardenNY*	Year	Number of years in the time series corresponding to this variable.

D.8 Terrestrial Food Web Module

The terrestrial food web module (TerFW) 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 (EcoEx) 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 5 cm). The spatial averages are defined by the home ranges and habitats that are delineated within the area of interest (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. Additional detail on the TerFW module can be found in U.S. EPA (1999j).

D.8.1 Functionality

The major computational functions performed by the Terrestrial Food Web module are the following:

- *Time series management*. The TerFW module determines the overall duration of the time period to be simulated (including concentration data from discontinuous time periods) and identifies the individual years within the overall duration that will be simulated.

- *Module loops over the time series, through habitats and home ranges.* The TerFW module has three basic loops: (1) over the time series, (2) over each habitat delineated at the site, and (3) over the four home range areas delineated within each habitat.

- *Calculation of time series soil and plant concentrations and minimum and maximum concentrations in terrestrial prey types (e.g., small mammals).* This is the fundamental structure of the TerFW module, namely, to develop soil and tissue concentrations for each year of the simulation that reflect the range of potential exposure concentrations. These concentrations are spatially explicit with regard to the home range for each ecological receptor.

The major steps performed by the Terrestrial Food Web module that are required to predict concentrations in soil (surficial and depth-averaged), plants, and other prey types can be summarized as follows:

- Select terrestrial habitat of interest (i.e., cropland, residential area, grassland, forest, shrub/scrub).

- Select home range within habitat (i.e., one of four home range areas).

- Calculate average soil concentration within home range for surficial soil and depth-averaged soil.

- Calculate concentration for all categories of terrestrial plants within home range.

- Calculate tissue concentration in soil fauna within home range (i.e., earthworms and other soil invertebrates).

- Calculate tissue concentrations in receptors assigned to home range (e.g., small mammals, omnivores).

- Loop through all home ranges within habitat of interest and repeat calculations of soil and tissue concentrations.

- Report minimum and maximum values for tissue concentrations in prey types other than terrestrial plants and soil fauna.

D.8.2 Assumptions and Limitations

The contaminant concentration calculations used in the Terrestrial Food Web module reflect a number of assumptions and limitations, which are listed below.

D.8.2.1 <u>Assumptions</u>

- *Study area is bounded at 2 km.* EPA assumed that significant exposures to source-related contaminants do not occur for ecological receptors that are beyond 2 km of the source. Consequently, tissue concentrations in food items located outside of the study (measured from the edge of the source to a point 2 km away) are presumed to be zero.

- *Uptake and accumulation of chemicals within categories of plants (e.g., exposed vegetables) is assumed to be similar.* The algorithms used to estimate biotransfer factors do not distinguish physiological differences across various kinds of plants. For example, the category "forage" includes forbs, grasses, fungi, shrubs, trees, and unclassified plants. Therefore, in estimating biotransfer factors for this category, it is implicitly assumed that the physiological differences in different plant species do not significantly affect chemical loadings in plant tissues. The use of empirical data on selected plant species (typically crops) also assumes similar mechanisms of uptake and accumulation.

- *No less than 10 percent of the diet is attributed to the study area.* In many instances, the home range for a given receptor exceeds the size of the habitat. In general we assumed that the percent of the home range that "fits" into the habitat is a suitable surrogate with which to scale exposure and predict tissue concentration. However, the purpose of this analysis is to determine acceptable waste concentrations assuming that the study area (e.g., forests) would be used as habitat by wildlife. Therefore, we assumed that no less than 10 percent of the diet

originated from the study area, even if the fraction of the home range inside the habitat fell below 10 percent.

A reasonable averaging depth for soil concentrations is 5 cm. In view of the multiple purposes of this soil concentration (e.g., evaluate risks to soil fauna; predict tissue concentrations in prey using soil-based bioaccumulation factors), this was selected as a depth that was ecologically meaningful (with regard to organisms occupying different soil horizons) and consistent with the goals for the ecological risk analysis. However, this assumption carries with it some uncertainty in its application within the exposure and risk modules.

D.8.2.2 Limitations

Concentrations in terrestrial prey are based on soil-to-prey bioaccumulation factors (BAFs). The most significant limitation in predicting tissue concentrations in terrestrial prey is the paucity of mechanistic models and data sources with which to estimate food web dynamics. For instance, the tissue concentration in small birds is generally predicted using a BAF for soil rather than a biotransfer factor (or BAF) from earthworms and insects into birds. As a result, the TerFW can not rely on the matrix solution technique used by the Aquatic Food Web module to solve for concentrations in various prey items.

Some chemicals rely heavily on empirical uptake data. This limitation is similar to that noted for the Farm Food Chain module. In essence, the paucity of data on uptake and accumulation of constituents in terrestrial food items introduces significant uncertainty into this module.

Estimates of tissue concentrations reflect a single home range setting. The TerFW module calculates tissue concentrations in prey items for a single random placement of four home range sizes.[3] As a result, the four home ranges in the site layout may not reflect the spatial variability in soil contamination, particularly for large habitats (i.e., habitats that cover substantially greater areas than most of the home ranges).

Resuspension and redeposition on plants are not considered. Plant concentrations are a function of the deposition on plants of the contaminants that have been emitted from the waste management unit. Plant concentrations do not reflect resuspension and redeposition, which can occur due to tillage, wind erosion, vehicular resuspension, and rainsplash

[3] As described in U.S. EPA (1999n), each receptor is assigned to one of four discrete home range sizes, depending on the receptor-specific home range size. The four home ranges overlap in a manner that reflects the predator-prey relationships.

D.8.3 Inputs

The concentration inputs required by the TerFW module are provided by the Air module, the Regional Watershed (RW) module, and two source modules: the Wastepile and Land Application Unit. The Air (Ar) module provides air concentrations and deposition rates relevant to plant loadings. The RW module provides surficial and depth-averaged soil concentrations for watersheds within the AOI, and the source modules provide soil concentrations within the drainage sub-basin that includes the source. The average chemical concentration in soil calculated for a given home range may include contributions from regional watersheds as well as from a source-related drainage sub-basin (referred to as the local watershed). These inputs include:

Air Module

- vapor concentration for each home range and habitat within the AOI
- wet vapor deposition rate for each home range and habitat within the AOI
- dry particle deposition rate for each home range and habitat within the AOI
- wet particle deposition rate for each home range and habitat within the AOI

Regional Watershed

- surficial soil concentration for each watershed within the AOI
- depth-averaged soil concentration for each watershed within the AOI

Source Modules

- surficial soil concentration for the each local watershed within the AOI
- depth-averaged soil concentration for each local watershed within the AOI

The terrestrial food web module receives inputs from its module-specific input file (tf.ssf), the generic site layout file (sl.ssf), the generic chemical properties file (cp.ssf), and modeled inputs from the following other modules: air module (ar.grf), watershed module (ws.grf), and those source modules outputting to a common grf file (sr.grf) a “true” for the soil-presence logical flag, SrcSoil. These sources are the land application unit, landfill, wastepile, and surface impoundment. The soil, plant, invertebrate, and worm concentration outputs are three-dimensional arrays indexed on time, space, and receptor. The small birds, small herpetofauna, small mammals, herbiverts, and omniverts are two-dimensional arrays indexed on time and space. All input variables are listed and described in Table D-17.

D.8.4 Outputs from the Terrestrial Food Web Module

The terrestrial food web module outputs are written to the tf.grf file. All output variables are listed and described in Table D-18.

Table D-17. Summary of Inputs for the Terrestrial Food Web Module

File	Input Parameters	Units	Description
tf.ssf	*Bv_ecf_plant*	unitless	Empirical correction factor for Bv.
tf.ssf	*Fw_<plant type>*	unitless	Fraction of wet deposition that adheres to the plant. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
tf.ssf	*MAF<plant type>*	percent	Moisture adjustment factor to convert DW into WW. (Note: "<plant type>" is replaced with exfruit, exveg, leaf, profruit, proveg, and root.)
tf.ssf	*MAFleaf*	percent	Moisture content in leaf.
tf.ssf	*rho_leaf*	g/L	Density of the leaf.
tf.ssf	*Rp_<plant type>*	unitless	Interception fraction. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
tf.ssf	*tp_<plant type>*	year	Length of plant exposure to deposition. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
tf.ssf	*VapDdv*	cen/sec	Vapor phase dry deposition velocity.
tf.ssf	*VGag_<plant type>*	unitless	Empirical correction factor. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
tf.ssf	*VGbg_root*	unitless	Empirical correction factor for roots.
tf.ssf	*Yp_<plant type>*	kg DW/m^2	Yield or standing crop biomass. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
sl.ssf	*focS*	mass fraction	Fraction organic carbon (soil).
sl.ssf	*HabRangeAirIndex*	NA	Index of air points that impacts a home range.
sl.ssf	*HabRangeAirFrac*	fraction	Fraction of home range impacted by air points.
sl.ssf	*HabRangeNumWSSub*	unitless	Number of watersheds that impact a home range.
sl.ssf	*HabRangeLWSSubAFrac*	fraction	Fraction of contributing local watershed subarea.
sl.ssf	*HabRangeWSSubFrac*	fraction	Fraction of home range impacted by watershed.
cp.ssf	*ChemBAF<animal>*	unitless	Bioaccumulation factor for small birds, herbiverts, small herpetofauna, invertebrates, small mammals, omniverts, and worms.
cp.ssf	*ChemBr_<plant type>*	(μg/g DW plant) / (μg/g soil)	Soil-to-plant bioconcentration factor. (Note: "<plant type>" is replaced with exfruit, exveg, forage, grain, profruit, proveg, root, and silage.)
cp.ssf	*ChemBv_ecf_plant*	unitless	Empirical correction factor for Bv.
cp.ssf	*ChemBv_<plant type>*	(μg/g DW plant) / (μg/g air)	Mass-based air-to-plant biotransfer factor. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)

(continued)

Table D-17. (continued)

File	Input Parameters	Units	Description
cp.ssf	*ChemHLC*	(atm-m^3) / mol	Henry's law constant.
cp.ssf	*ChemKoc*	mL/g	Organic carbon partition coefficient
cp.ssf	*ChemKow*	unitless	Octanol/water partition coefficient
cp.ssf	*ChemkpPar_<plant type>*	1/ year	Plant surface loss of particulate-bound constituent. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
cp.ssf	*ChemkpVap_<plant type>*	1/ year	Degradation loss of vapor phase constituents. (Note: "<plant type>" is replaced with exfruit, exveg, forage, and silage.)
cp.ssf	*ChemRCF*	(μg/g WW plant) / (μg/mL sl water)	Root concentration factor.
cp.ssf	*ChemType*	NA	Chemical type (O, M, Hg, S, or D)
ar.grf	*CVap*	μg/m3	Concentration of chemical in air vapor.
ar.grf	*CVapNY*	unitless	Number of years in the time series corresponding to this variable.
ar.grf	*CVapYR*	year	Time series of years corresponding to this variable.
ar.grf	*ParDDep*	g/m2/d	Particle dry deposition rate.
ar.grf	*ParDDepNY*	unitless	Number of years in the time series corresponding to this variable.
ar.grf	*ParDDepYR*	year	Time series of years corresponding to this variable.
ar.grf	*ParWDep*	g/m2/d	Particle wet deposition rate.
ar.grf	*ParWDepNY*	unitless	Number of years in the time series corresponding to this variable.
ar.grf	*ParWDepYR*	year	Time series of years corresponding to this variable.
ar.grf	*VapWDep*	g/m2/d	Vapor wet deposition rate.
ar.grf	*VapWDepNY*	unitless	Number of years in the time series corresponding to this variable.
ar.grf	*VapWDepYR*	year	Time series of years corresponding to this variable.
sr.grf	*CTda*	μg/g	Depth-averaged soil concentration across farm area.
sr.grf	*CTdaNY*	year	Number of years in the time series corresponding to this variable.
sr.grf	*CTdaYR*	unitless	Time series of years corresponding to this variable.

(continued)

Table D-17. (continued)

File	Input Parameters	Units	Description
sr.grf	*CTss*	μg/g	Surficial soil concentration across farm area.
sr.grf	*CTssNY*	year	Number of years in the time series corresponding to this variable.
sr.grf	*CTssYR*	unitless	Time series of years corresponding to this variable.
ws.grf	*CTdaR*	μg/g	Depth-averaged soil concentration for the regional watershed area.
ws.grf	*CTdaRNY*	year	Number of years in the time series corresponding to this variable.
ws.grf	*CTdaRYR*	unitless	Time series of years corresponding to this variable.
ws.grf	*CTssR*	μg/g	Surface soil concentration for the regional watershed area.
ws.grf	*CTssRNY*	year	Number of years in the time series corresponding to this variable.
ws.grf	*CTssRYR*	unitless	Time series of years corresponding to this variable.

NA = not applicable

Table D-18. Summary of Outputs from the Terrestrial Food Web Module

File	Output Parameters	Units	Description
tf.grf	*C<animals>_<max or min>NY*	unitless	Number of years in the time series corresponding to this variable.
tf.grf	*C<animals>_<max or min>*	mg/kg	Concentration of contaminant found in herbiverts and omniverts.
tf.grf	*C<animals>_<max or min>YR*	year	Time series of years corresponding to this variable.
tf.grf	*C<animals>_HabRange*	mg/kg	Concentration of contaminant found in invertebrates and worms.
tf.grf	*C<animals>_HabRangeNY*	unitless	Number of years in the time series corresponding to this variable.
tf.grf	*C<animals>_HabRangeYR*	year	Time series of years corresponding to this variable.
tf.grf	*C<animals>_sm_<max or min>*	mg/kg	Concentration of contaminant found in small birds, herpetofauna, and mammals.
tf.grf	*C<animals>_sm_<max or min>YR*	year	Time series of years corresponding to this variable.
tf.grf	*C<animals>_sm_<max or min>NY*	unitless	Number of years in the time series corresponding to this variable.
tf.grf	*CTdaAveHabRange*	μg/g	Average depth average soil concentration in each home range.
tf.grf	*CtdaAveHabRangeNY*	unitless	Number of years in the time series corresponding to this variable.
tf.grf	*CTdaAveHabRangeYR*	year	Time series of years corresponding to this variable.
tf.grf	*CTssAveHabRange*	μg/g	Average depth average soil concentration in each home range.
tf.grf	*CTssAveHabRangeNY*	unitless	Number of years in the time series corresponding to this variable.
tf.grf	*CTssAveHabRangeYR*	year	Time series of years corresponding to this variable.
tf.grf	*P<plant type>_HabRangeNY*	unitless	Number of years in the time series corresponding to this variable.
tf.grf	*P<plant type>_HabRangeYR*	year	Time series of years corresponding to this variable.
tf.grf	*P<plant type>_HabRange*	mg/kg	Concentration of contaminant found in exfruit, exveg, forage, grain, root, and silage.

D.9 Aquatic Food Web Module

The aquatic food web (AqFW) module calculates chemical concentrations in aquatic organisms that are consumed by human and ecological receptors (e.g., fish filet; 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 cold water and warm water aquatic habitats. It uses both property-based calculations and empirical data to estimate uptake and accumulation. Addition detail on the model design and construction, including governing equations, may be found in U.S. EPA (1999o).

D.9.1 Functionality

The major computational functions performed by the Aquatic Food Web module can be summarized as follows:

- *Time series management*. The AqFW module determines the overall duration of the time period to be simulated (including concentration data from discontinuous time periods) and identifies the individual years within the overall duration that will be simulated.

- *Module loops over the time series, through aquatic habitats, and reaches.* The AqFW module has three basic loops: (1) over the time series, (2) over each aquatic habitat delineated at the site, and (3) over the "fishable" reaches within each aquatic habitat. The module considers all reach order 3 streams, ponds, lakes, and certain types of permanently flooded wetlands as fishable by human and ecological receptors.

- *Calculation of time series tissue concentrations for fish and other aquatic organisms*. The AqFW module predicts concentrations for each year of the simulation for aquatic organisms assigned to each habitat. These concentrations are defined spatially for each reach even though a stream habitat or wetland may contain multiple reaches.[4] Similarly, the module predicts concentrations in ponds and lakes as though the system is fully mixed and at steady state.

The major steps performed by the Aquatic Food Web module that are required to predict concentrations in aquatic organisms may be summarized as follows:

- Select fishable reach of interest (i.e., stream or wetland reach, pond, or lake).

- Determine temperature and set aquatic habitat type (e.g., cold water stream).

- Construct dietary matrix for fish in aquatic habitat.

[4] Reaches are defined in the site layout file and modeled by the Surface Water module as homogeneous segments (i.e., there is no concentration gradient throughout the reach).

Calculate whole-body tissue concentrations (for ecological receptors)

- Identify chemical type (e.g., hydrophobic organic, metal, mercury).
- If chemical type is not readily metabolizable (i.e., special), check K_{ow} value.
- If chemical is hydrophobic (log $K_{ow} \geq 4.0$ is true), run matrix solution to estimate whole-body tissue concentrations.
- If chemical is hydrophilic (log $K_{ow} < 4.0$ is true), run regression models to estimate whole-body tissue concentrations.
- If chemical is metal, readily metabolizable, or mercury, get empirical bioaccumulation data and calculate whole-body tissue concentrations.

Calculate filet concentrations (for human receptors).

D.9.2 Assumptions and Limitations

The methodology used in the aquatic food web module reflects a number of assumptions and/or limitations, which are listed below. It should be noted that, because the AqFW module relies on the surface water module (U.S. EPA, 1999p) to provide concentrations in surface water and sediment, the assumptions and limitations identified for the SW module are relevant to the AqFW module. For example, the SW module provides annualized average concentrations for stream reaches and other waterbodies. Consequently, the methods developed to estimate tissue concentrations in aquatic organisms were developed to be use the annual average surface water concentrations predicted with the SW model. The assumptions and limitations implicit in the SW module are not discussed in this section.

D.9.2.1 <u>Assumptions</u>

*Study area is bounded at 2 km.* EPA assumed that significant exposures to source-related contaminants do not occur for ecological receptors that are beyond 2 km of the source. Consequently, concentrations were not calculated in aquatic organisms in waterbodies outside of the study area, measured from the corner of the source to a point 2 km away.

*All waterbodies that define aquatic habitats are fishable.* The module assumes that all third order stream reaches (and above), ponds, lakes, and certain permanently flooded wetlands support a multi-compartment aquatic food web. The simple food webs developed for each of these aquatic habitats provide a useful framework for predicting tissue concentrations in aquatic organisms for a national assessment. Nevertheless, it is a certainty that not all of the waterbodies designated as fishable in this analysis will be of sufficient quality to sustain a multi-compartment food web.

Variability in aquatic systems is reasonably represented. The underlying framework developed for the AqFW module (as applied in a national analysis) is the eight representative aquatic habitats. It is implicitly assumed that these eight habitats provide adequate resolution of the major types of freshwater systems within the constraints of available data and modeling tools.

Hydrophobic organics may be defined as organic chemicals with log $K_{ow} \geq 4.0$. Although a strict definition for hydrophobic organics has not appeared in the literature, the AqFW module assumes that a reasonable cutoff is a log K_{ow} value of 4.0. Comparisons of predicted bioaccumulation factors (BAFs) derived with mechanistic models versus BAFs derived using regression equations suggests that, below log K_{ow} = 4.0, the difference in BAF estimates is below the level of resolution that these models are capable of.

The model construct is applicable to waterbodies other than coldwater lakes. A number of journal articles (e.g., Morrison et al., 1997) and reference texts (e.g., Rand, 1995) were reviewed in evaluating appropriate mechanistic models to simulate the uptake and accumulation of hydrophobic organics in aquatic organisms. From that review, it was determined that the underlying theory for these models is remarkably similar and that there is no inherent advantage in selecting one model over another. Although the Gobas (1993) model was calibrated for coldwater lakes (i.e., Lake Ontario), it was determined that this model construct was appropriate for use on other aquatic systems under the general assumption of steady-state conditions.

D.9.2.2 <u>Limitations</u>

Steady-state conditions are generally assumed. Because annual average concentrations are provided by the SW module, the AqFW module assumes steady-state conditions. As a result, the module can not be used to evaluate the impacts from storm events nor can it be used to distinguish the impacts on tissue concentrations from peak events and subsequent averaging from long-term, low-level exposures. For example, a storm event may contaminate a given reach for relatively short periods of time, probably well below the duration required for organisms to reach steady-state for most chemicals.

The module relies heavily on empirical data for many chemicals. For chemicals that have not been shown to be readily metabolizable (e.g., other than PAHs, selected phthalates), mechanistic models are not used to predict tissue concentrations. Hence, the AqFW module estimates tissue concentrations by multiplying empirical factors (primarily bioconcentration factors, or BCFs) by water concentrations. As discussed in the data collection documentation on the AqFW parameters, these BCFs are measured under conditions that may not be relevant to all possible conditions (and species) included in the analysis.

- *The module does not allow for separate treatment of essential metals.* Bioconcentration of essential metals is not linear and modeling approaches are available to account for nonlinearity (see Bergman and Dorward-King, 1997). Bioconcentration of essential metals tends to be much greater at low concentrations than at higher concentrations since organisms actively seek to sequester necessary nutrients. Because many metals are regulated in biological systems, the apparent bioconcentration of metals at low concentrations may simply result in metal accumulation at "healthy" levels.

- *The module currently lacks the capability to use sediment concentrations directly in predicting tissue concentrations.* The AqFW module was developed, primarily, to utilize dissolved and total contaminant concentrations to predict tissue concentrations. Although sediment concentrations are used in predicting uptake and accumulation into benthic dwellers, the AqFW module lacks the necessary algorithms to use these data directly to predict concentrations in plants or fish. For certain constituents (e.g., dioxins), it may be useful to build this functionality into the module to provide greater flexibility in data use.

- *The module has not been validated in field studies.* Much of the modeling theory on which the AqFW module is based is widely accepted and has been used in numerous analyses. In particular, the methods used to predict concentrations of hydrophobic organics have been validated in coldwater lakes. However, the module has not been validated for other freshwater aquatic habitats, nor has it been validated *in toto* for application in a national-scale analysis.

D.9.3 Inputs

The only concentration inputs required by the AqFW module are provided by the surface water module (SW). These inputs include:

- average, reach-specific total concentration in sediment
- average, reach-specific total concentration in surface water
- average, reach-specific dissolved concentration in surface water

The aquatic food web module receives inputs from its module-specific input file, af.ssf, the generic site layout file (sl.ssf), the chemical properties file (cp.ssf), and modeled inputs from the surface water module (sw.grf). All AqFW module outputs are 3-dimensional arrays indexed on time, waterbody network, and reach. Input variables are listed and described in Table D-19.

D.9.4 Outputs from the Aquatic Food Web Module

The aquatic food web module outputs are written to the af.grf file. Output variables are listed and described in Table D-20.

Table D-19. Summary of Inputs for the Aquatic Food Web Module

File	Input Parameters	Units	Description
af.ssf	*a_fish*	unitless	Slope of BCF regression equation across all tissues in fish.
af.ssf	*a_mus*	unitless	Slope of BCF regression equation for muscle tissue in fish.
af.ssf	*b_fish*	unitless	Slope (2) of BCF regression equation across all tissues in fish.
af.ssf	*b_mus*	unitless	Slope (2) of BCF regression equation for muscle tissue in fish.
af.ssf	*BiotaTypeIndex*	unitless	Numerical index of each biota type.
af.ssf	*BwFish*	unitless	Fish body weight.
af.ssf	*c_fish*	unitless	Error term in BCF regression equation across all tissues in fish.
af.ssf	*c_mus*	unitless	Error term in BCF regression equation for muscle tissues in fish.
af.ssf	*FiletFrac*	unitless	Fraction of fish that is a filet based on lipid content.
af.ssf	*FishWaterFrac*	unitless	Water fraction across all tissues of fish.
af.ssf	*LipFrac*	unitless	Lipid fraction.
af.ssf	*LipFracMus*	unitless	Lipid fraction in fish muscle.
af.ssf	*MaxPreyPref*	unitless	Maximum dietary preference for item in the aquatic food web.
af.ssf	*MinPreyPref*	unitless	Minimum dietary preference for item in the aquatic food web.
af.ssf	*MusWaterFrac*	unitless	Water fraction in muscle of fish.
af.ssf	*NumBiotaTypes*	unitless	Number of biota types in the aquatic food web.
af.ssf	*rho_lip*	kg/L	Density of organic carbon.
af.ssf	*rho_oc*	kg/L	Density of lipids.
af.ssf	*T3EdibleFish*	unitless	Edible trophic level 3 fish for human consumption.
af.ssf	*T3NumEdibleFish*	unitless	Number of edible trophic level 3 fish in the aquatic food web.
af.ssf	*T3NumFish*	unitless	Number of trophic level 3 fish in the aquatic food web.
sl.ssf	*NumWBN*	unitless	Number of waterbody networks.
sl.ssf	*WBNFishableRchIndex*	unitless	Index of reaches that are fishable.
sl.ssf	*WBNNumFishableRch*	unitless	Number of fishable reaches.

(continued)

Table D-19. (continued)

File	Input Parameters	Units	Description
sl.ssf	*WBNRchArea*	m^2	Reach surface area.
sl.ssf	*WBNRchOrder*	unitless	Reach order of stream.
sl.ssf	*WBNRchBodyType*	unitless	Type of waterbody (e.g., pond, stream).
sl.ssf	*WBNTemp*	degrees Celsius	Median temperature of waterbody network.
sl.ssf	*WBNTempMax*	degrees Celsius	Maximum temperature of reaches in the waterbody network.
cp.ssf	*ChemT3musBAFm*	L/kg ww	Empirical bioaccumulation factor in filet of TL3 fish.
cp.ssf	*ChemT3fishBAFm*	L/kg ww	Empirical bioaccumulation factor in whole-body of TL3 fish.
cp.ssf	*ChemT4musBAFm*	L/kg ww	Empirical bioaccumulation factor in filet of TL4 fish.
cp.ssf	*ChemT4fishBAFm*	L/kg ww	Empirical bioaccumulation factor in whole-body of TL4 fish.
cp.ssf	*ChemaqmpBCFm*	L/kg ww	Empirical bioconcentration factor for aquatic macrophytes.
cp.ssf	*ChembenthffBAFm*	L/kg ww	Empirical bioaccumulation factor in benthic filter feeders.
cp.ssf	*ChemKm*	1/day	Metabolic rate constant for fish.
cp.ssf	*ChemKow*	unitless	Octanol/water partition coefficient.
cp.ssf	*ChemType*	NA	Chemical Type
sw.grf	*WBNConcBenthTot*	μg/g	Concentration of contaminant in benthic solids.
sw.grf	*WBNConcBenthTotNY*	unitless	Number of years in the time series corresponding to this variable.
sw.grf	*WBNConcBenthTotYR*	year	Time series of years corresponding to this variable.
sw.grf	*WBNConcWaterTot*	mg/L	Total contaminant concentration in surface water.
sw.grf	*WBNConcWaterTotNY*	unitless	Number of years in the time series corresponding to this variable.
sw.grf	*WBNConcWaterTotYR*	year	Time series of years corresponding to this variable.
sw.grf	*WBNConcWaterDiss*	mg/L	Freely dissolved contaminant concentration in surface water.
sw.grf	*WBNConcWaterDissNY*	unitless	Number of years in the time series corresponding to this variable.
sw.grf	*WBNConcWaterDissYR*	year	Time series of years corresponding to this variable.
sw.grf	*WBNfocBenth*	fraction	Benthivore fraction of organic carbon.

(continued)

Table D-19. (continued)

File	Input Parameters	Units	Description
sw.grf	*WBNfocBenthNY*	unitless	Number of years in the time series corresponding to this variable.
sw.grf	*WBNfocBenthYR*	year	Time series of years corresponding to this variable.

NA = not applicable

Table D-20. Summary of Outputs for the Aquatic Food Web Module

File	Code	Units	Description
af.grf	*Caqmp*	mg/kg ww	Concentration of contaminant in aquatic plants.
af.grf	*CaqmpNY*	unitless	Number of years in the time series corresponding to this variable.
af.grf	*CaqmpYR*	year	Time series of years corresponding to this variable.
af.grf	*Cbenthff*	mg/kg ww	Concentration of contaminant in benthic filter feeders.
af.grf	*CbenthffNY*	unitless	Number of years in the time series corresponding to this variable.
af.grf	*CbenthffYR*	year	Time series of years corresponding to this variable.
af.grf	*CT3Filet*	mg/kg ww	Concentration in filet of contaminant in TL3 fish.
af.grf	*CT3FiletNY*	unitless	Number of years in the time series corresponding to this variable.
af.grf	*CT3FiletYR*	year	Time series of years corresponding to this variable.
af.grf	*CT3Fish*	mg/kg ww	Whole-body concentration of contaminant in TL3 fish.
af.grf	*CT3FishNY*	unitless	Number of years in the time series corresponding to this variable.
af.grf	*CT3FishYR*	year	Time series of years corresponding to this variable.
af.grf	*CT4Filet*	mg/kg ww	Concentration in filet of contaminant in TL4 fish.
af.grf	*CT4FiletNY*	unitless	Number of years in the time series corresponding to this variable.
af.grf	*CT4FiletYR*	year	Time series of years corresponding to this variable.
af.grf	*CT4Fish*	mg/kg ww	Whole-body concentration of contaminant in TL4 fish.
af.grf	*CT4FishNY*	unitless	Number of years in the time series corresponding to this variable.
af.grf	*CT4FishYR*	year	Time series of years corresponding to this variable.

D.10 Human Exposure Module

The human exposure module calculates the applied dose (mg of constituent per kg of body weight), to human receptors from media and food concentrations calculated by other modules in the multimedia, multipathway and multiple receptor risk assessment (3MRA) methodology. These calculations are performed for each receptor, cohort, exposure pathway, and year at each exposure area.[5] The human exposure module calculates exposures for two basic receptor types: residential receptors (residents and home gardeners) and 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. The subcategories within residential receptors and farmers differ in the particular exposures they incur. For example, a resident (only) differs from a home gardener in that home gardeners are exposed to contaminated fruits and vegetables, but residents are not. Within each of the two basic receptor types, the human exposure module calculates exposures for 5 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). Additional detail about the background and implementation of the model is available in U.S. EPA (1999q).

D.10.1 Functionality

The major computational functions performed by the human exposure module are the following:

- *Time series management*. The human exposure module determines the overall duration of the time period to be simulated, which could possibly be discontinuous, and the individual years within this duration to be simulated.

- *Calculation of time series exposure concentrations and doses from time series media and food concentrations*. This is the fundamental purpose of the human exposure module and is performed by a set of equations specific to each exposure pathway and carcinogenic/noncarcinogenic chemical property.

Exposure to humans other than infants may occur through eight pathways: inhalation of ambient air, inhalation of shower air, ingestion of groundwater, ingestion of soil, ingestion of fruits and vegetables, ingestion of beef, ingestion of milk, and ingestion of fish. However, not all receptors are exposed via all of these pathways. Residents are exposed via inhalation of ambient air, inhalation of shower air, ingestion of groundwater, and ingestion of soil. Home gardeners have the same exposures as a resident, plus exposure via ingestion of fruits and vegetables. All farmers are exposed via inhalation of ambient air, inhalation of shower air, ingestion of groundwater, ingestion of soil, and ingestion of fruits and vegetables. In addition, beef farmers are exposed via ingestion of beef, and dairy farmers are exposed via ingestion of milk. Recreational fishers have the same exposures as one of the other receptor types plus fish ingestion. Not all age cohorts are exposed via all pathways; shower exposures are calculated only for adults and children ages 12 to 19 years.

[5] See Section 3.3.10 for the list of receptors and cohorts and applicable exposure pathways.

The media inputs for which the human exposure module calculates exposure concentrations and doses include ambient air concentration (both vapor and particulate), soil concentration, groundwater concentration, exposed vegetable concentration, protected vegetable concentration, exposed fruit concentration, protected fruit concentration, root vegetable concentration, beef concentration, milk concentration, and fish filet concentration for trophic level 3 and trophic level 4 fish. For vegetables and fruits, the terms "exposed" and "protected" refer to whether the edible portion of the plant is exposed to the atmosphere.

Infant exposure occurs via breast milk ingestion. The human exposure module tracks noninfant exposure by the eight pathways described above. For infant exposure via breast milk, the maternal exposure via all pathways must be summed. Therefore, infant exposures are calculated for eight maternal exposure configurations: resident, home gardener, beef farmer, dairy farmer, resident/recreational fisher, home gardener/recreational fisher, beef farmer/recreational fisher, and dairy farmer/recreational fisher. The mother is assumed to be an adult (as opposed to a teenager) for the purpose of calculating maternal dose in the infant breast milk pathway.

D.10.2 Assumptions and Limitations

The exposure characterization methodology used in the human exposure module reflects a number of assumptions and/or limitations, which are listed below.

- Study area is bounded at 2 km. EPA assumed that all significant exposure by human receptors occurs within 2 km of the source. Exposures are not evaluated for individuals residing outside of the 2-km study area, measured from the source periphery.

- *Human receptors are stationary.* EPA assumed in characterizing exposure that human receptors both reside and work at the receptor location identified for them during site characterization (i.e., the farm area for farmers or residential exposure area for nonfarmers). The point of exposure is, in general, the census block centroid for a resident and home gardener and the centroid of a farm for farmers. This assumption may overestimate or underestimate exposure, because it is possible that individuals may reside at the identified location within the study area but commute to work areas outside of the study area or could commute to more or less contaminated areas within the study area.

- *Incremental exposure is modeled.* The HWIR model generates incremental exposures in accordance with standard practice. No provision is made for considering background exposures for the purpose of generating cummulative or total risk, HQ, or MOE estimates for modeled receptors.

- *Homogeneous concentrations in fruits and vegetables are assumed.* The exposure methodology makes no provision for possible chemical concentration gradients within fruits or vegetables that might result in different concentrations in edible portions than when averaged throughout the food item.

- *Food preparation has no effect*. No diminution of chemical concentration in food items is assumed to occur through food preparation, e.g., washing of fruits and vegetables.

- Annual average concentrations/doses for exposure. No shorter term average or spikes evaluated. All outputs from this module are on an annual basis.

- Ingestion rates are age cohort specific. The ingestion and inhalation rates, as well as body weight, are based on the age cohort. For example, a 1 to 5-year-old child would ingest less water on a daily basis then a 6- to 10-year-old child.

D.10.3 Inputs for the Human Exposure Module

The human exposure module receives inputs from its module-specific input file, he.ssf, the generic site layout file (sl.ssf), the generic chemical properties file (cp.ssf), and the following modeled outputs from other 3MRA modules: ground water concentrations from the aquifer module (aq.grf); fish filet concentration for trophic level 3 and trophic level 4 fish from the aquatic food web module (af.grf); exposed vegetable concentration, protected vegetable concentration, exposed fruit concentration, protected fruit concentration, root vegetable concentration, beef concentration, and milk concentration from the farm food chain module (ff.grf)[6]; soil concentrations from the watershed module (ws.grf); ambient air concentration (both vapor and particulate) from the air module (ar.grf); and soil concentrations from those source modules outputting (to a common grf file, sr.grf) a "true" for the soil-presence logical flag, *SrcSoil*. (SrcSoil = true signifies that contaminated soil is present, which is an exposure pathway.) These sources are the land application unit, landfill, wastepile, and surface impoundment. All input variables for the human exposure module are listed and described in Table D-21.

D.10.4 Outputs from the Human Exposure Module

Human exposure module outputs are written to the he.grf file. All exposure outputs except infant breastmilk exposures are three-dimensional arrays indexed on time, space, and age cohort. The spatial component may be x-y coordinate representing receptor locations as the centroid of a census block or farm represented by a set of x,y coordinates. Infant breast milk exposures are two-dimensional arrays on time and space. They apply to only one age cohort, infants, so there is no third dimension. Output variables are listed and described in Table D-22.

[6] For vegetables and fruits, the terms "exposed" and "protected" refer to whether the edible portion of the plant is exposed to the atmosphere.

Table D-21. Summary of Input Parameters for the Human Exposure Module

File	Input Parameter	Units	Description
he.ssf	*Bri_<cr#>*	m^3/d	Cohort-specific inhalation rate for the four child resident cohorts (Note: "<cr#>" is replaced with the actual cohort designation in the variables used by the human exposure module)
he.ssf	*Bri_r*	m^3/d	Inhalation rate for the adult resident.
he.ssf	*BW<cr#>*	kg	Cohort-specific body weight for each of the four child cohorts (Note: this parameter is not differentiated for farmer versus non-farmer receptor)
he.ssf	*BW_r*	kg	Body weight for adult receptors
he.ssf	*CRb_cf_<#>*	gWW/kg/d	Beef consumption rate for the three farmer child cohorts 2-4 (Note: "<#>" is replaced with the actual cohort number in the variables used by the human exposure module)
he.ssf	*CRb_af*	gWW/kg/d	Beef consumption rate for the adult farmer
he.ssf	*CRbm_cf_1*	mL/d	Breast milk ingestion rate for the farmer infant
he.ssf	*CRfr_cf_<#>*	gWW/kg/d	Exposed fruit consumption rate for the three farmer child cohorts 2-4 (Note: "<#>" is replaced with the actual cohort number in the variables used by the human exposure module)
he.ssf	*CRfr_f*	gWW/kg/d	Exposed fruit consumption rate for the adult farmer
he.ssf	*CRfr_cg_<#>*	gWW/kg/d	Exposed fruit consumption rate for the three gardener child cohorts 2-4 (Note: "<#>" is replaced with the actual cohort number in the variables used by the human exposure module)
he.ssf	*CRfr_g*	gWW/kg/d	Exposed fruit consumption rate for the adult gardener
he.ssf	*CRfs_c_<#>*	gWW/kg/d	Home-caught fish consumption rate for the three child cohorts 2-4 (Note: "<#>" is replaced with the actual cohort number in the variables used by the human exposure module)
he.ssf	*CRfs_a*	gWW/kg/d	Home-caught fish consumption rate for the adult
he.ssf	*CRl_cf_-#-*	gWW/kg/d	Exposed vegetables consumption rate for the three farmer child cohorts 2-4 (Note: "<#>" is replaced with the actual cohort number in the variables used by the human exposure module)
he.ssf	*CRl_f*	gWW/kg/d	Exposed vegetables consumption rate for the adult farmer

(continued)

Table D-21. (continued)

File	Input Parameter	Units	Description
he.ssf	*CRl_cg_<#>*	gWW/kg/d	Exposed vegetables consumption rate for the three gardener child cohorts 2-4 (Note: "<#>" is replaced with the actual cohort number in the variables used by the human exposure module)
he.ssf	*CRl_g*	gWW/kg/d	Exposed vegetables consumption rate for the adult gardener
he.ssf	*CRpfr_cf_<#>*	gWW/kg/d	Protected fruit consumption rate for the three farmer child cohorts 2-4 (Note: "<#>" is replaced with the actual cohort number in the variables used by the human exposure module)
he.ssf	*CRpfr_f*	gWW/kg/d	Protected fruit consumption rate for the adult farmer
he.ssf	*CRpfr_cg_<#>*	gWW/kg/d	Protected fruit consumption rate for the three gardener child cohorts 2-4 (Note: "<#>" is replaced with the actual cohort number in the variables used by the human exposure module)
he.ssf	*CRpfr_g*	gWW/kg/d	Protected fruit consumption rate for the adult gardener
he.ssf	*CRpl_cf_<#>*	gWW/kg/d	Protected vegetables consumption rate for the three farmer child cohorts 2-4 (Note: "<#>" is replaced with the actual cohort number in the variables used by the human exposure module)
he.ssf	*CRpl_f*	gWW/kg/d	Protected vegetables consumption rate for the adult farmer
he.ssf	*CRpl_cg_<#>*	gWW/kg/d	Protected vegetables consumption rate for the three gardener child cohorts 2-4 (Note: "<#>" is replaced with the actual cohort number in the variables used by the human exposure module)
he.ssf	*CRpl_g*	gWW/kg/d	Root vegetables consumption rate for the adult gardener
he.ssf	*CRr_cf_<#>*	gWW/kg/d	Root vegetables consumption rate for the three farmer child cohorts 2-4 (Note: "<#>" is replaced with the actual cohort number in the variables used by the human exposure module)
he.ssf	*CRr_f*	gWW/kg/d	Root vegetables consumption rate for the adult farmer
he.ssf	*CRr_cg_<#>*	gWW/kg/d	Root vegetables consumption rate for the three gardener child cohorts 2-4 (Note: "<#>" is replaced with the actual cohort number in the variables used by the human exposure module)
he.ssf	*CRr_g*	gWW/kg/d	Root vegetables consumption rate for the adult gardener

(continued)

Table D-21. (continued)

File	Input Parameter	Units	Description
he.ssf	*CRw_cr_<#>*	gWW/kg/d	Drinking water consumption rate for the four child cohorts 1-4 (Note: "<#>" is replaced with the actual cohort number in the variables used by the human exposure module)
he.ssf	*CRw_r*	gWW/kg/d	Drinking water consumption rate for the adult receptor
he.ssf	*CRs_cr_<#>*	gWW/kg/d	Incidental soil ingestion rate for the three child cohorts 2-4 (Note: "<#>" is replaced with the actual cohort number in the variables used by the human exposure module)
he.ssf	*CRs_r*	gWW/kg/d	Incidental soil ingestion rate for the adult receptor
he.ssf	*CRm_cf_<#>*	gWW/kg/d	Milk consumption rate for the three child farmer cohorts 2-4 (Note: "<#>" is replaced with the actual cohort number in the variables used by the human exposure module)
he.ssf	*CRm_af*	gWW/kg/d	Milk consumption rate for the adult farmer receptor
he.ssf	*DD*	cm	Water droplet diameter
he.ssf	*EFr*	d/yr	Exposure frequency (adult resident)
he.ssf	*F<dietary item>_<receptor category>*	Unitless	Fraction of <dietary item> consumed (e.g., exposed fruit, exposed vegetables, beef, drinking water) that is contaminated (for the "f" farmer or "g" gardener). (Note: in the actual variable names, <dietary item> and <receptor category> are replaced with acronyms referring to appropriate terms - e.g., "m" for milk and "f" for farmer, respectively)
he.ssf	*fbp*	Unitless	Fraction of whole blood that is plasma
he.ssf	*ffm*	Unitless	Fraction of mother's weight that is fat
he.ssf	*fmbm*	Unitless	Fraction of fat in maternal breastmilk
he.ssf	*fpm*	Unitless	Fraction of mother's weight that is plasma
he.ssf	*Fs*	Unitless	Fraction of contaminated soil
he.ssf	*FT<#>fish*	Unitless	Fraction of fish consumed that is T# (i.e., T3 or T4)
he.ssf	*Hn*	cm	Shower nozzle height
he.ssf	*Rshower*	L/min	Shower rate
he.ssf	*t_sb*	min	Time in shower and bathroom
he.ssf	*t_shower*	min	Shower time
he.ssf	*Vbath*	m^3	Bathroom volume

(continued)

Table D-21. (continued)

File	Input Parameter	Units	Description
he.ssf	*Vn*	cm/s	Terminal velocity of shower droplet
he.ssf	*VRbh*	L/min	Bathroom to house ventilation rate
he.ssf	*Vrsb*	L/min	Shower to bathroom ventilation rate
he.ssf	*Vshower*	m^3	Shower volume
sl.ssf	*FarmAquIndex*	NA	Index of aquifer that impacts farm or crop area
sl.ssf	*FarmLWSIndex*	NA	Local watershed indices associated with each farm
sl.ssf	*FarmLWSSubAreaFrac*	Fraction	Fraction of contribution of subarea to farm
sl.ssf	*FarmLWSSubAreaIndex*	NA	Index of contributing subarea in local watershed indices associated with each farm
sl.ssf	*FarmNumLWSSubArea*	NA	Contributing subarea in local watershed indices associated with each farm
sl.ssf	*FarmNumWSSub*	Unitless	Number of watersheds that impact farm or crop area
sl.ssf	*FarmWBNIndex*	NA	Index of WBN that impacts farm or crop area
sl.ssf	*FarmWBNRchIndex*	NA	Index of WBN reach that impacts farm or crop area
sl.ssf	*FarmWSSubFrac*	Unitless	Fraction of each watershed on farm
sl.ssf	*FarmWSSubIndex*	NA	Index of watersheds that impact farm or crop area
sl.ssf	*focS*	Mass fraction	Fraction organic carbon (soil)
sl.ssf	*HumRcpAirIndex*	NA	Index of air points that impact receptor
sl.ssf	*HumRcpAquIndex*	Unitless	Index of aquifer that impacts receptor
sl.ssf	*HumRcpAquWellIndex*	Unitless	Index of well that impacts receptor for the given aquifer
sl.ssf	*HumRcpLWSIndex*	NA	Local watershed index for each human receptor
sl.ssf	*HumRcpLWSSubAreaInde*	NA	Local watershed subarea index for each human receptor
sl.ssf	*HumRcpPh*	pH units	Average shower water pH
sl.ssf	*HumRcpTemp*	° Celsius	Typical shower temperature
sl.ssf	*HumRcpWSSubIndex*	NA	Index of watershed that impacts receptor
sl.ssf	*NumFarm*	Unitless	Number of farm or crop areas
sl.ssf	*NumHumRcp*	Unitless	Number of human receptor points at a site
sl.ssf	*NumWBN*	Unitless	Number of waterbody networks
sl.ssf	*NyrMax*	Years	Maximum model simulation time

(continued)

Table D-21. (continued)

File	Input Parameter	Units	Description
sl.ssf	*TermFrac*	Fraction	Peak output fraction for simulation termination
sl.ssf	*WBNFishableRchIndex*	Unitless	Index of reaches that are fishable
sl.ssf	*WBNNumFishableRch*	Unitless	Number of fishable reaches
cp.ssf	*ChemBreast MilkExp*	Unitless	Causes breast milk exposure? (1=yes, 0=no)
cp.ssf	*ChemCSFfood*	$(mg/kg\text{-}d)^{-1}$	Cancer slope factor (food ingestion)
cp.ssf	*ChemCSFinhal*	$(mg/kg\text{-}d)^{-1}$	Cancer slope factor (inhalation)
cp.ssf	*ChemCSFwater*	$(mg/kg\text{-}d)^{-1}$	Cancer slope factor (drinking water ingestion)
cp.ssf	*ChemRfC*	mg/m^3	Reference concentration (inhalation)
cp.ssf	*ChemRfDfish*	mg/kg-d	Reference dose (fish ingestion)
cp.ssf	*ChemRfDfood*	mg/kg-d	Reference dose (food ingestion)
cp.ssf	*ChemRfDwater*	mg/kg-d	Reference dose (drinking water ingestion)
cp.ssf	*Chemfai*	Fraction	Fraction of ingested contaminant by the infant which is absorbed
cp.ssf	*ChemFam*	Fraction	Fraction of contaminant ingested by mother that is absorbed
cp.ssf	*ChemFbl*	Fraction	Fraction of contaminant in whole blood compartment
cp.ssf	*ChemFf*	Fraction	Fraction of contaminant stored in maternal fat
cp.ssf	*Chemkpm*	Unitless	Concentration proportionality constant between plasma and breast milk aqueous phase
cp.ssf	*ChemKrbc*	Unitless	Concentration proportionality constant between red blood cells and plasma
cp.ssf	*Chemt_halfb*	d	Biological half-life of chemical in lactating women
cp.ssf	*ChemADiff*	cm^2/s	Air diffusion coefficient
cp.ssf	*ChemHLC*	$(atm\ m^3)/mol$	Henry's law constant
cp.ssf	*ChemWDiff*	cm^2/s	Water diffusion coefficient
af.ssf	*CT3filet*	mg/kg WW	Chemical concentration in trophic level 3 fish filet
af.ssf	*CT4filet*	mg/kg WW	Chemical concentration in trophic level 4 fish filet
ff.ssf	*CTssAve_farm*	µg/g	Chemical concentration in surficial soil averaged over farm area

(continued)

Table D-21. (continued)

File	Input Parameter	Units	Description
ff.ssf	*CtssAve_farmYR*	Unitless	Time series of years corresponding to this variable
ff.ssf	*CTssAve_farmNY*	Unitless	Number of years in the time series corresponding to this variable
ff.ssf	*Abeef_farm*	mg/kg WW	Modeled beef concentration
ff.ssf	*Abeef_farmYR*	Unitless	Time series of years corresponding to this variable
ff.ssf	*Abeef_farmNY*	Unitless	Number of years in the time series corresponding to this variable
ff.ssf	*Amilk_farm*	mg/kg WW	Modeled milk concentration
ff.ssf	*Amilk_farmYR*	Unitless	Time series of years corresponding to this variable
ff.ssf	*Amilk_farmNY*	Unitless	Number of years in the time series corresponding to this variable
ff.ssf	*P<vegetable or fruit type>_farm*	mg/kg WW	Modeled concentration for specific fruit and vegetable categories (e.g., <vegetable or fruit type> would be replaced by: “exveg”, “proveg” or “root” for exposed vegetables, protected vegetables or root vegetables, respectively) raised on farms
ff.ssf	*P<vegetable or fruittype>_farmYR*	Unitless	Time series of years corresponding to this variable
ff.ssf	*P<vegetable or fruittype>_farmNY*	Unitless	Number of years in the time series corresponding to this variable
ff.ssf	*P<vegetable or fruittype>_garden*	mg/kg WW	Modeled concentration for specific fruit and vegetable categories (e.g., <vegetable or fruit type> would be replaced by: “exveg”, “proveg” or “root” for exposed vegetables, protected vegetables or root vegetables, respectively) raised in home gardens
ff.ssf	*P<vegetable or fruittype>_gardenYR*	Unitless	Time series of years corresponding to this variable
ff.ssf	*P<vegetable or fruittype>_gardenNY*	Unitless	Number of years in the time series corresponding to this variable
sr.ssf	*SrcSoil*	NA	Flag for soil presence
sr.ssf	*CTss*	µg/g	Soil concentration (annual average, all subareas)
sr.ssf	*CTssYR*	Unitless	Time series of years corresponding to this variable
sr.ssf	*CTssNY*	Unitless	Number of years in the time series corresponding to this variable

(continued)

Table D-21. (continued)

File	Input Parameter	Units	Description
ar.ssf	*PM10*	µg/m^3	Concentration of particles = 10 microns
ar.ssf	*PM10YR*	Unitless	Time series of years corresponding to this variable
ar.ssf	*PM10NY*	Unitless	Number of years in the time series corresponding to this variable
ar.ssf	*CVap*	µg/m^3	Concentration of chemical in air vapor
ar.ssf	*CVapYR*	Unitless	Time series of years corresponding to this variable
ar.ssf	*CVapNY*	Unitless	Number of years in the time series corresponding to this variable
ws.ssf	*CTssR*	µg/g	Surface soil concentrations for modeled watersheds
ws.ssf	*CTssYR*	Unitless	Time series of years corresponding to this variable
ws.ssf	*CTssNY*	Unitless	Number of years in the time series corresponding to this variable

NA = not applicable

Table D-22. Summary of Output Parameters for the Human Exposure Module

File	Input Parameter	Units	Description
he.grf	*IngBM<pathway>H*	mg/kg-d	Chemical- and pathway-specific average daily dose for the nonfarmer infant resulting from breast milk ingestion. (Note: "<pathway>" denotes the actual pathway name in the variables generated by the human exposure module.)
he.grf	*IngBM<pathway>HYR*	Unitless	Time series of years corresponding to this variable.
he.grf	*IngBM<pathway>HNY*	Unitless	Number of years in the time series corresponding to this variable
he.grf	*IngBM<pathway>F*	mg/kg-d	Chemical- and pathway-specific average daily dose for the farmer infant resulting from breast milk ingestion (Note: "<pathway>" denotes the actual pathway name in the variables generated by the human exposure module.)
he.grf	*IngBM<pathway>FYR*	Unitless	Time series of years corresponding to this variable
he.grf	*IngBM<pathway>FNY*	Unitless	Number of years in the time series corresponding to this variable
he.grf	*Cambient_Farm*	mg/m^3	Farm area-specific modeled ambient air concentration used in evaluating inhalation risk; separate estimates are generated for each modeled year
he.grf	*Cambient_FarmYR*	Unitless	Time series of years corresponding to this variable
he.grf	*Cambient_FarmNY*	Unitless	Number of years in the time series corresponding to this variable
he.grf	*Cambient_HumRcp*	mg/m^3	Residential location-specific modeled ambient air concentration used in evaluating inhalation risk; separate estimates are generated for each modeled year
he.grf	*Cambient_HumRcpYR*	Unitless	Time series of years corresponding to this variable
he.grf	*Cambient_HumRcpNY*	Unitless	Number of years in the time series corresponding to this variable
he.grf	*Csb_Farm*	mg/m^3	Farm area-specific modeled shower/bath air concentration used in evaluating inhalation risk; separate estimates are generated for each modeled year
he.grf	*Csb_FarmYR*	Unitless	Time series of years corresponding to this variable
he.grf	*Csb_FarmNY*	Unitless	Number of years in the time series corresponding to this variable
he.grf	*Csb_HumRcp*	mg/m^3	Residential location-specific modeled shower/bath air concentration used in evaluating inhalation risk; separate estimates are generated for each modeled year
he.grf	*Csb_HumRcpYR*	Unitless	Time series of years corresponding to this variable

(continued)

Table D-22. (continued)

File	Input Parameter	Units	Description
he.grf	*Csb_HumRcpNY*	Unitless	Number of years in the time series corresponding to this variable
he.grf	*Ing<pathway>_Farm*	mg/kg-d	Chemical- and pathway- specific average daily dose for the farmer resulting from ingestion of the dietary item identified as the "pathway" by the variable (Note: "<pathway>" denotes the actual pathway name in the variables generated by the human exposure module.)
he.grf	*Ing<pathway>_FarmYR*	Unitless	Time series of years corresponding to this variable
he.grf	*Ing<pathway>_FarmNY*	Unitless	Number of years in the time series corresponding to this variable
he.grf	*Ing<pathway>_HumRcp*	mg/kg-d	Chemical- and pathway- specific average daily dose for the non-farmer resulting from ingestion of the dietary item identified as the "pathway" by the variable (Note: "<pathway>" denotes the actual pathway name in the variables generated by the human exposure module.)
he.grf	*Ing<pathway>_HumRcp YR*	Unitless	Time series of years corresponding to this variable
he.grf	*Ing<pathway>_HumRcp NY*	Unitless	Number of years in the time series corresponding to this variable

D.11 Human Risk Module

The human risk module considers two basic human receptor types are considered: residential receptors (residents and home gardeners) and 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. This results in eight categories of human receptors: resident, resident gardener, resident fisher, resident gardener fisher, beef farmer fisher, dairy farmer fisher, beef farmer, and dairy farmer.

The eight receptor categories were developed in consideration of exposure pathways; for example, a residential resident is a receptor that is exposed only to the baseline exposure pathways, i.e., inhalation via air and shower and ingestion via soil and water. A resident gardener is a resident exposed through these exposure pathways plus ingestion of homegrown produce.

The human exposure module's output has eight-receptor resolution; the human risk module calculates risks and/or HQs for each of these eight receptor categories but then aggregates these eight categories into four[7] composite receptor categories: resident, resident gardener, fisher, and farmer, for purposes of developing the cumulative population[8] frequency histograms and critical years. For example, the composite "fisher" receptor population consists of subpopulations from the resident fisher, resident gardener fisher, beef farmer fisher, and dairy farmer fisher receptor categories. Similarly, beef farmers and dairy farmers are aggregated into a single, composite "farmer." For every receptor type (four or eight), five age cohort classes are considered[9]: Child 1 (0 to 1 year old), Child 2 (1 to 5 years old), Child 3 (6 to 11 years old), Child 4 (12 to 19 years old), and Adult (greater than 19 years old). For the Child 1 (infant) cohort, only the breast milk pathway applies.[10] The margin of exposure [MOE] (mg/kg-d) for the infant breast milk pathway is analogous to HQ for infant breast milk exposure.

D.11.1 Functionality

The human risk module processes modeled outputs from the human exposure module (human receptor exposure estimates) and performs three major functions using these data:

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[7] The 3MRA Exit Level Processor I (ELP I) preserves this receptor resolution, but also aggregates these four receptors into a fifth, "all receptors" category.

[8] Site-specific receptor populations were identified as part of the HWIR99 data collection activities and are specified by receptor category, exposure area (farm or census block), and distance ring. See US EPA (1999c) for discussion of the methodology.

[9] For purposes of storage efficiency, the ELP I combines the Child 2 and 3 cohort classes as output by the human risk module into a single composite cohort class (ages 1 to 11). Child 4 is also combined with the adult cohort class by the ELP I.

[10] For HWIR99, the infant breast milk pathway is evaluated only for a single chemical, the dioxin species 2,3,7,8 -TCDD TEQ [CAS No. 1746-01-6]. (That is, the logical flag *ChemBreastMilkExp* will be set to "true" only for this chemical in the chemical properties input file, cp.ssf.)

1. *It calculates risk and/or hazard quotient for each receptor, cohort, exposure pathway, exposure area, and year.* Whether risk, HQ, or both are calculated is determined as a function of the chemical under consideration. For carcinogenic chemicals, risks are calculated as average risks over a 9-year exposure duration. For noncarcinogens, HQs are calculated as a 1-year average.

2. *It constructs cumulative frequency histograms that quantify the distributions of receptor/cohort-specific populations among different levels of risk and/or HQ for each exposure pathway and aggregation of pathways*[11] *and year*. The populations consist of individual receptor/cohorts residing at the various exposure areas (residential areas and farms).

3. *It determines and outputs that critical year during which the maximum cumulative risk and/or HQ occurs across the population for each receptor/cohort combination and for each exposure pathway and pathway aggregation.*

These functions are performed three times, once for each of three radial distances outward from the centroid of the waste management unit. The purpose of distance-specific results is to assess the sensitivity of risk results to distance from the chemical source.

These functions are performed by the human risk module by a series of nested loops. Figures 3-17a through 3-17c illustrate the general looping structure used for a given radial distance. These illustrations are intended only to facilitate overall understanding of the module; the implementing computer code is significantly different to optimize performance.

D.11.2 Assumptions and Limitations

Calculations performed by the human risk module reflect a number of assumptions and/or limitations including:

- *Risks are calculated for a 2-km radius study area.* EPA assumed that all significant exposure and risk/HQ to human receptors occurs within 2 km of the source boundary based on the types of waste management unit sources currently in the 3MRA model.

- *Human receptors are stationary.* EPA assumed that human receptors both reside and work at the receptor location identified for them during site characterization. (Farmer receptors are on farms, and residential receptors are assumed to be at the centroid of census blocks within radial distance rings.) This assumption may overestimate or underestimate exposure, because it is possible that individuals

[11] Aggregation of risks occurring simultaneously over multiple pathways is the essence of multipathway risk assessment. For example, if a receptor is exposed to chemicals from both ingestion of contaminated groundwater and ingestion of contaminated fish, then it is appropriate to estimate the cumulative risk that is incurred across these pathways. In some instances, it is appropriate to aggregate risk across portals of entry (i.e., ingestion and inhalation).

may reside at the identified location within the study area but either commute to work outside of the study area or commute to more or less highly contaminated areas within the study area.

- *Incremental risk is considered.* No provision is made for considering background exposures and their risks for the purpose of generating total risk estimates.

- *Risk and HQ estimates are aggregated for certain receptors.* As mentioned, the four receptors considered—resident, residential gardener, farmer, and fisher—are fewer in number than the number of receptor categories output by the Human exposure module. Risks are aggregated for certain receptors to maintain output storage requirements at reasonable levels. Such aggregation results in some loss in risk resolution. For example, the risks specific to farmers who drink contaminated milk but do not ingest contaminated beef will not be available.

- *Lifetime and exposure duration for carcinogens.* For carcinogenic risk calculations, receptors are assumed to live 76.5 years. Of this lifetime, the exposure duration is assumed to be 9 years.

- *Carcinogenic risks are proportionately disaggregated from lifetime exposure to the assumed exposure duration.* Incurred risks are assumed to be lifetime risks that are reduced in direct proportion to the fraction of a lifetime actually exposed, i.e., 350 of 365 days per year (15 days away per year) for each year of exposure duration.

- *Synergistic or antagonistic effects among multiple chemicals and individual chemical speciation on risk estimates are not considered.* The human risk module is executed by the 3MRA system with a system-level chemical loop so that only one chemical is considered at any single execution. Chemicals are considered to be independent.

- *Cancer slope factors do not vary with cohort age.* Age-specific differences in exposure responses are not available and consequently are not considered.

- *Maximum HQ estimates are conservatively based on a single year of exposure.* Unlike carcinogenic risk estimates, which use a moving average over multiyear exposure periods (as discussed in the next section), HQ estimates treat each year independently, i.e., their time series reflects 1-year average values. Thus, a single high year of maximum exposure would not be "diluted" by a multiyear averaging period. This is a protective approach.

- *If any residents in a census block group ingest ground water,* all *residents in the component census blocks are assumed to ingest ground water*. The census data report the number of households within a census block group that are served by ground water wells. However, this information is available only at the census block group level, and it is not possible to determine from census data alone

whether individual census blocks within a block group with wells have wells or not. The human risk module loops over census blocks when considering residential exposure areas. Consequently, the actual fraction of residents on wells for any individual residential exposure area is uncertain. To resolve this lack of information, the protective assumption is made that, if any residents in the block group containing the residential exposure area (or census block) under consideration are on wells, then all residents in the exposure area are on wells. That is not to say, of course, that all well water is contaminated. Only those wells lying within the ground water plume from the source are potentially contaminated.

D.11.3 Inputs for the Human Risk Module

The human risk module receives inputs from its module-specific input file, hr.ssf, the generic site layout file (sl.ssf), the generic chemical properties file (cp.ssf), and modeled inputs from the human exposure module's output file, he.grf. Input variables are listed and described in Table D-23.

D.11.4 Outputs from the Human Risk Module

Human risk module outputs are written to hr.grf, and include all risk estimates necessary to determine risk by distance from the source, exposure pathway, exposure route, receptor type, and age cohort as well as total and maximum risk estimates. Output variables are listed and described in Table D-24.

Table D-23. Summary of Inputs for the Human Risk Module

File	Input Parameter	Units	Description
hr.ssf	*LifeTime*	years	Human lifetime used in carcinogenic risk calculation
hr.ssf	*ExDur_Car_Farm*	years	Exposure duration used for modeling carcinogenic risk for all farming receptor populations
hr.ssf	*ExDur_Car_Block*	years	Exposure duration used for modeling carcinogenic risk for all residential receptor populations
hr.ssf	*ExDur_NCar_Farm*	years	Exposure duration used for modeling noncarcinogenic HQ/MOE for all farming receptors.
hr.ssf	*ExDur_NCar_Block*	years	Exposure duration used for modeling noncarcinogenic HQ/MOE for all residential receptors.
hr.ssf	*RegPercentile*	percent	Regulatory criterion used in calculating total risk incurred by a given percentage of the population. *RegPercentile* is the percentage.
hr.ssf	*DoExposed*	unitless	Logical flag indicating whether the output CDFs comprise (1) only actually exposed receptors (true), or (2) all receptors (false).
sl.ssf	*BinRange_Min_C*	unitless	Carcinogenic risk values used to define the minimum value for each of the carcinogenic risk bins.
sl.ssf	*BinRange_Min_NC*	unitless	Noncarcinogenic HQ values used to define the minimum value for each of the noncarcinogenic HQ bins.
sl.ssf	*NumBinC*	unitless	Number of bins used in reporting cancer risk (i.e., number of bins used to define the cumulative risk distribution)
sl.ssf	*NumBinNC*	unitless	Number of bins used in reporting noncancer HQs (i.e., number of bins used to define the cumulative HQ distribution)
sl.ssf	*NumHumRcp*	unitless	Number of residential locations (i.e., number of human receptor points excluding farms)
sl.ssf	*NumFarm*	unitless	Number of beef and/or dairy farms
sl.ssf	*NumRing*	unitless	Number of concentric rings used to subdivide the site for purposes of estimating risk or HQ/MOE distributions conditional on distance from the source.
sl.ssf	*FarmPopulation*	unitless	Number of farmers associated with each of the farms/crop areas identified for a given site. These population estimates are farmer-, type-, and cohort-specific.
sl.ssf	*HumRcpPopulation*	unitless	Number of residents (nonfarmers) associated with each of the residential locations identified for a given site. These population estimates are receptor population- and cohort-specific.

(continued)

Table D-23. (continued)

File	Input Parameter	Units	Description
sl.ssf	*RingFarmFrac*	fraction	The fraction of a given farm that is located within a given ring. This variable is used to allocate farm population into different rings for purposes of ring-specific risk or HQ/MOE estimates when the farm occurs in multiple rings.
cp.ssf	*ChemC_Add*	unitless	Identifies whether carcinogenic risk for a given chemical can be added across routes.
cp.ssf	*ChemNC_Add*	unitless	Identifies whether noncarcinogenic HQ/MOEs for a given chemical can be added across routes.
cp.ssf	*ChemBreastMilkExp*	unitless	Identifies whether a given chemical should be assessed for breast milk exposure (i.e., does it bioconcentrate in breast milk)
cp.ssf	*ChemCSFinhal*	$(mg/kg\text{-}d)^{-1}$	Inhalation cancer slope factor
cp.ssf	*ChemCSFfood*	$(mg/kg\text{-}d)^{-1}$	Cancer slope factor used to evaluate dietary exposure and incidental soil ingestion (excluding drinking water)
cp.ssf	*ChemCSFwater*	$(mg/kg\text{-}d)^{-1}$	Cancer slope factor used to evaluate ingestion of drinking water
cp.ssf	*ChemRFC*	mg/m^3	Inhalation reference concentration
cp.ssf	*ChemRFDfood*	mg/kg-d	Reference dose used to evaluate dietary exposure and incidental soil ingestion (excluding drinking water and fish)
cp.ssf	*ChemRFDwater*	mg/kg-d	Reference dose used to evaluate ingestion of drinking water
cp.ssf	*ChemRFDfish*	mg/kg-d	Reference dose used to evaluate dietary exposure to fish
cp.ssf	*ChemBM*	mg/kg-d	Background-drived breast milk exposure value used in generating margin of exposure estimate for breast milk consumption in infants
he.grf	*IngBM<pathway>H*	mg/kg-d	Chemical- and pathway- specific average daily dose for the nonfarmer infant resulting from breast milk ingestion. (Note: "<pathway>" denotes the actual pathway name in the variables generated by the human exposure module.)
he.grf	*IngBM<pathway>HYR*	unitless	Time series of years corresponding to this variable.
he.grf	*IngBM<pathway>HNY*	unitless	Number of years in the time series corresponding to this variable.
he.grf	*IngBM<pathway>F*	mg/kg-d	Chemical- and pathway- specific average daily dose for the farmer infant resulting from breast milk ingestion. (Note: "<pathway>" denotes the actual pathway name in the variables generated by the human exposure module.)
he.grf	*IngBM<pathway>FYR*	unitless	Time series of years corresponding to this variable.

(continued)

Table D-23. (continued)

File	Input Parameter	Units	Description
he.grf	*IngBM<pathway>FNY*	unitless	Number of years in the time series corresponding to this variable.
he.grf	*Cambient_Farm*	mg/m^3	Farm-specific modeled ambient air concentration used in evaluating inhalation risk. Separate estimates are generated for each modeled year.
he.grf	*Cambient_FarmYR*	unitless	Time series of years corresponding to this variable.
he.grf	*Cambient_FarmNY*	unitless	Number of years in the time series corresponding to this variable.

NA = not applicable

Table D-24. Summary of Outputs from the Human Risk Module

File	Code	Units	Description
hr.grf	*Risk_1_Index; Risk_2_Index; Risk_3_Index*	unitless	Number of exposure pathway-specific (Risk_1_Index), exposure route-specific (Risk_2_Index), or total (Risk_3_Index) carcinogenic risk estimates generated for each receptor population/age cohort combination. Separate exposure pathway-, exposure route-, and total risk estimates are generated for each ring modeled. Risk results for each of these three categories are only reported for Tcrit (i.e., for the maximum risk year) and not for all modeled years.
hr.grf	*HQ_1_Index; HQ_2_Index; HQ_3_Index*	unitless	Number of exposure pathway-specific (HQ_1_Index), exposure route-specific (HQ_2_Index), or total (HQ_3_Index) non-carcinogenic HQ estimates generated for each receptor population/age cohort/chemical combination. Separate exposure pathway-, exposure route-, and total HQ estimates are generated for each ring modeled. HQ results for each of these three categories are only reported for Tcrit (i.e., for the maximum risk year) and not for all modeled years.
hr.grf	*Risk_1; Risk_2; Risk_3*	unitless	CDFs of population in risk bins for exposure pathway-specific (Risk_1), exposure route-specific (Risk_2), and total (Risk_3) carcinogenic risk. Separate CDFs are generated for each receptor/cohort/ring combination. These estimates are only reported for Tcrit.
hr.grf	*HQ_1; HQ_2; HQ_3*	unitless	CDFs of population in HQ bins for exposure pathway-specific (HQ_1), exposure route-specific (HQ_2) and total (HQ_3) non-carcinogenic HQ estimate. Separate CDFs are generated for each receptor population/cohort/ring combination. These estimates are only reported for Tcrit.
hr.grf	*Risk_1_TcrIndex; Risk_2_TcrIndex; Risk_3_TcrIndex*	years	Tcrit (critical year or maximum risk year) for carcinogenic risk. Separate Tcrits are identified for exposure pathways (Risk_1_TcrIndex), exposure routes (Risk_2_TcrIndex), and for total risk (Risk_3_TcrIndex).
hr.grf	*Risk_1_RingIndex; Risk_2_RingIndex; Risk_3_RingIndex*	unitless	The specific ring associated with each of the Tcrit values identified through the Risk_#_TcrIndex variables (i.e., Risk_1_RingIndex, Risk_2_RingIndex, and Risk_3_RingIndex).
hr.grf	*Risk_1_PathIndex; Risk_2_PathIndex; Risk_3_PathIndex*	unitless	The specific exposure pathway associated with each of the Tcrit values identified through the Risk_#_TcrIndex variables (i.e., Risk_1_RingIndex, Risk_2_RingIndex, and Risk_3_RingIndex).
hr.grf	*HQ_1_TcrIndex; HQ_2_TcrIndex; HQ_3_TcrIndex*	years	Tcrit (critical year or maximum HQ year) for noncarcinogenic HQ. Separate Tcrit values are identified for exposure pathways (HQ_1_TcrIndex), exposure routes (HQ_2_TcrIndex), and for total HQ (HQ_3_TcrIndex).
hr.grf	*HQ_1_RingIndex; HQ_2_RingIndex; HQ_3_RingIndex*	unitless	The specific ring associated with each of the Tcrit values identified through the HQ_#_TcrIndex variables (i.e., HQ_1_RingIndex, HQ_2_RingIndex, and HQ_3_RingIndex).
hr.grf	*HQ_1_PathIndex; HQ_2_PathIndex; HQ_3_PathIndex*	unitless	The specific exposure pathway associated with each of the Tcrit values identified through the HQ_#_TcrIndex variables (i.e., HQ_1_RingIndex, HQ_2_RingIndex, and HQ_3_RingIndex).

D.12 Ecological Exposure Module

The ecological exposure (EcoEx) 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 EcoEx module calculates exposures for each receptor home range placed within a terrestrial or freshwater aquatic habitat (as defined in the site layout). Thus, exposure is a function of: (1) the home range (or portion, thereof) to which the receptor is assigned; (2) the spatial boundaries of the 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 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). Supporting detail about the background and implementation of the model is available in U.S. EPA (1999l).

D.12.1 Functionality

The major computational functions performed by the ecological exposure module can be summarized as follows:

- *Time series management*. The EcoEx module determines the overall duration of the time period to be simulated (including concentration data from discontinuous time periods) and identifies the individual years within the overall duration that will be simulated.

- *Module loops over the time series, through habitats and receptors*. The EcoEx module has three basic loops: (1) over the time series, (2) over each habitat delineated at the site, and (3) over the mammalian, avian, and selected herpetofauna receptors assigned to each habitat.

- *Calculation of time series exposures from time series media and food concentrations*. This is the fundamental structure of the EcoEx module, namely, to develop exposure concentrations for each year of the simulation that include all relevant receptors, food items, and media. These exposure concentrations are spatially explicit with regard to the home range for each ecological receptor.

The major calculation steps performed by the ecological exposure module that are required to calculate an applied dose may be summarized as follows:

- Select receptor of interest.
- Get media concentrations from TerFW module, SW module, and SR module.
- Calculate average media concentrations to which receptor is exposed.
- Construct diet for receptor of interest (i.e., composition and preferences).
- Get plant and prey concentrations for dietary items from TerFW.
- Sum intake from media and food sources.

- Calculate potential applied dose by adjusting for body weight.
- Calculate applied dose by prorating dose by habitat / home range ratio.

D.12.2 Assumptions and Limitations

The exposure characterization methodology used in the ecological exposure module reflects a number of assumptions and/or limitations, which are listed below.

D.12.2.1 Assumptions.

- *Study area is bounded at 2 km.* EPA assumed that significant exposures to source-related contaminants do not occur for ecological receptors that are beyond 2 km of the source. Consequently, exposures are not evaluated for receptors outside of the study area, measured from the edge of the source to a point 2 km away.

- *All areas delineated as habitat support wildlife.* EPA assumed that habitats delineated at each site are capable of sustaining a variety of wildlife. Because the predator-prey interactions for each habitat are represented by a simple food web, we assumed each habitat to be of sufficient quality to support multiple trophic levels and at least one reproducing pair of upper trophic level predators. Hence, exposure estimates reflect essentially free access to any of the food items suggested in the database on ecological exposure factors.

- *There are no other chemical stressors in the study area.* Because this is a site-based (rather than site-specific) assessment we assumed that ecological receptors were not subjected to other stressors within the study area. Background concentrations of constituents were not considered in developing exposure estimates, nor were other potential nonchemical stressors such as habitat fragmentation.

- *No less than 10 percent of the diet is attributed to the study area.* In many instances, the home range for a given receptor exceeds the size of the habitat. In general we assumed that the percent of the home range that “fits” into the habitat is a suitable surrogate with which to scale exposures. However, the purpose of this analysis is to determine acceptable waste concentrations assuming that suitable portions of the study area (e.g., forests) would be used as habitat by wildlife. Therefore, we assumed that no less than 10 percent of the diet originated from the study area, even if the fraction of the home range inside the habitat fell below 10 percent.

- *Spatial averaging of exposures is defined by habitat and home range.* For this site-based assessment of representative habitats, we assumed that a reasonable approach to define the spatial extent of exposure for each receptor was to place the home range within the habitat boundaries. If the home range was larger than the habitat (i.e., extends beyond AOI) the exposure was averaged across the

habitat and then prorated. However, alternative approaches were considered, including the calculation of exposure point concentrations based on a random walk across various habitats.

D.12.2.2 <u>Limitations</u>.

Plant categories were defined by analogy. Vegetation categories relevant to wildlife were extrapolated from the plant categories defined for use in the Farm Food Chain (FFC) module. The cross reference for vegetative categories consumed by wildlife is presented in the Terrestrial Food Web module documentation.

Annual average concentrations define exposure. The exposure profiles generated with the EcoEx module are based on the average annual concentrations in food items and media. Consequently, concentration spikes due to episodic events (e.g., rain storms) or elevated source releases following waste additions are not evaluated. In addition the annual average approach does not capture elevated exposures during critical life stages.

Exposures are predicted only for adult animals. Because concentrations are annualized, the module predicts exposures only for adult animals; intrayear contaminant exposures to juveniles, often with very different dietary preferences, are not predicted.

Dietary preferences remain constant over the year. The EcoEx module constructs the dietary preferences for each receptor based on dietary data covering one or more seasons. Some of the seasonal variability in the diet is captured indirectly by the hierarchical algorithm used to determine the dietary preferences. However, the algorithm is implemented on data across multiple seasons and, therefore, does not necessarily reflect seasonal differences.

Exposure estimates reflect a single home range setting. The EcoEx module calculates the applied doses to receptors for a single random placement of four home range sizes.[12] As a result, the four home ranges in the site layout may not reflect the spatial variability in exposure patterns, particularly for large habitats (i.e., habitats that cover substantially greater areas than most of the home ranges).

D.12.3 Inputs for the Ecological Exposure Module

The concentration inputs required by the EcoEx module are provided by the terrestrial food web module (TerFW), the aquatic food web module (AqFW), the surface water module

[12] As described in U.S. EPA (1999n), each receptor is assigned to one of four discrete home range sizes, depending on the receptor-specific home range. The four home ranges are spatially linked in that the ranges overlap in a manner that reflects the dietary preferences of the predator species.

(SW), and the surface impoundment module (a common source output file). These inputs include:

Terrestrial Food Web (TF.GRF)

- Spatially averaged surficial soil concentration by home range
- Spatially averaged concentration in soil invertebrates by home range
- Spatially averaged concentration in various plant types by home range
- Minimum and maximum concentrations in various categories of vertebrates across the habitat (e.g., small mammals, small birds, omnivores)

Aquatic Food Web (AF.GRF)

- Average, reach-specific concentration in aquatic (water column) invertebrates
- Average, reach-specific concentration in benthic invertebrates
- Average, reach-specific concentration in aquatic macrophytes
- Average, reach-specific concentration in trophic level 3 (T3) fish
- Average, reach-specific concentration in trophic level 4 (T4) fish

Surface Water (SW.GRF)

- Average, reach-specific concentration in sediment
- Average, reach-specific concentration in surface water

Surface Impoundment (SR.GRF)

- Average concentration in surface impoundment water

The ecological exposure module receives inputs from its module-specific input file, ee.ssf, the generic site layout file (sl.ssf), and modeled inputs from the following other modules: terrestrial food web module (tf.grf), aquatic food web module (af.grf), surface water module (sw.grf), and those source modules outputting (to a common grf file, sr.grf) a “true” for the surface water logical flag, *SrcH2O*. In the HWIR application, these sources are the land application unit, landfill, wastepile, and surface impoundment; currently, only the surface impoundment reports true for this flag. Input variables are listed and described in Table D-25.

D.12.3 Outputs from the Ecological Exposure Module

The ecological exposure module outputs are written to the ee.grf file. All ecological exposure outputs are 3-dimensional arrays indexed on time, habitat, and receptor. Output variables are listed and described in Table D-26.

Table D-25. Summary of Input Parameters for the Ecological Exposure Module

File	Code	Units	Description
ee.ssf	*BodyWt_rec*	kg	Body weight of each receptor.
ee.ssf	*CR_food*	kg/d	Consumption rate of food items for each receptor.
ee.ssf	*CR_water*	L/d	Consumption rate of water for each receptor.
ee.ssf	*CRfrac_sed*	mass fraction	Consumption rate of sediment for each receptor.
ee.ssf	*CRfrac_soil*	mass fraction	Consumption rate of surficial soil for each receptor.
ee.ssf	*HabitatIndex*	unitless	Index of habitat types.
ee.ssf	*HabitatType*	NA	Description of habitat types.
ee.ssf	*MaxPreyPref_HabRange*	unitless	Maximum dietary preference for items found in a habitat range.
ee.ssf	*MinPreyPref_HabRange*	unitless	Minimum dietary preference for items found in a habitat range.
ee.ssf	*NumHabitat*	unitless	Number of habitat types represented.
ee.ssf	*NumPrey*	unitless	Number of potential prey items.
ee.ssf	*PreyIndex*	unitless	Numerical index of potential prey items.
ee.ssf	*PreyType*	NA	Description of each prey item.
sl.ssf	*HabArea*	m^2	Area of habitat.
sl.ssf	*HabIndex*	unitless	Index of habitat type.
sl.ssf	*HabNumRange*	unitless	Number of home ranges per habitat.
sl.ssf	*HabNumWBNRch*	unitless	Number of WBN reaches that impact each habitat range.
sl.ssf	*HabRangeAreaFrac*	fraction	Fraction of total home range area that falls within each habitat.
sl.ssf	*HabRangeFishWBNIndex*	unitless	Index of WBN containing fishable reaches that impact each habitat range.
sl.ssf	*HabRangeNumSISrc*	unitless	Number of surface impoundments that intersect each habitat range.
sl.ssf	*HabRangeNumWBNRch*	unitless	Number of WBN reaches found within each habitat range.
sl.ssf	*HabRangeNumWSSub*	unitless	Number of watersheds that impact each habitat range.
sl.ssf	*HabRangeRecIndex*	unitless	Receptor index associated with each habitat range.
sl.ssf	*HabRangeWBNIndex*	unitless	Index of WBN that impacts each habitat range.
sl.ssf	*HabRangeWBNRchIndex*	unitless	Index of WBN reaches that impact each habitat range.
sl.ssf	*HabRangeWSSubIndex*	unitless	Index of watershed that impacts each habitat range.
sl.ssf	*HabType*	NA	Type of representative habitat.

(continued)

Table D-25. (continued)

File	Code	Units	Description
sl.ssf	*HabWBNIndex*	unitless	Index of WBN that impacts each habitat.
sl.ssf	*HabWBNRchFrac*	unitless	Fraction of habitat range impacted by each reach.
sl.ssf	*HabWBNRchIndex*	unitless	Index of WBN reaches that impact each habitat.
sl.ssf	*HRangeFishWBNRchIndex*	unitless	Index of fishable reaches that impact each habitat range.
sl.ssf	*HRangeNumFishWBNRch*	unitless	Number of fishable reaches that cross each habitat range.
sl.ssf	*NumHab*	unitless	Number of habitats selected for site simulation.
sl.ssf	*NumReceptor*	unitless	Complete receptor list across all habitat types.
sl.ssf	*NumWBN*	unitless	Number of waterbody networks.
sl.ssf	*NumWSSub*	unitless	Number of watershed sub basins.
sl.ssf	*ReceptorIndex*	unitless	Indices assigned to each receptor.
sl.ssf	*ReceptorName*	NA	Name of receptor.
sl.ssf	*ReceptorType*	NA	Description of receptor.
sl.ssf	*WBNFishableRchIndex*	unitless	Index of reaches that are fishable.
sl.ssf	*WBNNumFishableRch*	unitless	Number of fishable reaches.
sl.ssf	*WBNNumRch*	unitless	Number of reaches for each waterbody network.
af.grf	*Caqmp*	mg/kg	Concentration of contaminant in aquatic plants.
af.grf	*CaqmpNY*	unitless	Number of years in the time series corresponding to this variable.
af.grf	*CaqmpYR*	year	Time series of years corresponding to this variable.
af.grf	*Cbenthff*	mg/kg	Concentration of contaminant in benthic organisms.
af.grf	*CbenthffNY*	unitless	Number of years in the time series corresponding to this variable.
af.grf	*CbenthffYR*	year	Time series of years corresponding to this variable.
af.grf	*CT3Fish*	mg/kg	Concentration of contaminants in trophic level 3 fish.
af.grf	*CT3FishNY*	unitless	Number of years in the time series corresponding to this variable.
af.grf	*CT3FishYR*	year	Time series of years corresponding to this variable.
af.grf	*CT4Fish*	mg/kg	Concentration of contaminants in trophic level 4 fish.
af.grf	*CT4FishNY*	unitless	Number of years in the time series corresponding to this variable.
af.grf	*CT4FishYR*	year	Time series of years corresponding to this variable.
sr.grf	*SrcH2O*	NA	Flag for surface water presence.
sr.grf	*SWConcTot*	mg/L	Contaminant concentration in surface water.

(continued)

Table D-25. (continued)

File	Code	Units	Description
sr.grf	*SWConcTotNY*	unitless	Number of years in the time series corresponding to this variable.
sr.grf	*SWConcTotYR*	year	Time series of years corresponding to this variable.
sw.grf	*WBNConcWaterTot*	mg/L	Dissolved concentration in surface water used as drinking water source by cattle.
sw.grf	*WBNConcWaterTotNY*	unitless	Number of years in the times series corresponding to this variable.
sw.grf	*WBNConcWaterTotYR*	year	Time series of years corresponding to this variable.
tf.grf	*C<animals>_<max or min>NY*	unitless	Number of years in the time series corresponding to this variable.
tf.grf	*C<animals>_<max or min>*	mg/kg	Concentration of contaminant found in herbiverts and omniverts.
tf.grf	*C<animals>_<max or min>YR*	year	Time series of years corresponding to this variable.
tf.grf	*C<animals>_HabRange*	mg/kg	Concentration of contaminant found in invertebrates and worms.
tf.grf	*C<animals>_HabRangeNY*	unitless	Number of years in the time series corresponding to this variable.
tf.grf	*C<animals>_HabRangeYR*	year	Time series of years corresponding to this variable.
tf.grf	*C<animals>_sm_<max or min>*	mg/kg	Concentration of contaminant found in small birds, herpetofauna, and mammals.
tf.grf	*C<animals>_sm_<max or min>YR*	year	Time series of years corresponding to this variable.
tf.grf	*C<animals>_sm_<max or min>NY*	unitless	Number of years in the time series corresponding to this variable.
tf.grf	*CTdaAveHabRange*	μg/g	Average depth average soil concentration in each habitat range.
tf.grf	*CTdaAveHabRangeNY*	unitless	Number of years in the time series corresponding to this variable.
tf.grf	*CTdaAveHabRangeYR*	year	Time series of years corresponding to this variable.
tf.grf	*CTssAveHabRange*	μg/g	Average depth average soil concentration in each habitat range.
tf.grf	*CTssAveHabRangeNY*	unitless	Number of years in the time series corresponding to this variable.
tf.grf	*CTssAveHabRangeYR*	year	Time series of years corresponding to this variable.
tf.grf	*P<plant type>_HabRangeNY*	unitless	Number of years in the time series corresponding to this variable.

(continued)

Table D-25. (continued)

File	Code	Units	Description
tf.grf	*P<plant type>_HabRangeYR*	year	Time series of years corresponding to this variable.
tf.grf	*P<plant type>_HabRange*	mg/kg	Concentration of contaminant found in exfruit, exveg, forage, grain, root, and silage.

NA = not applicable

Table D-26. Summary of Output Parameters for the Ecological Exposure Module

File	Code	Units	Description
ee.grf	*Dose_rec*	mg/kg-d	Dose of contaminant to receptor.
ee.grf	*Dose_recNY*	unitless	Number of years in the time series corresponding to this variable.
ee.grf	*Dose_recYR*	year	Time series of years corresponding to this variable.

D.13 Ecological Risk Module

The ecological risk (EcoRisk) module calculates hazard quotients[13] (HQs) for a suite of ecological receptors assigned to habitats delineated for study sites. These receptors fall into eight receptor groups: (1) mammals, (2) birds, (3) herpetofauna, (4) terrestrial plants, (5) soil community, (6) aquatic plants and algae, (7) aquatic community, and (8) benthic community. The spatial resolution of the EcoRisk module is, to a large degree, determined by both the home ranges and habitats delineated at each site.

The HQs for the 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. The HQ risk bins are used in developing cumulative distribution functions of risk and are defined as: (1) below 0.1, (2) between 0.1 and 1, (3) between 1 and 10, (4) between 10 and 100, and (5) above 100. Each of the HQs calculated by the EcoRisk 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 km to 2 km, or across the entire site) is important in understanding the spatial character of potential ecological risks.

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). It is important to note that 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.

D.13.1 Functionality

The major computational functions performed by the ecological risk module may be summarized as follows:

- *Time series management*. The EcoRisk module determines the overall duration of the time period to be simulated (including concentration data from discontinuous time periods) and identifies the individual years within the overall duration that will be simulated.

- *Module loops over the time series, through habitats, and receptors.* The EcoRisk module has three basic loops: (1) over the time series, (2) over each habitat, and (3) over each receptor assigned to the habitat.

[13] Hazard quotients are defined as: (1) the ratio between applied dose received from the ingestion of contaminated media and food items and an ecological benchmark (EB in units of dose), and (2) the ratio between the concentration in the medium of interest (soil, sediment, or surface water) and a chemical stressor concentration limit (CSCL in units of concentration).

- *Calculation of time series hazard quotients for ecological receptors.* The EcoRisk module predicts HQs for each year of the simulation for receptors in each habitat. These HQs are defined in terms of a number of attributes to facilitate clarity in the risk characterization.

The major steps performed by the EcoRisk module that are required to predict ecological risks are summarized as follows:

- Select the ecological distance ring of interest (i.e., 0 to 1 km; 1 to 2 km, entire site).

- Read in all data required to calculate HQs for all receptors (e.g., EBs, CSCLs, site layout characteristics such as water hardness).

- Calculate HQs for all receptors within the area of interest for each year of the simulation.

- Calculate probability density functions for each year of the simulation (this is performed in much the same manner as with the Human Risk module).

- Identify and output the cumulative density functions for various receptor and habitat groups for the year in which the maximum total HQ was experienced.

- Identify and output information about the receptor experiencing the maximum HQ across all years of the simulation and the year in which the maximum occurred.

D.13.2 Assumptions and Limitations

The methodology used in the ecological risk module reflects a number of assumptions and/or limitations, which are listed below. Several key assumptions listed for the ecological exposure module (see Section D.12.1) are also relevant to the EcoRisk module. For example, the assumption that all areas delineated as habitat support wildlife also applies to the EcoRisk module in that HQs calculated within each habitat are presumed to reflect potential risks to ecological receptors. For convenience, these assumptions are included below as well as assumptions and limitations that are unique to the EcoRisk module.

D.13.2.1 Assumptions

- *Study area is bounded at 2 km.* We assumed that significant risks to source-related contaminants do not occur for ecological receptors that are beyond 2 km of the source. Consequently, HQs were not calculated for receptors outside of the study area, measured from the corner of the source to a point 2 km away.

- *All areas delineated as habitat support wildlife.* It is assumed that habitats delineated at each site are capable of sustaining a variety of wildlife. Since the predator-prey interactions for each habitat are represented by a simple food web,

each habitat is assumed to be of sufficient quality to support multiple trophic levels and, at least, one reproducing pair of upper trophic level predators. Hence, risk calculations assume that the receptors of interest are present in each habitat.

There is only one source for each chemical stressors in the study area. Background concentrations of constituents were not considered in developing exposure estimates. Contributions to ecological exposures from other sources, or pre-existing conditions such as a fish advisory were not addressed.

The most appropriate endpoints for population sustainability are reproductive and developmental effects. In calculating HQs for populations of mammals and birds, it is implicitly assumed that endpoints associated with the populations' ability to reproduce and grow are an appropriate surrogate for true population-level endpoints (e.g., adverse effects leading to a 10% reduction in the population size).

One and only one population of each wildlife species is carried by a given habitat. For example, although there may be a number of receptors assigned to a habitat, multiple populations of shrews or robins are not evaluated. Each receptor population has the same spatial characteristics, as defined by the home range. Hence, there is one HQ calculated for each receptor in each habitat.

Maximum HQ estimates are based on a single year of exposure. The ecological HQ estimates are based on annual averages: the smallest increment of time that for which the 3MRA system is designed. This time step represents much longer than lifetime exposures for some receptors, and substantially less than lifetime for other receptors.

D.13.2.2 Limitations

The HQs are not calculated at the population or community level; ecological risks must be inferred to higher levels of biological organization. Ecosystems are enormously complex, and our understanding of even simple community dynamics is limited. Data on chemical stressors are seldom available above the level of an individual organism; that is, the study endpoints focus on individual organisms rather than processes crucial to assemblages of organisms. Even the CSCLs developed to evaluate risks to communities are derived by statistical inference on toxicity data for individual organisms. Therefore, the data are generally insufficient to allow us to truly evaluate effects at the population or community levels. This is currently a limitation in the state-of-the-science, particularly for national analyses.

It is not possible to verify that reproductive and developmental endpoints are, in all cases, sufficient to protect the assessment endpoints for wildlife populations. The endpoints for certain wildlife populations (i.e., mammals, birds) were almost exclusively taken from reproductive and developmental studies. Although

reproductive and developmental endpoints have been recognized by EPA as relevant to population sustainability, they are not always the critical effect associated with a chemical stressor. The assumption that other effects that may occur at lower environmental concentrations are not significant with respect to the population sustainability limits confidence in predicting ecological risk. Studies regarding this question are inconclusive and, therefore, there is some uncertainty in using only reproductive and developmental studies to address the assessment endpoint of population sustainability.

The HQ estimates are generated based on one, and only one, home range area. For the purposes of creating the site layout file, four home range areas are placed in each habitat. Once these areas are delineated and appropriate receptors are assigned, the spatial characteristics of the risk for each home range is established. Variability associated with exposures in different areas of the habitat is not reflected in this scheme. This limitation may result in significant differences for receptors with small home ranges, and can influence the risk estimates for predators with large home ranges (i.e., home range ≈ habitat) since tissue concentrations in prey items are constrained by the same spatial characteristics. As a result, the representativeness of the HQs with regard to the spatial character of the exposure is limited.

The effects of multiple stressors (chemical and non-chemical) are not considered in developing estimates of potential ecological risk. This is a source of considerable uncertainty in the HQ estimates. The EcoRisk module is executed within the FRAMES system within a system-level chemical loop such that only a single chemical is evaluated per iteration of the model. As a result, risks are predicted assuming a single chemical exposure. Data availability on the antagonistic and synergistic effects associated with multiple stressors are extremely limited at this time (with the possible exception narcotic contaminants in aqueous systems) and prevented the development of a multi-stressor analytical approach for the HWIR universe of constituents. Data limitations notwithstanding, the inability to consider multiple stressors is a limitation in our ability to interpret the risk results generated by this module.

The HQ estimates for the aquatic and benthic communities, respectively, are resolved at the habitat, rather than reach level. There is some uncertainty associated with calculating risks to aquatic life across an entire habitat (as defined within the study area). Species of fish such as brown trout tend to utilize certain segments of stream habitats and, therefore, HQs at the reach level may be more appropriate. Conversely, establishing artificial boundaries between stream reaches is contrary to the goals of the assessment strategy, namely, to evaluate ecological risks using the habitat as the fundamental unit.

The HQ estimates reflect different endpoints at varying levels of effect. The HQ methodology - the ratio of an exposure to a benchmark - is applied uniformly across all ecological receptors. However, the data supporting the HQ calculation

vary in that they include endpoints from lethality to reproductive fitness and address and community-level effects by inference. To some degree, the HQ estimates for different receptor groups represent different risk metrics. The interpretation of these HQ estimates is, therefore, limited by our understanding of the potential ecological significance of the measures of effect as well as overall confidence in the data used to support the calculations.

D.13.3 Inputs for the Ecological Risk Module

The concentration and dose inputs required by the EcoRisk module are provided by the ecological exposure (EcoEx) module, the Terrestrial Food Web module (TerFW), and the Surface Water (SW) module. These inputs include:

Ecological Exposure (ee.grf)

- applied dose to receptors by home range and habitat

Terrestrial Food Web (tf.grf)

- spatially-averaged surficial soil concentration by home range

Surface Water (sw.grf)

- average, reach-specific total concentration in sediment
- average, reach-specific total concentration in surface water
- average, reach-specific dissolved concentration in surface water

The ecological risk module receives inputs from its module-specific input file, er.ssf, the generic site layout file (sl.ssf), the chemical properties file (cp.ssf), and modeled inputs from the surface water module (sw.grf), terrestrial food web module (tf.grf), and the ecological exposure module (ee.grf). Input variables are listed and described in Table D-27.

D.13.4 Outputs

The ecological risk module outputs are written to the er.grf file. All ecological risk outputs are 3-dimensional arrays indexed on time, habitat, and receptor. Output variables are listed and described in Table D-28.

Table D-27. Summary of Inputs for the Ecological Risk Module

File	Code	Units	Description
er.ssf	EcoRegPercentile	unitless	Policy criterion for selecting critical year for maximum HQ
sl.ssf	NumEcoBin	unitless	Number of bins for cumulative distribution function
sl.ssf	EcoRingNumHab	unitless	Number of habitats in each ecoring
sl.ssf	EcoBinRange_Min	unitless	Minimum HQ for each ecobin
sl.ssf	NumEcoRing	unitless	Number of ecorings at the site
sl.ssf	EcoRingHabIndex	unitless	Habitat index for a habitat in a given ecoring
sl.ssf	HabNumRange	unitless	Number of ranges in a given habitat
sl.ssf	HabNumWBNRch	unitless	Number of reaches in a given habitat
sl.ssf	HabType	NA	String description of the habitat type for a given habitat
sl.ssf	ReceptorType	NA	String description of the receptor type for a given receptor
sl.ssf	ReceptorName	NA	Receptor name
sl.ssf	RecGroup	NA	String description of receptor group
sl.ssf	RecTrophicLevel	NA	String description of receptor trophic level
sl.ssf	HabRangeRecIndex	unitless	Index for a given receptor in a given habitat
sl.ssf	WBNWaterHardness	mg CaCO3 eq/L	Water hardness for a given waterbody network type
sl.ssf	HabWBNIndex	unitless	Waterbody network index for a given reach in a given habitat
sl.ssf	HabWBNRchIndex	unitless	Reach index for a given reach in a waterbody network in a given habitat
sl.ssf	WBNRchBodyType	NA	String description of reach body type for a given reach in a given waterbody network
cp.ssf	ChemCASID	NA	Chemical abstracts service registry number for the chemical
cp.ssf	ChemType	NA	Chemical type
cp.ssf	ChemKoc	mL/g	Organic carbon partition coefficient for the chemical
cp.ssf	ChemEBRec	mg/kg-day	Ecological benchmark for the chemical for a given receptor
cp.ssf	ChemCSCLWaterDissRec	mg/L	Chemical stressor concentration limit for the chemical dissolved in water for a given receptor
cp.ssf	ChemCSCLWaterTotRec	mg/L	Chemical stressor concentration limit for the total chemical in water for a given receptor

(continued)

Table D-27. (continued)

File	Code	Units	Description
cp.ssf	ChemCSCLSediment Rec	ug/g	Chemical stressor concentration limit for the chemical in sediment for a given receptor
cp.ssf	ChemCSCLSoilRec	ug/g	Chemical stressor concentration limit for the chemical in soil for a given receptor
sw.grf	WBNNumChem	NA	Number of chemical species for the chemical
sw.grf	WBNConcWaterDiss	mg/L	Dissolved concentration of chemical in a given WBN reach in a given year
sw.grf	WBNConcWaterTot	mg/L	Total concentration of a chemical in a given WBN reach in a given year
sw.grf	WBNConcBenthTot	ug/g	Total concentration of a chemical in the benthic column of a given WBN reach in a given year
sw.grf	WBNfocBenth	fraction	Fraction organic carbon in the benthic column of a given WBN reach in a given year
tf.grf	CTdaAveHabRange	ug/g	Depth-averaged total chemical concentration in soil, averaged over a given habitat and range in a given year
ee.grf	Dose_rec	mg/kg-day	The chemical dose experienced by a receptor in a given habitat and range in a given year

NA = not applicable

Table D-28. Summary of Outputs for the Ecological Risk Module

File	Code	Units	Description
er.grf	HQcdf_HabGroup	unitless	Cumulative percentile of receptor HQs, by habitat group for each ecoring for the
er.grf	HQcdf_HabType	unitless	Cumulative percentile of receptor HQs, by habitat type
er.grf	HQcdf_RecGroup	unitless	Cumulative percentile of receptor HQs, by receptor group
er.grf	HQcdf_RGHabGroup	unitless	Cumulative percentile of receptor HQs, by receptor group and habitat group (ecoring 3 only)
er.grf	HQcdf_TLHabGroup	unitless	Cumulative percentile of receptor HQs, by trophic level and habitat group (ecoring 3 only)
er.grf	HQcdf_TrophicLevel	unitless	Cumulative percentile of receptor HQs, by trophic level
er.grf	HQHabTypeTcrit	year	Time output at which maximum HQ occurs for each habitat type
er.grf	HQHabGroupTcrit	year	Time output at which maximum HQ occurs for each habitat group
er.grf	HQMax	unitless	Maximum HQ across the ecoring
er.grf	HQMaxHabGroup	unitless	Habitat group index for the maximum HQ in the ecoring
er.grf	HQMaxHabType	NA	Habitat type for the maximum HQ in the ecoring
er.grf	HQMaxRec	unitless	Receptor index for the maximum HQ in the ecoring
er.grf	HQMaxRecGroup	NA	Receptor group for the maximum HQ in the ecoring
er.grf	HQMaxTcrit	year	Year with maximum HQ across all eco receptors in the ecoring
er.grf	HQMaxTrophicLevel	unitless	Trophic level of receptor for the maximum HQ in the ecoring
er.grf	HQRecGroupTcrit	year	Time output at which maximum HQ occurs for each receptor group
er.grf	HQRGHabGroupTcrit	year	Time output at which maximum HQ occurs for each receptor group/habitat group combination
er.grf	HQTLHabGroupTcrit	year	Time output at which maximum HQ occurs for each trophic level/habitat group combination
er.grf	HQTrophicLevelTcrit	year	Time output at which maximum HQ occurs for each trophic level

NA = not applicable