EPA/NUMBER
October, 1998

Peer Review Draft

ORD/OSW INTEGRATED RESEARCH AND DEVELOPMENT PLAN FOR THE HAZARDOUS WASTE IDENTIFICATION RULE (HWIR)

Jointly produced under partnership agreement by:

Office of Research and Development
Office of Solid Waste

U.S. Environmental Protection Agency
Washington, D.C.

ORD/OSW INTEGRATED RESEARCH AND DEVELOPMENT PLAN FOR THE HAZARDOUS WASTE IDENTIFICATION RULE (HWIR)

EXECUTIVE SUMMARY viii

1.0 BACKGROUND AND PURPOSE 11
1.1 Purpose and Organization of Research and Development Plan 12
1.2 The HWIR Technical Assessment Problem 12
1.3 Summary of Major Review Comments from 1995 HWIR Proposal 13

2.0 HWIR RISK ASSESSMENT: OBJECTIVES AND ORGANIZATION 18
2.1 Research and Development Objectives 18
2.2 Interoffice Organizational Plan 18

3.0 REVISED RISK ASSESSMENT METHODOLOGY: TECHNICAL APPROACH 21
3.1 Assessment Strategy 29
3.1.1 HWIR99 Strategy for Developing National Exit Criteria 29
3.1.1.1 Risk Matrices: HWIR Technical Assessment Output 30
3.1.1.2 Protection Measures for Establishing HWIR99 Regulatory Limits . . 30
3.1.1.2.1 Protection Measure based on Receptor Risk 31
3.1.1.2.2 Protection Measure based on Protected Sites 32
3.1.1.3 Nationwide Aggregation of Protection Measures 32
3.1.1.4 Regulatory Scheme 34
3.1.1.5 Alternative Measures of Protection 36
3.1.2 Monte-Carlo Approach 36
3.1.2.1 Monte-Carlo Objectives 36
3.1.2.2 Monte Carlo Implementation Strategy 37
3.1.2.2.1 Ideal Conditions 37
3.1.2.2.2 Limitations in Implementation of the Monte Carlo Approach 38
3.1.2.2.3 HWIR99 Site Based Approach Monte Carlo 39
3.2 HWIR99 Site-based Assessment Model 43
3.2.1 Source Modules (Land Application Unit, Waste Pile, and Landfill) 44
3.2.1.1 Purpose 44
3.2.1.2 Summary of Major Comments from 1995 Proposal 44
3.2.1.3 Requirements for HWIR99 and Approaches Considered 45
3.2.1.4 Module Description 46
3.2.1.5 Limitations 47
3.2.2 Source Modules (Tanks and Surface Impoundments) 47
3.2.2.1 Purpose 47
3.2.2.2 Summary of Major Comments from 1995 Proposal 47
3.2.2.3 Requirements for HWIR99 and Approaches Considered 48
3.2.2.4 Module Description 49
3.2.2.5 Limitations 49
3.2.3 Atmospheric Module 50

3.2.3.1 Purpose 50
3.2.3.2 Summary of Major Comments from 1995 Proposal 50
3.2.3.3 Requirements for HWIR99 and Approaches Considered 50
3.2.3.4 Module Description 51
3.2.3.5 Limitations 51
3.2.4 Unsaturated Zone Module 51
3.2.4.1 Purpose 51
3.2.4.2 Summary of Major Comments from 1995 Proposal 52
3.2.4.3 Requirements for HWIR99 and Approaches Considered 52
3.2.4.4 Module Description 52
3.2.4.5 Limitations 52
3.2.5 Saturated Zone Module 52
3.2.5.1 Purpose 53
3.2.5.2 Summary of Major Comments from 1995 Proposal 53
3.2.5.3 Requirements for HWIR99 and Approaches Considered 53
3.2.5.4 Description of Module 53
3.2.5.5 Limitations 54
3.2.6 Watershed Module 54
3.2.6.1 Purpose 54
3.2.6.2 Summary of Major Comments from 1995 Proposal 54
3.2.6.3 Requirements for HWIR99 and Approaches Considered 54
3.2.6.4 Module Description 55
3.2.6.5 Limitations 55
3.2.7 Surface Water Module 56
3.2.7.1 Description of Module Purpose 56
3.2.7.2 Summary of Major Comments from 1995 Proposal 56
3.2.7.3 Requirements for HWIR99 and Approaches Considered 56
3.2.7.4 Description of Module 57
3.2.7.5 Limitations 59
3.2.8 Aquatic Food Web (AqFW) Module 59
3.2.8.1 Purpose 59
3.2.8.2 Summary of Major Comments from 1995 Proposal 60
3.2.8.3 Requirements for HWIR99 and Approaches Considered 60
3.2.8.4 Module Description 60
3.2.8.5 Limitations 63
3.2.9 Farm Food Chain (FFC) Module 63
3.2.9.1. Purpose 63
3.2.9.2 Summary of Major Comments from 1995 Proposal 63
3.2.9.3 Requirements for HWIR99 and Approaches Considered 63
3.2.9.4 Module Description 64
3.2.9.5 Limitations 65
3.2.10 Terrestrial Food Web (TerFW) Module 65
3.2.10.1 Purpose 65
3.2.10.2 Summary of Major Comments from 1995 Proposal 65
3.2.10.3 Requirements for HWIR99 and Approaches Considered 65
3.2.10.4 Description of Module 66
3.2.10.5 Limitations 67

3.2.11 Ecological Exposure (EcoEx) Module 67
3.2.11.1 Purpose 67
3.2.11.2 Summary of Major Comments from 1995 Proposal 68
3.2.11.3 Requirements for HWIR99 and Approaches Considered 68
3.2.11.4 Module Description 68
3.2.11.5 Limitations 70
3.2.12 Human Exposure Module 70
3.2.12.1 Purpose 70
3.2.12.2 Summary of Major Comments from 1995 Proposal 70
3.2.12.3 Requirements for HWIR99 and Approaches Considered 71
3.2.12.4 Module Description 71
3.2.12.5 Limitations 72
3.2.13 Risk Module 72
3.2.13.1 Purpose 73
3.2.13.2 Summary of Major Comments from 1995 Proposal 73
3.2.13.3 Requirements for HWIR99 and Approaches Considered 73
3.2.13.4 Module Description 74
3.2.13.5 Limitations 75
3.3 Assessment Data 75
3.3.1 Site-based Data 76
3.3.1.1 Spatial Framework 77
3.3.1.2 Data Storage and Processing 78
3.3.1.3 QA/QC and Record-Keeping 78
3.3.1.4 Methodology and Data Collection 79
3.3.1.5 Case Studies 80
3.3.2 Human Health Effects Benchmarks 80
3.3.3 Ecological Health Effects Benchmarks 81
3.3.4 Chemical Property Data 81
3.3.4.1 Basic Properties of Organic Chemicals 81
3.3.4.2 Basic Properties of Metals and Inorganics 88
3.3.4.3 Transformation Reactions 90
3.4 Assessment Technology 92
3.4.1 Summary of the FRAMES-HWIR Technology Software System Requirements 93
3.4.1.1 FRAMES-HWIR Technology Software System Components 94
3.4.1.2 FRAMES-HWIR Technology Software System Structure 95
3.4.2 System User Interface (SUI) 96
3.4.2.1 Summary of SUI Requirements 96
3.4.2.2 SUI Structure 97
3.4.3 Distribution Statistics Processor (DSP) 98
3.4.3.1 Summary of DSP Requirements 99
3.4.3.2 Regional and National Environmental Setting Distribution Statistics Databases 100
3.4.3.3 Regional and National Statistics Databases 102
3.4.4 Site Definition Processor (SDP) 103
3.4.4.1 Summary of the SDP Requirements 103
3.4.4.2 Databases Supplying Information to the SDP 104

3.4.5 Computational Optimization Processor (COP) 106
3.4.5.1 Summary of the COP Requirements 107
3.4.6 Multimedia Multipathway Simulation Processor (MMSP) 108
3.4.6.1 Summary of MMSP Requirements 108
3.4.6.2 Module Requirements 109
3.4.7 Exit Level Processor (ELP) 110
3.4.7.1 Summary of ELP Requirements 110
3.4.7.2 ELP Implementation 111
3.5 Science Support Activities 111
3.5.1 Science Support Activities Related to HWIR Source Module 112
3.5.1.1 Source Module Activity #1 112
3.5.1.2. Source Module Activity #2 114
3.5.1.3. Source Module Activity #3 115
3.5.2 Science Support Activities Related to HWIR Intermedia Transport 116
3.5.2.1 Intermedia Transport Activity #1 116
3.5.3 Science Support Activities Related to HWIR Air Module 117
3.5.3.1 Air Module Activity #1 117
3.5.3.2 Air Module Activity #2 117
3.5.4 Science Support Activities Related to HWIR Groundwater Module 118
3.5.4.1 Groundwater Module Activity #1 118
3.5.5 Science Support Activities Related to HWIR Surface Water Module 119
3.5.5.1. Surface Water Module Activity #1 119
3.5.5.2 Surface Water Module Activity #2 120
3.6 Peer Review Plan 121

4.0 SCHEDULE 171

5.0 GLOSSARY 173

6.0 ACRONYMS 180

REFERENCES 181

APPENDIX A 185
A.1 Uncertainty and Variability in HWIR99 185
A.2 Source of Variability and Uncertainty 185
A.3 Separating Variability And Uncertainty 186
A.4 References 191

List of Figures

Figure 3.1 Exposure pathways for human receptors. 125
Figure 3.2 Exposure pathways for ecological receptors. 126
Figure 3.3 Relationship between exposure concentration and pathway risk. 127
Figure 3.4 Pathway risks and exposure route risks for Site f. 128
Figure 3.5 N_f X N_i Pathway Risk Matrix Output. 129
Figure 3.6 General assessment flowchart. 131
Figure 3.7 Exit level determination flowchart. 134
Figure 3.8 Probability that percent protection is less than P for a given waste concentration and target risk level. 137
Figure 3.9 Percent of receptors protected for different risk levels and $C_w = 10^{-3}$ for N_i Monte Carlo iterations. 138
Figure 3.10 Percent of receptors protected for different waste concentrations and risk levels. 139
Figure 3.11 Graphical illustration of MMSP modules. 142
Figure 3.9. Site-Specific Spatial Overlays for HWIR99 Spatial Framework (GIS Analysis) 143
Figure 3.13 Overall diagram of the FRAMES-HWIR technology software system. 144
Figure 3.14 Overall diagram of the protocols for implementing a two-stage Monte Carlo analysis. . 145
Figure 3.15 View of the distribution statistics processor. 146
Figure 3.16 View of the site definition processor. 147
Figure 3.17 View of the inner loop. 148
Figure 3.18 View of the Computational Optimization Processor. 149
Figure 3.19 View of multimedia multipathway simulation processor. 150
Figure 3.20 General interactions of the multimedia multipathway simulation modules. 151
Figure 3.21 View of exit level processor. 152
Figure 3.22 Overview of the exit level processor. 153
Figure 3.23 Interactions in exit level processor I. 154
Figure 3.24 Interactions in exit level processor II. 155
Figure A.1 Distribution of risk under uncertainty. 189
Figure A.2 Distribution of risk under no uncertainty. 190

List of Tables

Table 1.1 Principal Review Comments for HWIR95 Technical Assessment (General) 15
Table 1.2 Principal Review Comments for HWIR95 Technical Assessment (Detailed) 16
Table 2.1 HWIR99 Research and Development Objectives 20
Table 3.1 HWIR99 Multimedia Risk Assessment Dimensions. 156
Table 3.2 Technical Requirements for HWIR99 Assessment. 158
Table 3.3 HWIR99 parameterization approaches by data type. 160
Table 3.4 Input data type by HWIR99 model component. 161
Table 3.5 Data collection activities for sites representing National distribution and case studies. . . . 162
Table 3.6 Physical/chemical properties for organic chemicals. 163
Table 3.7 Physical/chemical properties for metals and inorganics. 164
Table 3.8 Principal Review Comments for HWIR95 Technical Assessment (General) 165
Table 3.9 Summary of variables used to describe the HWIR99 Risk Assessment Methodology. 167

EXECUTIVE SUMMARY

This research plan is the result of activities following the Agency's December 1995 proposal to amend existing regulations for the disposal of hazardous waste under the Resource Conservation and Recovery Act (RCRA). That proposal outlined a new Hazardous Waste Identification Rule (HWIR 95) establishing constituent-specific exit levels for low risk solid wastes. During an extensive series of reviews by the EPA's Science Advisory Board (SAB), the Office of Research and Development (ORD), and numerous industrial and environmental stakeholders, a collective conclusion was reached that the technical basis of the proposed rule was not sufficient to allow the rule to promulgated. The Office of Solid Waste (OSW) and ORD have since entered into a cooperative effort to revise the methodology in accordance with the review comments. The development of the new approach, referred to as HWIR99, is the subject of the present research plan.

The overall goal of this development effort is to develop a methodology suitable for determining constituent-specific waste stream concentrations that represent a threshold below which Subtitle C disposal will not be required, and thus the waste stream may "exit" the hazardous waste management system. Since HWIR99 is to be a risk-based rule, the intent is to set exit levels such that no significant risk to human or ecological health shall occur as the result of implementing the new exit levels. In characterizing risks, HWIR99 will employ mathematical models to simulate the multimedia release of contaminants from land-based waste management units, their multimedia transport, and the subsequent exposure and risk to human and ecological receptors. This plan reflects the early strategy for developing such a methodology. In so doing, it is intended to address the major review comments obtained on the earlier proposal. Some of the most important of these are summarized in Tables 1.1 and 1.2.

The HWIR99 methodology described herein embodies six general objectives: 1) developing a revised risk-based assessment strategy, 2) developing a site-based multimedia, multi-pathway exposure and risk model, 3) developing the required assessment databases, 4) developing a computer-based technology for implementing the strategy, 5) developing a sound science foundation for the assessment, and 6) conducting the necessary peer reviews. A list of the key technical requirements underlying these objectives is presented in Section 3.1.1. In addition, the methodology under development is framed by a number of assumptions that are elaborated in Section 3.1.2 of the plan. In brief, these are: 1) concentration limits to be determined are chemical-specific, 2) receptors of concern are within a 2 km radius of the site, 3) human and ecological impacts of exposure are based on near-field, long term exposure, 4) the total mass of a given chemical in the waste management unit (WMU) is finite, 5) mass balance is conserved at the source, 6) calculation of measures of protection is performed at the site level and aggregated over sites to estimate National statistics, 7) waste management units are located as indicated in OSW's industrial Subtitle D database, 8) impacts on receptors are calculated from the beginning of the site operation and until a maximum time when all impacts are included, and 9) receptors will be subject to exposures from all pathways simultaneously.

From the logistical standpoint, this research plan is being implemented through a unique agreement between ORD and OSW in which both groups are working in unison to design and build the required assessment strategy and implementation technology. In this agreement OSW will provide expertise on policy and regulatory-based technical risk assessment, and ORD will provide its science and engineering expertise. The two groups are implementing this agreement through a working structure defined by eight formal research teams charged with addressing various aspects of the overall effort. These teams are listed below:

1. Sources Team
2. Atmospheric Fate and Transport Team
3. Groundwater Fate and Transport Team
4. Surface Water Team
5. Exposure Pathways and Receptors Team
6. Risk Characterization Team
7. Chemical and Biological Fate Team
8. Steering /Integration Team

All the teams are constituted by a mix of personnel from OSW and ORD with technical skill mixes appropriate for the subjects to be dealt with. All the teams also receive contract support as needed. Together, these teams are pursuing a model development approach that embodies the following summary characteristics:

The HWIR99 assessment will be a screening-level risk-based assessment of potential human and ecological health risks resulting from long-term (chronic) exposure to HWIR chemicals released from land-based waste management units (WMUs) containing currently 'listed' waste streams. The assessment of potential health risks will be conducted for both human and ecological receptors. The assessment will be national in scale and site-based, that is, risks will be assessed at individual sites across the U.S. where HWIR WMU's may be located. The resulting national distribution of site-based risks will form the basis for establishing exit criteria. For each site, statistically sampled from a national database of WMUs, the simultaneous release of chemicals from the WMU to each environmental medium, the fate and transport of the chemical through a multimedia environment, and the receptor-specific exposures and risks will be simulated. Human receptors include child and adult; residents, home gardeners, beef and dairy farmers, and recreational fishers. Exposure pathways include inhalation of outdoor air and shower air and ingestion of contaminated drinking water, garden and farm products and fish. Ecological exposure and risk will focus on population effects related to key species within habitats found in the proximity of sites. The assessment includes an estimation of the potential exposures per exposure pathway/receptor and aggregated across pathways followed by an estimate of the resulting carcinogenic and noncarcinogenic health effects. The end point of the technical assessment is a "rolling-up" of the site-based risks to form a national scale joint distribution reflecting the relationship between chemical concentration in wastestreams and human and ecological health risk. Specific exit levels will be selected from these distributions on the basis of Agency policy concerning appropriate degrees of protectiveness. The resulting chemical-specific exit levels represent threshold waste concentrations below which the associated wastestream is not considered hazardous and therefore does not require Subtitle C type disposal. The exit levels will be applicable to all wastestreams and all locations, i.e., nationally.

While the exit criteria to be developed are intended for National application, the modeling strategy is a "tiered site-based" approach. This reflects an agency decision to base exit levels on an assessment of potential risk occurring at Subtitle D facilities where WMU's may be located. In this approach, the individual site-based assessments are embedded in a two-stage Monte Carlo simulation procedure designed to produce sufficient site-based risk assessments to result in a national-scale statistical distribution of risk. The Monte Carlo analysis also provides explicit quantification of variability and uncertainty associated with the risk estimates and is flexible enough to accommodate alternative policy formulations.

A central feature of the HWIR99 technical approach is the comprehensive, multimedia, multi-pathway and multireceptor simulation processor (MMSP), which represents a site-based risk assessment model. This model simulates the release, fate and transport, exposure and risk associated with disposed chemicals. The MMSP is made up of several individual modeling components and is housed in a larger software framework system (FRAMES-HWIR) designed to automate implementation of the overall assessment strategy. The components of the MMSP (referred to as modules) are roughly grouped by function into four categories (source, media, food chain and exposure / risk) and include the following:

Source	Media	Food Chain	Exposure / Risk
Landfill	Atmospheric	Terrestrial	Ecological Exposure
Land Application	Watershed	Aquatic	Human Exposure
Waste Pile	Surface Water	Farm	Ecological Risk
Surface Impoundment	Vadose Zone		Human Risk
Tank	Saturated Zone		

These modules and their associated sub-modules encompass a wide array of input data requirements in the following categories: facility location data, waste management unit data, waste properties data, meteorological data, land use data, topography data, water body and water quality data, soils data, aquifer data, human receptor types and locations, ecological receptor types and locations, farm food chain data, terrestrial and aquatic food web data, human exposure factors, ecological exposure factors, human health benchmarks, ecological benchmarks, and chemical properties data. Some of these data needs are satisfied on site-specific basis, some are available on regional basis, and some are available only nationally. The HWIR approach employs a tiered protocol for collecting the necessary inputs.

To facilitate manageable implementation times for generating the required risk estimates, the HWIR99 methodology employs a technology software system (FRAMES-HWIR) consisting of a user interface and a series of five processors within a system framework. These include the following:

1. Distribution Statistics Processor (DSP) - randomly samples for statistical distributions;
2. Site Definition Processor (SDP) - organizes all required site definition data;
3. Computation Optimization Processor (COP) - formulates the exposure and risk scenario;
4. Multimedia Multipathway Simulation Processor (MMSP) - implements the release, transport, exposure and risk/hazard protocols; and
5. Exit Level Processors (ELP I and ELP II) - translate the MMSP simulations into national distributions of protectiveness vs. waste concentrations (from which exit levels are determined).

Peer review of the HWIR99 methodology will occur in several stages. In Phase I, the present document will undergo a ballot format review to determine how well the planned research and development efforts are addressing earlier review comments on the HWIR95 Multiple Pathway Receptor Analysis approach proposed earlier. Following that, a series of Phase II reviews will be conducted on individual modeling components (modules) that are under development. These too will be conducted using the ballot format. Considerations are also underway for conducting a Phase III consultation review with the Science Advisory Board following Phase II.

1.0 BACKGROUND AND PURPOSE

In December of 1995 the Agency proposed to amend existing regulations for disposal of listed hazardous wastes under the Resource Conservation and Recovery Act (RCRA). The December 1995 proposal (60 FR 6634, December 21, 1995) outlined the new Hazardous Waste Identification Rule (HWIR) that was designed to establish constituent-specific exit levels for low risk solid wastes. Wastes applicable under HWIR were those designated as hazardous because they were listed, or had been mixed with, derived from, or contained the listed wastes. Under the HWIR proposal, waste generators of listed wastes that could meet the new exit level criteria defined by the HWIR methodology, would no longer be subject to the hazardous waste management system specified under Subtitle C of RCRA for those wastes. Basically, this established a risk-based "floor" for low risk hazardous wastes that would encourage pollution prevention, waste minimization, and the development of innovative waste treatment technologies. The purpose of the rulemaking was to reduce possible over-regulation arising from the older "mixture" and "derived-from" rules promulgated earlier. Note that, in a number of cases, wastes were listed on the basis of containing both toxic hazardous constituents and exhibiting one or more of the hazardous waste characteristics that do not relate to chemical toxicity (e.g., ignitability, corrosivitiy, reactivity). If such a waste still exhibits any characteristic after complying with the exemption criteria proposed in the HWIR, it must continue to be managed as a characteristically hazardous waste.

The "mixture" rule and the "derived-from" rule were promulgated as part of the first comprehensive regulatory program for the management of hazardous wastes under RCRA in May of 1980. The mixture rule defined as a hazardous waste any solid waste that is mixed with one or more listed wastes, and the derived-from rule labeled as hazardous waste any solid waste generated from the treatment, storage, or disposal of a listed hazardous waste. Both were / are considered important definitions in regulating the disposal of hazardous wastes consistent with reducing risk to human health and the environment; however, since they apply regardless of the concentration or mobility of hazardous constituents associated with the solid wastes, the potential for over-regulation is a possibility. One of the primary purposes of HWIR was to provide a risk-based methodology for identifying possible instances of over-regulation, and to provide an avenue for relief from the Subtitle C disposal regulations as appropriate.

Extensive reviews of the original proposal were conducted by the EPA Science Advisory Board (SAB), the Office of Research and Development (ORD), and numerous industrial and environmental stakeholders. The collective conclusion resulting from the reviews was that the technical basis of the proposed rule was not sufficient to allow the rule to be promulgated.

As part of a consent decree entered in the U.S. District Court on April 7, 1997, the EPA agreed to an accelerated schedule for the development of a methodology and for the promulgation of a revised HWIR. The decree specified that the Agency will propose a rule by October 31, 1999 and will finalize the rule by April 30, 2001 [ETC vs Browner, CA No. 94-2119 (DDC 1997)]. At this point ORD, at the request of Office of Solid Waste (OSW), agreed to become full partners in the development of the next phase of HWIR (HWIR99). The primary focus of the joint effort was to revise the HWIR95 technical assessment strategy in response to the major review comments and to develop and document the science and engineering foundation for HWIR99. This research and development plan represents a joint OSW/ORD effort to plan, coordinate, and execute HWIR99.

1.1 Purpose and Organization of Research and Development Plan

This research and development plan is intended to organize and document the essential elements of the revised HWIR technical assessment (referred to as HWIR99). This plan is organized to present first a description of the HWIR technical problem. This is followed, in Section 1.3, by a summary of the major review comments related to HWIR95. Section 2 presents the specific research and development goals to be achieved, an EPA interoffice organizational plan for conducting the work, key technical criteria that must be satisfied in the development of a revised risk-based assessment for HWIR, and a list of technical assumptions that will be fundamental to developing HWIR99. Section 3 presents an overview of the planned technical approach. Sections 3.1, 3.2 and 3.3 present the technical requirements, assumptions, and analytic basis of the approach; assessment strategy; and HWIR model, respectively. Section 3.4 presents the strategies for collecting data and Section 3.5 presents the computer-based technology for automating the assessment. Section 3.6 presents a number of science support activities intended to address important specific technical issues and Section 3.7 presents plans for peer review of HWIR99 methodology. Section 4 presents the schedule for the project, Section 5 includes a glossary of terms used in this document and Section 6 includes a list a acronyms.

The technical approach outlined in Section 3.0 represents the current vision for HWIR99. Because there are many technical issues that remain to be resolved and will influence the final form of the technical approach this document must be considered a work in progress. That is, as results of various scientific support activities (see Section 3.6) are produced, specific aspects of the overall technical approach will be reviewed and modified appropriately.

1.2 The HWIR Technical Assessment Problem

The underlying premise of the HWIR is that there are wastestreams currently included in hazardous waste listings that are effectively non-hazardous, that is, the wastestreams, if disposed of in accordance with Subtitle D regulations (as opposed to the hazardous waste requirements of Subtitle C), would not pose a significant health threat to human and ecological receptors. To quantify specific criteria for determining which wastestreams may "safely" exit the hazardous waste disposal program, the Agency must perform a technical assessment of the potential health risks related to the reduced requirements of Subtitle D disposal. The primary exit criterion for HWIR is related to the wastestream concentration of HWIR chemicals-of-concern. Wastestreams containing concentrations below Agency specified thresholds would exit thd hazardous waste system. Conversely, those wastestreams containing concentrations of any HWIR constituent above the chemical-specific threshold would remain in the hazardous waste program.

Given this background, the HWIR technical assessment problem can be defined as

> *Problem Statement: To determine constituent-specific wastestream concentrations that represent a threshold below which Subtitle C disposal will not be required and thus the wastestream may "exit" the hazardous waste management system and can be managed in a Subtitle D (non-hazardous) waste management system.*

The HWIR is a risk-based rule, thus the constituent specific waste exit levels are set such that no significant risk to human or ecological health will occur as a result of the disposal of the waste in non-hazardous waste management units. Also, the HWIR is a national ruling, thus the exit levels must apply

to all wastestreams under all Subtitle D waste management scenarios.

Thus, the HWIR99 assessment will be a screening-level risk-based assessment of potential human and ecological health risks resulting from long-term (chronic) exposure to HWIR chemicals released from land-based waste management units (WMUs) containing currently 'listed' waste streams. The assessment of potential health risks will be conducted for both human and ecological receptors. The assessment will be national in scale and site-based, that is, risks will be assessed at individual sites across the U.S. where HWIR WMU's may be located. The resulting national distribution of risks will form the basis for establishing exit criteria. For each site, statistically sampled from a national database of WMUs, the simultaneous release of chemicals from the WMU to each environmental medium, the fate and transport of the chemical through a multimedia environment, and the receptor-specific exposures and risks will be simulated. Human receptors include child and adult; residents, home gardeners, beef and dairy farmers, and recreational fishers. Exposure pathways include inhalation of outdoor air and shower air and ingestion of contaminated drinking water, garden and farm products and fish. Ecological exposure and risk will focus on individual effects related to population and community viability within habitats found in the proximity of sites. The assessment includes an estimation of the potential exposures per exposure pathway/receptor and aggregated across pathways followed by an estimate of the resulting carcinogenic and noncarcinogenic health effects. The end point of the technical assessment is a "rolling-up" of the risks to form a national scale joint distribution reflecting the relationship between chemical concentration in wastestreams and human and ecological health risk. Specific exit levels will be selected from these distributions on the basis of Agency policy (e.g., appropriate degrees of protectiveness, receptor types, sites, distance from units, geographic location). The resulting chemical-specific exit levels represent threshold waste concentrations below which the associated wastestream is not considered hazardous and therefore does not require Subtitle C type disposal.

In characterizing risks resulting from the disposal of waste, the HWIR technical assessment attempts to simulate, using mathematical models, the multimedia release of contaminants from waste management units, the subsequent multimedia transport of these contaminants, and the resulting exposure and risk to human and ecological receptors. The HWIR99 risk assessment approach and its components are discussed in Section 3.

As stated earlier, the original HWIR was proposed in December, 1995 and included "exit" levels based on a technical assessment of human and ecological health risks. The review of the assessment methodology was sufficiently critical to cause the Agency to respond to criticisms. The Agency decided to develop and implement a revised methodology under a new court-ordered deadline of October 31, 1999 for a proposed rule and April 30, 2001 for a final rule. The next section of this plan describes the major review comments on the HWIR95 proposal. This is followed, in Section 2, with a description of the research and development goals for the next phase of HWIR (HWIR99), and specific technical criteria and assumptions that will be applied to the new approach to the HWIR technical assessment.

1.3 Summary of Major Review Comments from 1995 HWIR Proposal

The December 21, 1995 HWIR proposal was available for public comment up through April 22, 1996. It also underwent extensive reviews by the Office of Research and Development (ORD) and the Agency's Science Advisory Board (SAB). Overall, hundreds of comments were received from industrial, scientific, and environmental stakeholder communities. For the purpose of preparing this research and

development plan, comments were placed into two broad categories; 1) general comments related to the overall risk-based assessment strategy for developing national exit criteria, and 2) detailed comments related to individual components of a risk assessment (e.g., source characterization, groundwater fate and transport, human exposure, etc.). The major review comments are listed in Table 1.1 (General) and Table 1.2 (Detailed).

Table 1.1 Principal Review Comments for HWIR95 Technical Assessment (General)

- Integration of Groundwater and Non-Groundwater Multipathway Risk Assessment (MPRA): The groundwater pathway and MPRA approach (i.e., non-groundwater pathways) represent fundamentally different approaches to the exposure and risk assessment and as such result in a technically confusing and inconsistent rulemaking.
- MPRA Methodology: The MPRA does not represent a true multimedia approach, "... the proposed method of calculating exit criteria is actually based on individually calculating each of many exposure pathways. This approach fails to maintain mass balance and may lead to significant, but unknown, errors in the exposure estimates". This approach should be abandoned in favor of true multi-pathway calculations in which a receptor receives contaminants from a source via all pathways concurrently.
- Characterization of High-end Exposures: The approach for assigning high-end or central-tendency values to model parameters results in an inconsistent and unquantifiable representation of high-end exposures across human and ecological pathways. To ensure a consistent and uniform approach the Agency should conduct a systematic examination of parameter sensitivity and consider implementation of Monte Carlo simulation for the purpose of quantifying the national distribution of exposures and risks.
- Ecological Assessment: The ecological analysis in HWIR is fundamentally flawed because lack of toxicity data has been implicitly equated with lack of adverse ecological effect throughout the analysis. The Agency should discard the proposed ecological risk screening procedure for selecting an initial subset of chemicals for ecological analysis and instead require that a minimum data set be satisfied before ecological based exit criteria are calculated.
- Validation: The total construct of the HWIR methodology has not been validated against actual data derived from laboratory or field experiments or observations. Substantial validation of the overall methodology and its components is essential to developing any degree of confidence in the scientific defensibility of the resulting exit criteria. Recognizing that this approach to validation is not feasible in the near term an alternative is to consult readily accessible, published sources of data for cases that permit comparisons with calculations based on relevant pathways or portions of pathways.
- Temporal Scale of Assessment: The assessment methodology does not address pollutant transport associated with episodic events, such as intense rainfall or wind storms. The significance, with respect to underestimation of exposure and risk to both human and ecological receptors, should be determined.
- Documentation: The documentation of the HWIR methodology for calculating exit criteria lacks clarity and organization. The HWIR documentation should be reorganized and rewritten for both clarity and ease of use. Further, the documentation, with respect to methodology, should distinguish clearly between scientific judgment and EPA policy decisions.
- Quality Assurance: The purpose of QA in this context is to ensure that the methodology for calculating exit criteria is implemented without error. Upon review of the HWIR methodology and specific example calculations reviewers expressed concern that QA issues have not been adequately addressed. The Agency should conduct a thorough examination of all aspects of QA prior to subsequent publication of exit criteria.
- Science Support: The Agency should actively seek the substantive participation, input, and peer review of Agency scientists, and outside peer review groups as necessary, to contribute to and evaluate the overall design and individual elements of a revised methodology.

Table 1.2 Principal Review Comments for HWIR95 Technical Assessment (Detailed)

Source Modules

- The waste management scenarios are poorly developed and do not incorporate established engineering design and operation practices.
- A mass balance approach is necessary for the HWIR analysis and was lacking in the HWIR95 analysis.
- Need to model constituent concentrations (C_S) in soil as a function of time and depth. -- In HWIR95 constituent concentrations in soil (for the LAU) were assumed uniform in a given depth of soil and were incremented only with the addition of constituent mass, with no decrement in C_S due to losses to the atmosphere and no upper limit on C_S. Criticisms of this modeling approach focused on its lack of mass balance and also its lack of ability to recognize a C_S sufficiently large as to be indicative of the presence of a non-aqueous phase liquid (NAPL).
- Need to consider other removal processes including first order biological and chemical degradation.
- Simplistic treatment of partition coefficients -- Concern was expressed that HWIR made extensive use of partition coefficients (i.e., K_d, soil-water partition coefficients) without adequate treatment of the factors that can affect K_d such as characteristics of the chemical, the medium, and the method of measurement.

General Fate and Transport

- Biodegradation and chemical transformation are inadequately represented throughout the assessment. "There are adequate data on biodegradation rates for a number of the chemicals listed to generate generic loss terms."

Regional Watershed

- The method for addressing the overland pathway resulting from soil erosion is not physically based. The implementation of the USLE and other equations used to calculate soil erosion resulted in higher concentrations at the receptor than in the source.

Aquatic Food Web

- Bioaccumulation models that simulate the uptake and accumulation of hydrophobic organics in aquatic biota have not been calibrated or validated over a sufficiently broad variety of aquatic systems.

Farm Food Chain

- The food chain model does not reflect the expertise of scientists in ORD.
- Input parameters for biotransfer factors were not consistent with published values.

Terrestrial Food Chain

- Major comments specific to the terrestrial food web module were not received. However, a number of commenters suggested that ecological exposure concentrations estimated by the HWIR95 model were overly conservative.

TABLE 1.2 (contd.)

Ecological Exposure

- A national assessment of ecological risks from waste management units is not defensible. Instead, ecological risks should be evaluated on a site-specific basis.
- The two generic ecosystems (terrestrial and freshwater) are insufficient to characterize the variability across ecosystems. This was considered one of the most significant limitations in the ecorisk methodology in HWIR95.
- The suite of ecological receptors is incomplete and should include other species (e.g., bats). Threatened and endangered species are not included among the suite of ecological receptors.
- Exposure estimates for ecological receptors are overly conservative because 100% of the diet is presumed to originate from the contaminated area.

Human exposure

- Human exposures should include all relevant exposure pathways and exposure routes, where appropriate. The most limiting pathway approach of HWIR95 was viewed as a major limitation of that analysis.
- The variability and uncertainty in exposures should be explicitly quantified where possible. This includes temporal and spatial variability from exposure area to exposure area at a facility, as well as, variability and uncertainty in exposure parameters.

Risk estimation

- Variability and uncertainty in the risk estimates should be explicitly quantified where possible.
- Human health risk should include all relevant exposure pathways and represent an aggregate risk across pathways and exposure routes where appropriate.
- Health benchmarks for dermal routes of exposure which are based on oral toxicity data should be reviewed in terms of similar toxicokinetics. Further review of the use of oral toxicity data for characterizing risk via dermal routes of exposure should be conducted.
- The absence of ecological benchmarks has been equated with the absence of ecological risk for HWIR constituents that were not included in the ecological risk assessment.
- Ecological risks should not be evaluated by inference from data on individual effects (e.g., reproductive effects). Ecological risks should be evaluated for entire communities and ecosystems.
- The ecological toxicity data represents a collection of species-level benchmarks that are used to define a value that protects some fraction (e.g., 95 percent) of the species. Thus, the assessment represents risks to populations and not communities and ecosystems as presented in the HWIR documentation.
- The use of no effects levels to develop estimates of ecological risk is overly conservative.

2.0 HWIR RISK ASSESSMENT: OBJECTIVES AND ORGANIZATION

2.1 Research and Development Objectives

There are two primary goals associated with this effort. First and foremost is the development of a science-based human and ecological exposure and risk assessment capability for HWIR99. A second goal (a relatively longer term goal) is to establish a base multimedia risk assessment technology that can be used to conduct technical assessments for regulatory development and implementation across the Agency, and to provide Agency scientists a centralized multimedia modeling technology for conducting research and developing new models.

Table 2.1 lists the specific objectives that must be achieved in order to accomplish the technical goals. The details of the approach for achieving these objectives is contained in Section 3.0.

The following definitions are presented in an effort to be clear with respect to the meaning of terms used in the objectives. The assessment strategy represents a detailed description of the technical approach designed to generate the HWIR constituent-specific waste concentration exit levels. The assessment strategy lays out, on paper, the individual technical components of the HWIR problem and the individual steps of the problem solution. Multimedia models are designed to simulate the constituent release, fate and transport, exposure, and risk occurring via multiple pathways involving soil, air, groundwater, surface water, and biota. The assessment data includes all chemical, site, source, exposure, and risk data required by the HWIR assessment. The assessment technology represents the computer-based technology (i.e., software and hardware) that will automate the HWIR assessment strategy. Included here are 1) a software system designed to manage execution of the assessment strategy, 2) the technical algorithms for each module (e.g., atmospheric transport), and 3) the numerous types and large quantity of data required to conduct the HWIR simulations. The science foundation for HWIR involves directly connecting and explaining the assessment strategy in the context of current science and modeling state-of-the art. The screening level approach to be taken in conducting the HWIR technical assessment of exposures and risk reflects a simplified view of the actual environmental system. The simplifications are made because, if performed properly, the resulting screening level assessment is sufficient to address the objectives of HWIR. More sophisticated strategies and tools may be available, but they would require resources (time and data) that are not available or necessary. Simplifications are made on the basis of the science and an understanding of the relationship between system behavior and the problem being solved. Peer review is a fundamental means by which to establish acceptance of the technical approach in the greater scientific community.

2.2 Interoffice Organizational Plan

This research and development plan is unique in that the EPA's Office of Research and Development and the EPA's Office of Solid Waste have committed to working together to design and build the assessment strategy and technology required for the Hazardous Waste Identification Rule. The OSW, with its perspective and expertise in regulatory development (i.e., policy and regulatory-based technical assessment) is joined by the ORD with its science and engineering expertise. While satisfaction of the short-term HWIR-specific objectives is the principal priority both OSW and ORD foresee the results of this effort significantly accelerating the realization of high priority long-term research, development, and other regulatory goals. OSW views the multimedia, multipathway, and multireceptor assessment technology that will result from this effort as the basis for a number of additional regulations under its charge. Having a single, state-of-the-art modeling technology will greatly enhance consistency

among programs. For ORD the long-term vision includes merging the science and modeling assessment of human and ecological exposure and risk. This movement is toward holistic understanding and the resulting assessment technology associated with multimedia, multipathway, and multireceptor exposure and risk assessment.

After a series of discussions it was decided that personnel from ORD and OSW would combine to form eight (8) regulatory-based research and development teams, each focusing on a major component of the HWIR. The eight research teams formed include:

1. Sources (i.e., Waste Management Units) Team,
2. Atmospheric Fate and Transport Team,
3. Groundwater Fate and Transport Team,
4. Surface Water / Watershed Fate and Transport Team,
5. Exposure Pathways and Receptors Team,
6. Risk Characterization Team,
7. Chemical and Biological Fate Team, and
8. Steering / Integration Team.

The teams are composed of a mix of personnel from OSW, ORD, and contract support, and with a mix of technical skills and experience appropriate for the tasks at hand. Each component team selected a team leader, developed a general charge statement, and conducted independent weekly conference calls beginning in April of 1997. In addition, the team leaders have participated in weekly conference calls of the Steering / Integration Team, which is charged with resolving the cross-cutting and coordination issues. To further support the fruitful debate, the teams entertained scientific inputs from various outside sources as appropriate. All these efforts resulted in the development of a unified approach to the refinement of the HWIR methodology that is responsive to the review comments, consistent with research and development capabilities and funding levels, and that is intended to satisfy the mandated regulatory schedules.

Table 2.1 HWIR99 Research and Development Objectives

- Develop revised risk-based technical assessment strategy
- Design site-based, multimedia, multipathway and multireceptor exposure and risk model
- Develop required assessment data (physical (site), chemical, biological, exposure and risk data)
- Develop computer-based assessment technology for implementing the assessment strategy
- Develop science foundation of the HWIR assessment strategy
- Conduct necessary peer reviews

3.0 REVISED RISK ASSESSMENT METHODOLOGY: TECHNICAL APPROACH

The conceptual foundation of the technical approach to achieving the HWIR99 goals is the risk paradigm and the associated relationship between a source of contaminant, its release to and transport through the environment, subsequent contact (i.e., exposure) with human and ecological receptors, and the resulting risk of health effects.

The objectives for HWIR99 presented in Section 2.1 reflect the major components and implementation tasks required in order to design, build, and apply a revised science-based technical assessment for HWIR. As discussed there are six principal components to the effort; an assessment strategy, a site-based multimedia multipathway exposure and risk model, assessment data, assessment technology, science support activities, and peer review. The following subsections are organized to describe the essential features of each of the components. First, technical basis of HWIR99 is presented in three subsections: technical requirements, assumptions and analytic basis underlying the HWIR99 effort are presented. Then, the HWIR99 technical assessment strategy is presented. The assessment strategy describes how the combination of exposure/risk models and data will be used to establish the exit criteria and develop regulatory thresholds. A description of the multimedia multipathway model is presented next. The model follows the risk paradigm and includes modules (i.e., sub-models) to simulate source release, transformation and transport, exposure, and risk. A description of the assessment data and the data collection strategies is then presented, followed by a description of the assessment technology intended to automate the assessment strategy. An important part of the overall approach for HWIR99 is to ensure that the technical assessment strategy reflects current environmental science and engineering based on the available computational resources and the regulatory time constraints. To this end a series of science support activities are planned. To complete the discussion of the technical approach a description of plans for peer review of the complete HWIR99 technical effort is presented.

To provide a risk assessment context to the discussions that follow, Table 3.1 presents the dimensions of HWIR99 Integrated Multimedia Risk Assessment, and Figures 3.1 and 3.2 depict the exposure pathways for human and ecological receptors, respectively.

Technical Requirements

In responding to the need to revise the HWIR assessment, the EPA has engaged in both HWIR related policy discussions as well as technical discussions to determine the specific direction to pursue in the next phase of HWIR (i.e., HWIR99). While these discussions are ongoing, results to date are significant and allow for the establishment of the research and development plan outlined in this document. Forming the foundation for the revised HWIR is a combination of technical requirements and key technical assumptions and policy decisions. The key technical requirements that must be satisfied by the technical assessment for HWIR99 are listed in Table 3.2.

Key Decisions and Assumptions

In addition to the list of requirements there are a number of key decisions and assumptions regarding the assessment of exposures and risks as well as the methods for establishing national exit criteria and for driving the national threshold levels. These decisions and assumptions reflect the manner in which certain requirements will be satisfied and form the analytic underpinning for the HWIR99 assessment strategy. They are presented to help frame the presentation of the detailed technical approach in subsequent sections.

- Regulatory threshold waste concentration limits are determined for each constituent of concern. The threshold levels are based on the evaluation of the nationwide impacts to the health of receptors of concern resulting from the management of the given chemical in Subtitle D units located throughout the U.S.

- The impacts to receptors of concern are evaluated for each chemical independent of the effects of other chemicals. The cumulative effects of different chemicals, acting simultaneously on a receptor are not considered.

- A waste concentration limit for each WMU type is derived independently.

- Nationwide impacts are determined by aggregating the impacts of individual waste management facilities. The individual waste management facilities represent actual sites located throughout the U.S. The location and physical characteristics of the sites (e.g., surface area, volume, number and type of waste management units) were determined from a statistical sample of industrial Subtitle D facilities. The sample represents a "snapshot" of industrial waste management facilities for the year 1986 throughout the U.S. The resulting impacts for the individual facilities in the sample are aggregated and extrapolated to the population of sites in the U.S. by using the sampling weights associated with each individual facility.

- Monte Carlo simulation methods that allow the calculation of uncertainty and variability in the measures of protection will be employed. The incorporation of uncertainty in the protection levels allows for the development of regulatory rules that result in more conservative regulatory levels as the uncertainty in risk predictions increases.

- The approach is designed to rely as much as possible on a site-specific data collection and modeling approach for the source (other than waste characteristics), fate and transport, and exposure characteristics of a facility. In the absence of site-specific data, data from regional and national distributions will be used.

- A waste management facility (WMF) can contain more than one type of waste management unit (WMU), and more than one WMU of each type. However, the impact of the sources is represented by modeling a single unit with source characteristics (e.g. area and volume) given by the average of the individual units.

- The assessment of the impact of a single waste management facility on receptors of concern is based on the consideration of near-field, long-term (chronic) impacts from the operation and closure of the waste management unit.

- The effects of the different WMU types within a site are considered separately in the exit-level determination decision context.

- For purposes of assessing risk the geographic boundary of a given site is defined by the area contained within a two-kilometer distance from the WMU boundary as defined by the unit area.

- Each site encompasses one or more exposure areas (or sectors). Receptors of each type in each exposure area are represented by a single receptor (representative receptor) with a weight

corresponding to the total number of receptors of that type in that exposure area.

- Receptors of concern include both human and ecological receptors that are located within the geographic boundary defined above. Both human and ecological receptors include receptors of different types (see Table 3.1).

- A receptor may be exposed simultaneously via multiple pathways, each involving different combinations of contact media and exposure routes.

- Human exposure routes to be considered include inhalation and ingestion. The dermal contact route is not being considered because of limited data as compared with those available for ingestion and inhalation and has been excluded from the risk assessment for HWIR99. Exposure media for human receptors include groundwater, soil, air, biota (vegetables, meat, dairy products, etc.).

- Ecological exposure routes include ingestion and direct contact. Exposure media for ecological receptors include surface water, soil, and biota.

- The evaluation of the impact on receptors of concern is performed for a fixed time, beginning at time t_0 until T_{max}. The value of T_{max} varies for different chemicals, but will not exceed 10,000 years as set by Agency policy.

- The total mass of a given chemical constituent that is managed in a WMU is a finite value, M_{Total}. The value of M_{Total} can be different for different unit types in a facility, but the waste concentration, C_w, is the same for all unit types in all facilities The total volume V_{Total} in which M_{Total} resides must not exceed the total available capacity of the WMU which is a measured site-specific quantity. The total mass of a constituent can be accumulated incrementally throughout the WMU's operating life.

$$M_{Total} = M(t_0) + \int_{t_0}^{t_{oplife}} Q_m(t)dt \qquad \textbf{(1)}$$

where: $M(t_0)$ = Mass of given chemical at time t_0

M_{Total} = Total mass of given chemical

t = Time ϵ $[t_0, T_{max}]$

$Q_m(t)$ = Net rate with which waste mass of given chemical is changed in the unit

= 0, when $t > t_{oplife}$

$$= \frac{d}{dt}(C_w \rho_{HW} V_{Win} - C_{Wout} \rho_{Wout} V_{Wout})$$

t_{oplife} = Unit operating life

C_W = Incoming waste concentration of given chemical

C_{wout} = Concentration of given chemical in the waste volume removed from the WMU

ρ_{HW} = Density of regulated (hazardous) waste.

ρ_{Wout} = Density of the waste volume removed from the WMU.

For some types of WMU, such as landfill, the total available storage capacity of the WMU is assumed finite and fixed, and no additional mass beyond the storage capacity can be added to the WMU (see Equation **(2)** below). Whereas for other types of WMUs, e.g., waste piles, waste mass is removed and replenished periodically during the operational lifetime of the WMU.

$$V_{Total} = V(t_0) + \int_{t_0}^{t_{oplife}} Q_V(t)dt \leq S_{WMU} \quad \textbf{(2)}$$

where: $V(t_0)$ = Waste volume at time t_0
V_{Total} = Total unit volume
$Q_V(t)$ = Net rate with which waste volume is changed in the unit
= $\frac{d}{dt}(V_{Win} - V_{Wout})$
= 0, when $t > t_{oplife}$
V_{Win} = Waste volume entering the WMU at time t
V_{Wout} = Waste volume removed from the WMU at time t
S_{WMU} = WMU's available storage capacity

- Mass balance in the waste management unit is maintained at all times. If the mass in the unit is exhausted through releases to the environment and/or degradation, no additional releases can occur from the unit.

Mass balance in the proposed approach is based on the following mass conservation equation:

$$\frac{dM(t)}{dt} = Q_m(t) - \sum_{ipr=1}^{N_{Pr}} R_{ipr}(t) \quad \textbf{(3)}$$

Integrating the above equation yields,

$$M(t+\Delta t) = M(t) + Q_m(t)\Delta t - \sum_{ipr=1}^{N_{Pr}} R_{ipr}(t)\Delta t \quad \textbf{(4)}$$

where $R_{ipr}(t)$ = Rate with which mass is released through process *ipr*
Δt = Time step size; and
N_{pr} = Number of physico-bio-chemical processes by which the mass is released from the waste management unit.

- The fate/transport components take the source releases from a WMU and distribute the mass through each medium to determine the concentrations of the chemical for each contact medium (e.g., air, groundwater, soil, surface water, plants) in each exposure area from time t_0 to T_{max}. The contaminant concentration for any contact medium at any point within an exposure area at a given time is given by the spatial average over the exposure area.

- Each receptor type in an exposure area within a site is represented by a series of T_{max} longitudinal cohorts. Each longitudinal cohort corresponding to a given receptor type has identical exposure

characteristics with the exception that the initial exposure conditions are lagged by one-year intervals from time t_0 to T_{max}. If t represents time in years, we can refer to each longitudinal cohort uniquely as cohort t. Each cohort t is assumed to be exposed to annual contact medium concentrations from the age of a years to $a + d_{fgh}$ years (from time t to time $t + d_{fgh}$), where d_{fgh} is the total exposure duration defined in Equation **(5)** below. Each cohort is allowed to age naturally and is immediately preceded and followed by two identical cohorts t - 1 and t +1, respectively, with $t = t_0$, $t + 1$, ..., T_{max}. Each receptor type for humans represents a distinct age group (the age at which exposure begins) and for each age group there is a series of cohorts. With the exception of the exposure concentration, the characteristics (e.g., exposure characteristics; location of receptors; exposure areas; number of receptors in an exposure area) of each cohort are the same. In general, each receptor type is assumed to reside within the exposure area during the exposure duration. A nationwide probability distribution based on the EPA's Exposure Factors Handbook data (USEPA 1997) will be used to simulate the exposure factors for each receptor type. The exposure factors for ecological receptors will be based on the EPA's Wildlife Exposure Factors Handbook (USEPA 1993).

- The response variables (e.g., CSF - cancer slope factor of the dose, population-level benchmarks) can vary between chemicals, receptor types (ecological receptors only), and exposure routes, but are assumed as a matter of policy to not exhibit variability (or uncertainty) between individual receptors of the same type within an exposure area.

- Some of terms used in this document are defined below for ready reference:

  Exposure pathway - The course a chemical takes from the source(s) to an exposed organism. Each exposure pathway includes a source, an exposure route, a contact medium, and the location of a representative receptor in an exposure area.

  Contact medium - The substance that transports the constituent(s) from the environment to an exposed organism. Contact media include, for example, surface water, groundwater, air, and soil.

  Exposure route - The manner in which a chemical(s) come(s) into contact with, or introduced into, an exposed organism. For example, exposure routes include inhalation, and ingestion.

  Exposure area - For each site, one or more exposure areas are defined in which receptors are located. In each exposure area, receptors of the same type are replaced by a representative receptor randomly located within the exposure area.

- The impact to each receptor type is evaluated in terms of risk measures (e.g., risk or hazard quotient) that provide a measure of the impact. In the case of carcinogens, (or non-carcinogens where inhalation and ingestion act on the same organ) the individual exposure route risks can be aggregated to estimate the aggregate risks.

- Risks can be described by pathway, media, and exposure route. If there are:

  b = 1, 2..., nb WMU types;
  e = 1, 2..., ne chemicals;
  f = 1, 2..., nf sites;
  g = 1, 2..., ng(f) exposure areas;

h = 1, 2..., nh receptor types;
i = 1, 2,..., ni(k) contact media;
j = 1, 2,..., nj(i,k) pathways associated with exposure route k and contact medium i;
k = 1, 2,..., nk exposure routes, and

for a representative receptor of type h in exposure area g of site f, then the pathway, media and exposure route risks are defined as follows:

8) The pathway specific risk ($PR_{befghijkt}(C_w)$) for chemical e at waste concentration $C_{w,}$ for an individual cohort t (that starts exposure at time t) associated with representative receptor type h for pathway j, involving exposure route k and contact medium i, in exposure area g, in WMU of type b in site f is given by the sum of the concurrent doses (doses in the same exposure period) to the receptor during exposure duration d_{fgh} :

$$PR_{befghijkt}(C_w) = \sum_{T=t}^{t+d_{fgh}} \frac{C_{befgijkT} \cdot I_{fghikT} \cdot EF_{fghikT} \cdot \beta_{ehk} \cdot \delta_d}{\Delta_e \cdot W_{fghT} \cdot 365} \quad \textbf{(5)}$$

where: $C_{befgijkT}$ = Annual concentration of constituent e, in contact medium over the exposure area associated with exposure route k and pathway j in exposure area g of site f in year T due to waste concentration C_w in WMU type b

I_{fghikT} = Daily intake (kg/day) of contact medium i associated with exposure route k and pathway j by cohort t associated with a representative receptor of receptor type h in exposure area g of site f in year T

EF_{fghikT} = Exposure frequency (days/yr) for cohort t associated with a representative receptor of receptor type h from media i associated with exposure route k in exposure area g of site f in year T

d_{fgh} = Exposure duration (yrs) for cohort t associated with a representative receptor of receptor type h in exposure area g of site f in year T

β_{ehk} = Carcinogenic risk potency (and the inverse of the reference dose RfD for non-carcinogens) for exposure route k for chemical e for cohort t associated with individual receptor m of receptor type h $(mg/kg/day)^{-1}$

Δ_e = Averaging time for chemical e (yrs)

W_{fghT} = Body weight for cohort t associated with a representative receptor of receptor type h in exposure area g of site f in year T

δ_d = Time step (1 year).

Figure 3.3 shows the relationship between the annual concentration in contact medium i associated with exposure route k and pathway j, $C_{befgijkt}$ (obtained from fate and transport component modules), and the pathway risk associated with the contact medium for a single cohort, $PR_{befghijkt}$. The figure demonstrates that the pathway-specific risk for a single longitudinal cohort t_1 is based on medium concentration averaged between time t_1 and time $t_1 + \Delta t$, where Δt is the exposure duration.

9) The contact medium specific risk ($MR_{befghikt}(C_w)$) for media i associated with exposure route k from chemical e for cohort t associated with representative receptor type h in exposure area g of site f for waste concentration C_w in WMU type b is given by the sum of the concurrent individual pathway risks corresponding to the exposure route and contact medium:

$$MR_{befghikt}(C_w) = \sum_{j=1}^{nj(i,k)} PR_{befghijkt}(C_w) \quad \textbf{(6)}$$

Media risks can be evaluated directly from media concentrations without the necessity to calculate pathway risks.

The pathway risk, as described in Equation **(5)**, is presented here in the event that the determination of pathway risks is necessary or of interest. However, for HWIR99, pathway risks may not be calculated due to the anticipated difficulties resulting from the computer storage and computational constraints.

10) The exposure route specific risk ($ER_{befghkt}(C_w)$) for a receptor cohort t associated with representative receptor of type h for exposure route k at time t, in exposure area g, for chemical e at site f for waste concentration C_w in WMU type b is given by the sum of the concurrent risks of the cohort from each medium i associated with exposure route k over the exposure duration d_{fgh}:

$$ER_{befghkt}(C_w) = \sum_{i=1}^{ni(k)} MR_{befghikt}(C_w) \quad \textbf{(7)}$$

- There are two types of aggregate risks, for cohort t of receptor type h, which are of interest: contact medium-specific aggregate risk, and receptor-specific aggregate risk.

In the case of a carcinogen (or a non-carcinogen where the exposure routes act on the same organ), the medium-specific aggregate risk ($AMR_{befghikt}(C_w)$) for medium i associated over all exposure routes from chemical e for cohort t associated with representative receptor of type h in exposure area g of site f from waste concentration C_w in WMU type b is given by the sum of the concurrent individual medium risk (defined by Equation **(6)**) for each exposure route:

$$AMR_{befghit}(C_w) = \sum_{k=1}^{nk} MR_{befghikt}(C_w) \quad \textbf{(8)}$$

The contact medium-specific aggregate risk may be used as an indicator of the relative significance of the medium in conveying risks to the receptor.

Similarly, the receptor-specific aggregate risk, $AR_{befght}(C_w)$, in the case of a carcinogen (or a non-carcinogen where the exposure routes act on the same organ), for a receptor cohort t associated with representative receptor of type h in exposure area g at time t from chemical e at site f and waste concentration C_w in WMU type b is given by the sum of the concurrent risks (ER) from each exposure route:

$$AR_{befght}(C_w) = \sum_{k=1}^{nk} ER_{befghkt}(C_w) \quad \textbf{(9)}$$

For carcinogens, if the receptor-specific aggregate risk exceeds a predetermined target risk or the maximum allowable risk threshold for the receptor, the receptor is said to be unprotected.

- Ecological risks are formulated in terms of a risk/hazard quotient type measure comparable to the human receptors. However, unlike human risk, ecological risk applies at the community and population level rather than at the individual receptor level.

  For example, the toxicity quotient for species that is exposed to constituent *e*, at site *f*, at time *t* is determined by

$$TQ_{befght} = \frac{CDI_{befght}}{CSCL_{eh}} \quad \textbf{(10)}$$

  where: TQ_{befght} = Toxicity quotient for chemical *e*, at site *f*, over exposure area *g*, for species *h*, at time *t*
  CDI_{befght} = Chronic daily intake for chemical *e*, at site *f*, over exposure area *g*, for species *h*, at time *t* (mg/L)
  $CSCL_{eh}$ = Chemical stressor concentration limit for chemical *e* and species *h* (mg/L)

  The chronic daily intake rate for species *h* that is exposed to chemical *e*, at site *f*, at time *t*, CDI_{befght}, is primarily a function of the following:

  Concentration of chemical in whole body prey (mg/kg)
  Daily quantity of prey ingested (kg/day)
  Fraction of contaminated material ingested
  Concentration of chemical in soil (mg/kg)
  Daily quantity of soil ingested (kg/day)
  Concentration of chemical in water (mg/L)
  Daily quantity of water ingested (L/day)
  Species-specific body weight (kg)

- Given that the impacts of different pathways can occur over significantly different time frames at a site and for a given individual receptor, all aggregations of doses and risks for a given cohort are carried out concurrently in time. Similarly all aggregations of protection measure statistics (e.g., number of receptors within a site that exceed a given target risk level) at the site are carried out concurrently in time.

  Figure 3.4 shows an example to illustrate how risks are aggregated concurrently in time. The example describes a case with two exposure pathways and one exposure route (ingestion of soil and ingestion of contaminated groundwater) for a representative receptor of type *h* for exposure area *g* at site *f* for a given waste concentration C_w of chemical *e* in a WMU of type *b*. The first two graphs show the pathway specific risks for each cohort t ($t = t_0, \ldots, T_{max}$) associated with the

receptor. The last graph shows the exposure route (ingestion) specific risk for each cohort at the site that results from the concurrent aggregation of the individual pathway risks at the given exposure area.

3.1 Assessment Strategy

The HWIR99 assessment strategy represents the conceptual approach for applying the combination of models and data to develop national exit criteria. The assessment strategy for HWIR99 includes a "regional site-based" approach. The regional site-based approach was developed as part of EPA's Composite Model for leachate Migration with Transformation Products (EPACMTP) and was approved by EPA's Science Advisory Board (USEPA 1995).

The assessment approach for HWIR99 reflects an Agency decision to base exit levels on an assessment of potential health risks occurring at Subtitle D facilities (i.e., sites) where HWIR99 waste management units may be located. The objective here is to base the national exit criteria (i.e., allowable wastestream concentration per HWIR constituent) on an assessment of risks under the widely varying environmental conditions, and receptor exposures associated with actual waste management units and locations.

The regional site-based approach embeds individual site-based assessments within a two-stage Monte Carlo simulation procedure. The overall objective of the iterative Monte Carlo procedure is to develop the nationwide distributions of risks and their uncertainty, as summarized by risk matrices, which can be queried to provide the basis for the development of the HWIR99 regulatory limits. The approach for describing the assessment strategy is to present first, in Section 3.1.1: the risk matrices, the intended output of the HWIR99 Technical Assessment; the protection measures which can be obtained by querying the risk matrices; and the regulatory framework, based on the proposed measures of protection, that establishes the procedure for determining the HWIR regulatory limits. Section 3.1.2 then describes the details of the Monte Carlo-based approach, including the general algorithm, and presents examples that illustrate the use of the proposed protection measures to establish the HWIR99 regulatory limits. A more comprehensive treatment of the HWIR99 Assessment Strategy is documented in a report entitled: "A Preliminary Framework for Finite-Source Multimedia, Multipathway and Multireceptor Risk Assessment: 3MRA"(USEPA 1998).

3.1.1 HWIR99 Strategy for Developing National Exit Criteria

The objective of the HWIR99 strategy for developing national exit criteria is to develop a national database of site-based exposure and risk information, the risk matrices, that can be queried in different ways to support Agency decision makers in the establishment and implementation of exit criteria. This section explains the contents of the database, the protection measures which define the different ways the database can be queried, and how the database/protection measures may be used to develop national exit criteria.

Section 3.1.1.1 defines the risk matrices that summarize the output of the HWIR99 Technical Assessment at each site. Section 3.1.1.2 presents the proposed protection measures that can be estimated by querying the risk matrices at each site. Section 3.1.1.3 outlines the process for aggregating the protection measures of the individual sites to estimate nationwide impacts. Section 3.1.1.4 outlines the regulatory framework for establishing the HWIR99 regulatory limits based on the nationwide measures of protection presented in Section 3.1.1.3, and extends the approach to the case where the protection

measures are characterized by uncertainty as well as variability. Finally, Section 3.1.1.5 discusses alternative measures of protection.

3.1.1.1 Risk Matrices: HWIR Technical Assessment Output

The HWIR technical assessment output can be summarized through risk matrices that facilitate the process of developing exit criteria. Four general risk matrix summaries are considered: pathway, contact medium, exposure route, and aggregate risk matrices.

Pathway Risk Matrix. For each site *f*, the baseline impacts for a given waste concentration C_w of chemical *e* in a WMU of type *b* can be summarized in a pathway risk matrix, $\boldsymbol{PR}_{bef}(C_w)$. The matrix consists of the pathway specific risks ($\boldsymbol{PR}_{befghijkt}(C_w)$) for each pathway *j* associated with each contact medium *i* and exposure route *k* for each cohort *t* associated with representative receptor of type *h* at each exposure area *g*. The pathway risks provide a baseline from which contact medium risks, exposure route risks, and aggregate risks can be computed for each cohort/receptor.

Contact Medium Risk Matrix. Contact medium risks can be summarized for each site by matrices for given values of the WMU type, chemical, and waste concentration. A contact medium matrix, $\boldsymbol{MR}_{bef}(C_w)$, consists of the contact medium specific risks ($\boldsymbol{MR}_{befghikt}(C_w)$) for each contact medium *i* which are the respective sums of pathway specific risks from nj(i,k) pathways connecting contact medium *i* and exposure route *k* for each cohort *t* associated with each representative receptor type *h* at each exposure area *g* of site *f* for a given waste concentration (C_w) of chemical *e* in WMU type *b*.

Exposure Route Risk Matrix. Exposure route risks can be summarized for each site by matrices for given values of the WMU type, chemical, and waste concentration. An exposure route matrix, $\boldsymbol{ER}_{bef}(C_w)$, consists of the exposure route specific risks ($\boldsymbol{ER}_{befghkt}(C_w)$) for each exposure route *k* for each cohort *t* associated with each representative receptor type *h* at each exposure area *g* of site *f* for a given waste concentration (C_w) of chemical *e* in WMU type *b*.

Aggregate Risk Matrix. An aggregate risk matrix, $\boldsymbol{AR}_{bef}(C_w)$, consists of the aggregate risks ($\boldsymbol{AR}_{befghkt}(C_w)$) for each cohort *t* associated with each representative receptor type *h* at each exposure area *g* of site *f* for a given waste concentration (C_w) of chemical *e* in WMU type *b*.

3.1.1.2 Protection Measures for Establishing HWIR99 Regulatory Limits

A protection measure is a quantified degree of protection provided to sites, receptors, etc. Protection measures are used to determine whether the impacts on human health and the environment are acceptable. Examples of protection measures include: percentage (or number) of receptors of type *h* that are exposed to risks below a predefined risk threshold or target risk; percentage (or number) of all receptors exposed to risks below the predefined target risk; and percentage (or number) of sites wherein all receptors (or greater than certain predefined percentage of all total receptors) are exposed to risks below a given target risk.

There are a number of alternative protection measures that provide a basis for establishing the HWIR99 regulatory limits. Some of these are presented in Sections 3.1.1.4 and 3.1.1.5; others will be developed as the process of selecting exit levels progresses through the implementation stage. In order to outline how regulatory exit levels will be developed, two candidate protection measures are presented in this section. The first proposed measure of protection is the nationwide distribution of risks for receptors

of concern. Specifically, a regulatory limit is acceptable if the percent of nationwide receptors of concern that exceed a given risk level falls below an acceptable number. This protection measure can be applied, without loss of generality, to individual receptors, or combinations of receptors, as required by policy consideration. The second measure of protection is the nationwide distribution of sites that are protected. A regulatory limit is acceptable under the second protection measure if the percentage of protected sites nationwide is greater than a given target level.

3.1.1.2.1 Protection Measure based on Receptor Risk

The estimation of the number of receptors that exceed a given risk level (i.e., pathway specific risk, contact medium risk, exposure route risk, or aggregate risk) at a given site is calculated from the corresponding risk matrix. Since all receptors are being exposed from the same source, all inferences at the site level are based on concurrent year/exposure duration comparisons. Therefore, for a given site, all calculations are carried out individually for each concurrent year/cohort. The calculation consists of two steps. First, the number of concurrent cohorts that exceed the target risk level is determined for each exposure area; and second, the number of concurrent cohorts from different exposure areas that exceed the target level are added together. The result is the number of receptors that exceed the target level at the given site.

The remainder of this section will focus on aggregate (receptor-specific) risk, since the principles apply equally to the other types of risks, there is no loss in generality in limiting the discussion to the aggregate risk case. More formally, let $RIND_{befght}(C_w, TR)$ represent an indicator that is set to 1 if the risk to cohort/year t associated with receptor m of type h in exposure area g of site f for waste concentration C_w of chemical e in WMU type b exceeds the target risk level TR; and is set to zero otherwise. Then in the case of human receptors, $RIND_{befght}(C_w, TR)$ is given by:

$$RIND_{befght}(C_w, TR) = \begin{cases} 1 & \text{if } AR_{befght}(C_w) \geq TR \\ 0 & \text{otherwise} \end{cases} \quad \textbf{(11)}$$

And in the case of ecological receptors, $RIND_{befght}(C_w, TR)$ is given by:

$$RIND_{befght}(C_w, TR) = \begin{cases} 1 & \text{if } TQ_{befght}(C_w) \geq 1 \\ 0 & \text{otherwise} \end{cases} \quad \textbf{(12)}$$

where $TQ_{befght}(C_w)$ = Target toxicity quotient.

Then the number of receptors of type h in year t in site f that exceed the target risk, TR, for waste concentration C_w of chemical e in WMU type b is given by

$$NXR_{befht}(C_w, TR) = \sum_{g=1}^{ng(f)} W_R(fgh)\ RIND_{befght}(C_w, TR) \quad \textbf{(13)}$$

where: $ng(f)$ = Number of exposure areas in site f
$W_R(fgh)$ = Weight for receptor type h in exposure area g in site f which is given by the number of receptors of type h in exposure area g in site f.

In the case of ecological receptors, information relating to population size of each representative receptor type h (species/community h) is not available, appropriate values for $W_R(fgh)$, other than unity,

may be assigned to respective representative receptor types, to reflect the relative importance of the species.

3.1.1.2.2 Protection Measure based on Protected Sites

The implementation of this protection measure requires the definition of a protected site. Again, there are a number of alternative definitions. In general, a site can be defined as protective for a given receptor type *h* if the percentage of receptors of concern of a given type *h* that exceed a target risk level, *TR*, is less than or equal to an acceptable value $q(h)\%$. In the most conservative case, $q(h)\%$ is set to zero for all *h*, so that a site is considered protective only if no receptors of the given type are exposed to risk levels above the target level.

More formally, let $SIND_{befht}(C_w, TR)$ represent an indicator that is set to 1 if site *f* is protective for cohort/year *t* associated with representative receptor of type *h* for waste concentration C_w of chemical *e* in WMU type *b*; and is set to zero otherwise. Then $SIND_{befht}(C_w, TR)$ is given by

$$SIND_{befht}(C_w, TR) = \begin{cases} 1 & \text{if } PXS_{befht}(C_w,TR) \le q(h)\% \\ 0 & \text{otherwise.} \end{cases} \quad (14)$$

where

$$PXS_{befht}(C_w,TR) = \frac{NXR_{befht}(C_w,TR)}{\sum_{g=1}^{ng(f)} W_R(fgh)} \times 100 \quad (15)$$

with: $W_R(fgh)$ = Number of receptors of type *h* in exposure area *g* at site *f*
$ng(f)$ = Number of sectors in site *f*

Alternatively, the definition of a protected site can be extended to include all receptors, so that a site is protected if the percentage of receptors of concern of a given type *h* that exceed a target risk level, *TR(h)*, is less than or equal to an acceptable value *q(h)%*, for all *h*.

More formally, let $ASIND_{beft}(C_w, TR)$ represent an indicator that is set to 1 if site *f* is protective for cohort/year *t* associated for waste concentration C_w of chemical *e* in WMU type *b*; and is set to zero otherwise. Then $ASIND_{beft}(C_w, TR)$ is given by:

$$ASIND_{beft}(C_w,TR) = \begin{cases} 1 & \text{if } PXS_{befht}(C_w,TR) \le q(h)\% \text{ for all } h; \\ 0 & \text{otherwise} \end{cases} \quad (16)$$

As in the case of the site based protection measure, since all receptors are being exposed from the same source, all inferences at the site level are based on concurrent year/exposure duration comparisons.

3.1.1.3 Nationwide Aggregation of Protection Measures

The previous section presented measures of protection that can be applied at a specific site. This

section presents the method used to extrapolate the site specific results to a nationwide level.

The first step in determining the protection measures at the nationwide level is to repeat the site specific assessment described in the previous section to all facilities which have been selected in the sample design. The result, as shown in a column in the $N_f \times N_i$ matrix in Figure 3.5 would be a vector of size N_f; where each element (cell), corresponding to each of the N_f sites, consists of a risk matrix summarizing the corresponding risks for each receptor/cohort, in each exposure area for the corresponding site. This vector of risk matrices can then be queried to determine the protection measures at the nationwide level for each receptor type for any given waste concentration, chemical and WMU type.

In general, if the number of receptors of type *h* in year *t* at site *f* that exceed the target risk, *TR*, for waste concentration C_w of chemical *e* in WMU type *b* is given by $NXR_{befht}(C_w, TR)$ as defined above, then the percentage of nationwide receptors of type *h*, $PXR_{beht}(C_w, TR)$, over all sites that exceed the target risk, *TR*, is given by:

$$PXR_{beht}(C_w,TR) = \frac{\sum_{f=1}^{nf} W_S(f) \cdot NXR_{befht}(C_w,TR)}{\sum_{f=1}^{nf}\sum_{g=1}^{ng(f)} W_R(fgh) \cdot W_S(f)} \times 100 \qquad \textbf{(17)}$$

where: $W_S(f)$ = Sampling weight for site *f*
$W_R(fgh)$ = Number of receptors of type *h* in exposure area *g* at site *f*
$ng(f)$ = Number of exposure areas in site *f*

The percentage of receptors that exceed a target risk level can also be calculated by combining all receptors. For example, the percentage of the nationwide total receptors, $APXR_{bet}(C_w, TR)$, that exceed the target risk, *TR*, is given by:

$$APXR_{bet}(C_w,TR) = \frac{\sum_{h=1}^{nh}\sum_{f=1}^{nf} W_S(f) \cdot NXR_{befht}(C_w,TR)}{\sum_{h=1}^{nh}\sum_{f=1}^{nf}\sum_{g=1}^{ng(f)} W_R(fgh) * W_S(f)} \times 100 = \sum_{h=1}^{nh} PXR_{beht}(C_w,TR) \qquad \textbf{(18)}$$

These equations apply equally to pathway, contact medium, exposure route and aggregate risk matrices.

Alternatively, the measure of the impacts can be described as the percentage of receptors of type *h* that are protected for the target risk level. Thus we can define the protection measure as the percentage of nationwide receptors $PPR_{bet}(C_w, TR)$ over all sites whose risk is below the target risk, *TR*. More formally, the nationwide percent protection for receptors of type *h* in year *t* for target risk, *TR*, for waste concentration C_w of chemical *e* in WMU type *b* is given by:

$$PPR_{beht}(C_w,TR) = 100\% - PXR_{beht}(C_w,TR) \qquad \textbf{(19)}$$

Similarly, the nationwide percent protection for all receptors, $APPR_{beht}(C_w, TR)$, in year *t* for target risk, *TR*, for waste concentration C_w of chemical *e* in WMU type *b* is given by:

$$APPR_{bet}(C_w,TR) = 100\% - APXR_{bet}(C_w,TR) \quad \textbf{(20)}$$

In the case where the protection measure is based on the percentage of protected sites, then the analogous definition of protection is $PPS_{beht}(C_w, TR)$, the nationwide percentage of sites that are protected for receptors of type *h* in year *t* for target risk, *TR*, for waste concentration C_w of chemical *e* in WMU type *b*, which is given by:

$$PPS_{beht}(C_w, TR) = \frac{\sum_{f=1}^{nf} W_S(f) \cdot SIND_{befht}(C_w, TR)}{\sum_{f=1}^{nf} W_S(f)} \times 100 \quad \textbf{(21)}$$

Similarly, the analogous definition of protection for all receptors is $APPS_{bet}(C_w, TR)$, the nationwide percent of sites that are protected for all receptors, in year *t* for target risk, *TR*, for waste concentration C_w of chemical *e* in WMU type *b*, which is given by:

$$APPS_{bet}(C_w, TR) = \frac{\sum_{f=1}^{nf} W_S(f) \cdot ASIND_{beft}(C_w, TR)}{\sum_{f=1}^{nf} W_S(f)} \times 100 \quad \textbf{(22)}$$

3.1.1.4 Regulatory Scheme

The previous section outlined a procedure for deriving an estimate of the nationwide impacts to receptors of concern. The impacts are defined by a "protection measure" based on either the percentage of receptors that are below the target risk level or the number of protected sites. A defined protection measure is determined for each site and exposure area by querying the relevant risk matrices that provide the raw risk data for all receptors. Depending on the protection measure and the specific constituent, the relevant risk matrices can include pathway specific, contact medium specific, exposure route specific, and aggregate risk specific matrices for a single type of receptor, for groups of selected receptor types, or for all receptor types.

In general, the derivation of a regulatory limit for a given chemical consists of two steps. First, derive for each WMU type a waste concentration limit that satisfies the protection measure criteria for the given WMU type; and second, set one or more regulatory limit (exit criteria) from the WMU specific concentration limits on the basis of policy decisions.

The remainder of the discussion is based on the receptor based protection measure for the criteria based on all receptors. The procedure outlined below is also applicable to the site based protection measure. Extension of the discussion to the site based protection measure would only require the replacement of every instance of $APPR_{be}(C_w,TR)$ with $APPS_{be}(C_w,TR)$. The extension to the receptor type specific case would require a similar replacement of the applicable notation.

For a given WMU type, the regulatory waste concentration is selected as the largest waste

concentration that meets the protection measure criteria. For the purposes of this discussion, the protection measure criteria are met if at least p% of the nationwide receptors have risk below the target risk for every concurrent set of cohorts. For the given protection measure, the relevant percent protection, $APPR_{be}(C_w,TR)$, for a given chemical and WMU type, occurs in the year with the minimum level of protection, i.e.:

$$APPR_{be}(C_w,TR) = MIN_t \ (APPR_{bet}(C_w,TR) \mid t_0 \leq t \leq T_{max}) \quad \textbf{(23)}$$

Focusing on the year with the minimum level of protection guarantees that every concurrent set of nationwide cohorts meets the protection measure. Given the protection criteria, a concentration waste limit, $C_{w,limit,b,e}$, for chemical e is selected as the regulatory limit for a given WMU type b, if $C_{w,limit,b,e}$ is the largest waste concentration such that:

$$APPR_{be}(C_{w,limit,b,e},TR) \geq p\% \quad \textbf{(24)}$$

Once the limits for each WMU type are determined, one or more regulatory concentration waste limits $C_{w,limit,b,e}$ for chemical e are selected from the WMU specific limits based on policy considerations.

The protection measures, however, are characterized by uncertainty. In the presence of uncertainty, the protection measure is modified to include the additional criterion that the percent protection must be met with at least a specified level of confidence. An example of this modified protection measure is that 90% of the nationwide receptors of concern would be exposed to risks less than 10^{-6} with at least a 95% level of confidence (probability).

For the uncertainty case, the output data base used to derive the protection measures consists, as shown in Figure 3.5, of a matrix rather than a vector of risk matrices. In effect, the $N_f x N_i$ output risk matrix consists of N_i iterations of the single vector of risk matrices presented in a column in Figure 3.5; where each column represents an alternative realization of the risk matrices resulting from the uncertainty in the characteristics that describe a given simulation scenario.

For a given chemical waste concentration, each column (IT=1,...,N_i) of the output data base can be queried separately to determine IT different values of the minimum nationwide percentage of receptors that are protected for a given target risk level, $APPR_{be}(C_w,TR,IT)$ for a given chemical and WMU. This effectively results in N_i separate estimates of $APPR_{be}(C_w, TR, IT)$, IT=1,2,...,N_i that reflect the uncertainty in their prediction. Together, the N_i iterations of APPR can be used to establish confidence levels (or probability values in a Bayesian context) that the given protection measure will be met. A description of the Monte Carlo algorithm used to generate the $N_f x N_i$ output risk matrix, as well as examples describing how the nationwide exit levels are derived are presented in section 3.1.2.

This discussion applies to both human and ecological receptors. Each can be addressed with the proposed framework, but must be addressed separately. In the case of humans, the primary protection measures will involve the nationwide percentage of protected individual receptors; while in the case of ecological receptors, the primary measures involve the nationwide percentage of receptor species/communities. The measures are not directly comparable. Therefore, a separate regulatory limit is derived for humans and for ecological receptors. The final limit(s) is (are) given by the most restrictive of the two.

There are other alternative measures of protection that could be used to derive regulatory limits. The protection measure based on the percentage of all receptors protected at a given aggregate target risk level

provides a convenient starting point for presenting the methodology. One alternative is to focus on the number of protected sites rather than receptors. A discussion of other alternative measures of protection is presented in Section 3.1.1.5.

3.1.1.5 Alternative Measures of Protection

The previous section outlined a regulatory framework based on two protection measures. The first is a function of the percent of nationwide receptors that are exposed to risks less than a given target risk level. The second is a function of the percentage of nationwide that are protected. There are a number of other alternative definitions of protection which could be queried from the output database. One alternative measure is a variation on the receptor-based percent protection measure that involves both primary and secondary criteria. The primary criteria would be met if at least p% of all of the receptors have risk below the target risk level; and the secondary criteria would be met if no less than q% of any given type of receptor have risk below the target risk level with p%>q%. Both criteria would have to be met with a minimum level of confidence in order to satisfy the overall protection criteria.

Another alternative involving primary and secondary criteria would be to use the same primary criteria, but select the secondary criteria to include a separate criteria for the average risk (or some other statistical measure) of all receptors, or subsets of receptors, that exceed the primary criteria. Thus for example, a given waste concentration would meet this protection measure criterion if at least p% of all receptors had risk less than the primary target risk, and the average risk of the receptors, for receptors that exceeded the primary target risk, is below a secondary target risk level. Again, both criteria would have to be met with a minimum level of confidence in order to satisfy the overall protection criteria.

There are numerous other possibilities that could be queried from the output risk matrices, including variations on the site-based protection measure, and variations on the concurrent cohort requirements. In particular, the regulatory framework presented in Section 3.1.1.4 for both the risk and site based protection measures is based on concurrent cohorts both within a site as well as between sites. An alternative is to develop the regulatory framework so that the requirement for concurrent cohorts within a site is maintained as discussed in Sections 3.1.1.2.1 and 3.1.1.2.2, but does not require concurrent cohorts between sites.

Ultimately, the criteria will take the form that a regulatory waste concentration is selected if it meets the adopted measure of protection with a given level of confidence. The proposed two-stage Monte Carlo framework is sufficiently general to accommodate these options.

3.1.2 Monte-Carlo Approach

This section presents a general outline of the Monte Carlo approach proposed for the production of the $N_f \times N_i$ output matrix that forms the basis for the regulatory framework outlined in Section 3.1.1.2. The remainder of this section is organized as follows. The objectives of the Monte Carlo procedure are presented in Section 3.1.2.1. The proposed Monte Carlo implementation strategy is presented in 3.1.2.2. The latter section includes a general outline of the proposed Monte Carlo method, together with sample queries and outputs.

3.1.2.1 Monte-Carlo Objectives

The proposed Monte-Carlo procedure is designed to meet the following objectives:

- Provide an estimate of the uncertainty in the estimated measures of protection associated with a regulatory waste concentration (C_w);
- Provide a mechanism for accounting separately for variability and uncertainty through a two-stage Monte Carlo algorithm;
- Provide a (value of information) basis for comparing the potential benefit (reduced prediction uncertainty) versus cost of future sample collection efforts;
- Provide a flexible framework that can accommodate alternate policy formulations including different definitions of measure of protection, and both waste and leachate concentration regulatory limits; and
- Comply with the U.S. EPA's Guiding Principles for Monte Carlo Analysis.

3.1.2.2 Monte Carlo Implementation Strategy

3.1.2.2.1 Ideal Conditions

The validity of a Monte Carlo implementation depends ultimately on the amount, type, and quality of the data available to estimate the probability distributions of the Monte Carlo inputs. The fundamental question that the proposed framework is designed to answer for a given chemical can be stated in the following way: If a "receptor of concern" is defined as all receptors of a given type that currently reside within a specified radius of all currently existing Subtitle D waste management facilities in the continental U.S., then what percent of the total number of current receptors of concern would be exposed to risk/hazard quotient levels above specified target levels if each facility were to manage the chemical at the same concentration at all facilities.

Clearly, any attempt to determine nationwide risks is a challenge. Performing a risk assessment at a site-specific level is difficult enough. Extending the site-specific effort to a nationwide scale introduces an additional, and significant, layer of difficulty. Ideally the nationwide risk assessment would be performed in four steps. First, identify all current Subtitle D waste management facilities in the continental U.S. Second, collect all of the site-specific data necessary to characterize each facility and associated site/receptor characteristics, and relevant processes. Third, develop a site-specific mathematical model to predict the impacts at each site; and fourth, run the site-specific model at each of the sites and aggregate risks to predict the nationwide impacts to the "receptors of concern".

Under ideal conditions, the HWIR99 Monte Carlo approach would be based on the following database:

11) A statistically designed sample of waste management units from the target population of WMUs in the U.S.
12) Direct measurement of the facility/site characteristics (e.g., unit area and volume; depth to groundwater; aquifer thickness; hydraulic conductivity; hydraulic gradient; distance to nearest well; number, location and physiologic/behavioral characteristics of receptors) at each sampled site; and
13) Availability of calibration/validation data sets to estimate data measurement and component model prediction error structures.

This ideal data set, together with sufficient computational resources, provides a solid foundation for the identification and estimation of the relative magnitude of applicable sources of uncertainty (e.g., sampling errors, data errors, model prediction errors, non-sampling errors) and variability; and the development of a two-stage Monte Carlo algorithm that incorporates and separates the effects of uncertainty and variability. This separation allows for the estimation of uncertainties associated with given measures of variability, which form the basis of the regulatory framework presented in Sections 3.1.1.2. For an introduction to the topic of uncertainty and variability in HWIR99, the reader is referred to Appendix A. The appendix provides a summary of the various sources of uncertainty and variability, and a discussion of the importance of separating uncertainty and variability.

3.1.2.2.2 Limitations in Implementation of the Monte Carlo Approach

In reality, data limitations, constraints on time and computational resources, and the limits of our scientific knowledge impose a number of departures from the ideal conditions. First, the physical, chemical, biological and behavioral processes involved are complicated and our knowledge is limited. The required analysis, by necessity, involves a mathematical modeling approximation of the complex causal relationships between waste concentration and the impacts to receptors.

Second, the development of a site-specific model for each facility is impractical. This implies that a generic model will need to be developed that can be applied at all sites. A generic model is generally less able to approximate causal relationships than a site-specific model. Additionally, scheduling constraints require that the generic model must be computationally efficient, which forces even greater pressure to make trade-offs between model simplicity and model validity.

Third, resource constraints dictate that the analysis can only be performed at a subset of all of the facilities in the U.S. Ideally the subset of sites represents a statistically representative sample of the target population so that inferences from the sample can be extrapolated to all of the facilities in the U.S. However, the sample size will directly affect the uncertainty of the inferred nationwide impacts.

Fourth, resource constraints dictate that only a part of the model input data can be collected for all sampled facilities at the site-specific level. The remainder of the model inputs must be characterized through regional and/or national data bases, which raises the question of the representativeness of the data to the target population. Examples of parameters that cannot be practically obtained at the site specific level for all sites include receptor exposure/response physiologic and behavioral factors, most hydrogeologic parameters, and climatic characteristics. Finally, computational constraints, data storage requirements, and the spatial resolution of available data impose the need for spatial and temporal averaging at potentially large scales at all levels of the analysis, including the fate/transport and receptor models.

Under these limitations, additional sources of errors will be introduced in the analysis (e.g, errors due to non-representative data), and not all sources of uncertainty or variability (e.g., correlations) can be estimated or identified readily, even in the long run. As a result, estimates of uncertainty in estimated measures of variability obtained from a two stage Monte Carlo will only reflect the identified sources of uncertainty for part of the variability. The unestimated sources of uncertainty will either not be reflected in the uncertainty (e.g., sampling errors, prediction model errors), or remain combined with the variability and not be reflected in the uncertainty (e.g., data measurement errors).

Ultimately, the issue is not whether to incorporate all sources of uncertainty and variability, but

rather whether the sources of variability and/or uncertainty that are not included have a significant effect on the regulatory decisions. The key is to eliminate the sources of variability and uncertainty that have the least impact while meeting the budgetary, scheduling, and computational capacity constraints imposed on the problem.

3.1.2.2.3 HWIR99 Site Based Approach Monte Carlo

This section presents a proposed Monte Carlo structure to support the regulatory framework outlined in section 3.1.1.4. Although this data base is a departure from the ideal situation discussed above, it provides a number of advantages within the data, budgetary and scheduling constraints imposed on the problem. The structure reflects the anticipated compromises made to adjust to limitations associated with the available data and computational constraints, while retaining to the extent possible the site-specific and probability sample characteristics of the ideal data set. In particular, the currently available data set consists of a combination of site-specific measurements at existing WMU facilities selected on the basis of a stratified random sample for selected parameters, together with regional and national databases of surrogate parameters. Specific elements of the data base include:

1) A probability subsample of 200 WMU facilities from a stratified sample national survey of WMU facilities (USEPA 1986). This data set provides site specific measurements for facility characteristics including location and WMU geometries.
2) Site specific evaluations conducted at each of the 200 WMUs in the subsample to determine site-specific parameters.
3) Regional databases consisting of non-probability samples of surrogate hydrogeologic parameters and meteorologic parameters that allow correlation structures to be established; and
4) National databases consisting of non-probability samples of surrogate environmental media characteristics, the (physiologic and behavioral) exposure and response characteristics of the receptors, and the physical, chemical, and biochemical properties of the chemical constituents.

Given the limitations in the available data, it is anticipated that the initial focus of the Monte Carlo implementation effort will be on significant sampling error sources of uncertainty, and between site spatial variability of facility/site characteristics. Between individual variability of receptor characteristics, data measurement errors and model prediction errors will not be addressed initially. They will only be addressed as schedule and resource constraints permit, and as dictated by the results of sensitivity analyses. Additionally, the limitations in the data structure introduce potential non-sampling errors whose magnitude would be difficult to estimate. These errors will not be addressed. As a result, the estimated uncertainties will underestimate the true uncertainties

The Monte Carlo algorithm will follow the general form of the two stage Monte Carlo presented in Section 3.1.2.2.3.1. The exact form of the algorithm will depend on the type and amount of available data, the number and types of variability and uncertainties that will be incorporated, and the methods used to model the variability/uncertainty terms. The development of the algorithm will be incremental, moving forward in different stages of refinement as dictated by different testing protocols, including sensitivity analysis and computational benchmarks, and any additional data that may become available in the future.

In addition, the methods used to estimate/model the variability and uncertainty terms will depend

on the amount and type of available data, and the computational burden associated with estimation/simulation procedure. It is anticipated that the initial approach will use a combination of empirical and fitted distributions to describe variability. Parametric and non-parametric bootstrap methods are available to address uncertainty due to site sampling errors. In all cases, the estimation and reporting of the variability and uncertainty terms will conform to the principles of good practice for the use of Monte Carlo techniques adopted by the U.S. EPA (1997)

3.1.2.2.3.1 General Monte Carlo Algorithm

A general and idealized form for the HWIR99 Monte Carlo approach is presented in the flowchart in Figure 3.6. The flowchart is designed to illustrate and help explain the general steps of the approach for the primary protection measure described in previous sections. Specific details of the algorithm are not included since these will depend on the protection measure adopted, the type and amount of data available to estimate the needed probability distributions, the sources of variability and uncertainty that are significant, correlations among parameters, the methods used to estimate and model the various sources of variability and uncertainty, and computational efficiency considerations.

In its present form, the algorithm produces an output $N_f x N_i$ matrix that can be queried, as described in Section 3.1.2.2.3.2, to determine whether a given waste concentration meets the protection measure criteria within a given level of confidence. For the purpose of this illustration, each cell of the $N_f x N_i$ matrix, $MR_{bef}(C_w,IT)$ corresponds to the contact medium risk for a given waste concentration, chemical, WMU type, site, and iteration (*IT*). Alternatively, the algorithm could also have been written so that each cell corresponds to the pathway specific risk. In practice, since the storage of the risk matrices at the pathway risk level may impose excessive computational requirements, the output database will likely be based on the contact medium risk matrices. The algorithm is sufficiently general that the basic elements apply whether interest is on the pathway or contact medium matrices.

Each row of the matrix corresponds to a sampled facility; and each column represents an alternative realization of the risk matrices resulting from the uncertainty that characterizes a given simulation scenario. The level of confidence is derived by determining the protection measure independently for each iteration. The resulting N_i estimates of the protection measure represent a conditional distribution that allows the estimation of the probability (confidence level) that a given measure of protection will be met for a given waste concentration, C_w.

At this stage of development, the conditional distribution represents the uncertainty in the protection level only due to sampling error for a given value of C_w. It does not address data measurement errors, or model prediction component errors. Additionally, it does not address the more general case that includes uncertainties due to misspecification of the probability distribution functions (pdf) and parameters used to describe the different uncertainties, misspecification of the assumed pdf models that describe variability, errors associated with non-probability samples, or sampling of non-target populations. Such sources of uncertainty can be evaluated through subjective measures, but are not addressed in this example. Ultimately, the decision on whether to incorporate a source of uncertainty will depend on the results of sensitivity testing to determine the significance of each source relative to the selection of the regulatory waste concentrations.

For this example, sampling error uncertainty for input parameters not measured directly at each site is incorporated through a Bayesian and/or parametric bootstrap approach. In the actual case, a combination of parametric and nonparametric methods are possible. The specific form that will be

adopted will depend on the type and amount of data available to estimate the needed probability distributions.

Sampling error uncertainty in input parameters that are measured directly at each site for this example is simulated in the algorithm by a nonparameteric bootstrap of the facility within the inside loop. Each time the facility is selected in a bootstrap sample, all of the site-specific information measured at the facility is included in the sample.

The algorithm starts at the outer loop by generating and storing the parameters of the probability distribution functions that describe the between site variability of the various model input parameters that are not collected at each site. That is, those parameters whose between site variability will be based on regional and/or national distributions. The probability distribution function parameters are generated from probability distributions that reflect the uncertainties in their estimation. Examples of input parameters that will not be collected at the site-specific level include climatic, hydrogeologic, ambient water quality, physiologic and behavioral receptor exposure factors, and chemical specific characteristics.

Note that the pdf parameters generated in the outer loop remain fixed for all facilities for a given iteration. For example, suppose the pdf that describes the between facility variability of groundwater temperature at the national scale is normally distributed with some mean and variance. Then in order to generate the groundwater temperature for each of the N_f facilities in the given iteration, the mean and variance of the groundwater temperature pdf are generated in the outer loop. Assuming that the mean and variance generated in the outer loop are 20°C and 40 $(°C)^2$, respectively, the groundwater temperatures for all N_f facilities in the given iteration are generated from a normal distribution with mean of 20 °C and variance of 40 $(°C)^2$. The pdf for the groundwater temperature in the next iteration would have a different mean and variance which reflect the uncertainty in the parameters due to sampling error. In the case of parameters that are characterized by regional probability distributions, the pdf parameters will vary between regions within an iteration, but the pdf parameters of a given region will remain constant for all sites within a region within an iteration.

The inner loop begins after generating in the outer loop the parameters of the pdfs that describe the between facility variability of the input parameters that are not measured at the site. Facilities in the sample were randomly selected to represent the nation-wide population of industrial facilities that generate Subtitle D non-hazardous waste and handle it on-site. Bootstrap sampling/analysis can be used. Weights can be incorporated into this process which account for several known sources: sampling with replacement from finite population; and size of facilities.

The next step in the algorithm involves generating the remaining input parameters that were not measured at the site but are needed to describe a simulation scenario for the given site. These parameters are generated using the corresponding pdfs, conditional on the fixed pdf parameters generated in the outer loop. The conditional pdfs reflect variability of the parameters between sites, between sectors at a site, and within a site as applicable, as well as any relevant correlations between parameters.

Once the site/facility scenario is generated, the next twenty steps of the algorithm involve the calculation of the pathway risk matrices, $PR_{bef}(C_w(v), IT)$ for every pathway, or contact medium risk matrices, $MR_{bef}(C_w(v), IT)$ for every contact medium, for the representative receptor of every receptor type at the site for every chemical, WMU type and waste concentration. There are a number of intermediate steps involved in the calculation of the risk matrices that are not shown in the algorithm. The first of these steps involves using the input parameters generated for the facility to calculate the exposure zone

concentrations for each contact medium associated with each pathway and each cohort of each representative receptor of each type at the site for each chemical, WMU type and waste concentration.

The next step involves using the exposure factors (e.g., exposure duration) generated in the second step for each representative receptor of each type at the site to calculate the risk matrices for each cohort of each representative receptor of each type, for each chemical, WMU type and waste concentration. The calculation of risk, by policy decision, does not incorporate model error.

These steps are repeated for all N_f selected sites to calculate the N_f set of risk matrices for all sites in the given iteration. The outer loop is then repeated N_i times to produce the $N_f x N_i$ sets of risk matrices that provide the database that is queried in the next section of the algorithm.

3.1.2.2.3.2 Output Queries

In general, for any measure of protection, each of the N_i columns in the $N_f x N_i$ matrix can be queried to produce one estimate of the protection measure. Together, the N_i estimates of the protection measure can be used to create a probability distribution that a) describes the uncertainty in the protective measure; and b) provides an estimate of the probability (uncertainty) that the protection measure will be met.

The rest of the algorithm, as presented in Figure 3.7 illustrates how the querying of the $N_f x N_i$ sets of matrices can be used to select a regulatory limit for each chemical in the case where the protection measure is the nationwide percentage of all receptors that are protected for a given target risk level.

The query process is initiated by specifying a trial waste concentration, C_{wbe}, for a given chemical and WMU type. The first step involves calculating from the corresponding sets of N_f pathway risk matrices, $PR_{bef}(C_{wbe},IT)$, f=1,...,N_f, for the given chemical, waste concentration and WMU type b, the nationwide percentage of receptors that are protected at the target level risk TR for each cohort t in iteration IT, $APPR_{bet}(C_{wbe},TR,IT)$. Note that if C_{wbe} was not specifically included as one of the waste concentrations used in calculation of the $N_f x N_i$ matrices in the first part of the algorithm, the nationwide percent protection can be estimated by interpolating values of the matrices corresponding to waste concentrations that bound C_{wbe}.

The nationwide percentage of receptors that are protected at the target level risk TR for the given waste concentration $\mathbf{C_{wbe}}$, WMU type b and chemical e, for iteration IT, $APPR_{be}(C_{wbe},TR,IT)$, is then calculated by selecting the concurrent cohort/year t that gives the minimum percent protection:

$$APPR_{be}(C_{wbe},TR,IT) = MIN_t \left(APPR_{bet}(C_{wbe},TR,IT) \mid t_0 \le t \le T_{max}\right) \quad \textbf{(25)}$$

Repeating the process for all iterations, gives N_i values of the measure of protection, $APPR_{be}(C_{wbe},TR,IT)$, IT=1,2,...,N_i that can then be used to estimate whether the trial waste concentration, C_{wbe}, meets the percent protection criteria for the given WMU type and chemical with a sufficiently high probability.

If the trial waste concentration does not meet the protection criteria, a new waste concentration is tried until the largest concentration that meets the protection criteria is found. Although not explicitly addressed in the flowchart, it should be noted that the process of selecting alternate waste concentrations can be optimized by using efficient search techniques.

The process is repeated for each WMU type for the given chemical to yield the largest waste concentration limit, $C_{w,limit,b,e}$ for each WMU type (b=1,...,N_b) that meets the protection criteria. One or more regulatory limits for the given chemical, $C_{w,limit,e}$, is selected among the limits established for each WMU type on the basis of policy considerations. The process is repeated for each chemical to obtain a regulatory waste concentration limit for each chemical.

3.1.2.2.3.3 Example Monte Carlo Output

This section presents examples of output that can be obtained by querying the data base generated by the two-stage Monte Carlo algorithm discussed in the previous section. Figure 3.8 presents an example corresponding to a query for a target risk level of 10^{-6} from the N_i (columns) iterations of risk matrices corresponding to a waste concentration of 10^{-3} mg/kg. The figure indicates that there is a 5% chance that the level of protection (% of receptors that would be protected at the target risk level for the given waste concentration) would be less than or equal to 85%. Similarly, there is a 25% chance that less than or equal to 93% of the receptors would be protected at the target risk level for the given waste concentration.

The result of repeating the query for different target risk levels for the same waste concentration 10^{-3} mg/kg is illustrated by Figure 3.9, which presents the uncertainty in the percent of protected receptors for each risk level. From Figure 3.9, it can be inferred that there is a 95% chance that setting the waste concentration regulatory limit to 0.001 mg/kg, would result in at least 85% of the receptors protected to a 1E-6 risk level (*or 5% chance that, at the risk level of 1E-6, less than 85% of the receptors will be protected*), and at least 90% of the receptors protected to a 1E-5 risk level. Similarly, there would be a 95% chance that at least 95% of the receptors would be protected to the 1E-4 risk level, and at least 50% of the receptors would be protected to the 1E-7 risk level.

Querying the output data base for different waste concentrations can produce the set of graphs such as those shown in Figure 3.10. The figure shows how the percent protection varies as a function of the target risk, the waste concentration and the confidence limit; and can be used to select the waste concentration that meets a specified protection measure. These types of figures could also be produced for subsets of receptors to investigate the effects of selecting a waste concentration on secondary protection measures.

In particular, if the exit level criteria requires that at least 85% of the receptors must be protected at the 1E-6 risk with at least a 95% confidence level, then the exit level would be 0.001 mg/kg. If on the other hand, if the exit level criteria requires that at least 90% of the receptors must be protected at the 1E-6 risk with at least a 95% confidence level, then the exit level would have to be less than 0.001 mg/kg. In this case, Figure 3.10(a), would be used to determine the appropriate exit level.

As is evident by the figures presented in this section, the most notable effect of introducing uncertainty in the estimation of the protection measures is that the regulatory criterion for accepting a waste concentration limit must be modified to incorporate a minimum probability that the protection level will be obtained.

3.2 HWIR99 Site-based Assessment Model

At the core of the HWIR99 technical approach is a modeling-based protocol for estimating the release, fate and transport, exposure, and risk associated with the disposal of hazardous chemicals at

Subtitle D facilities. To satisfy technical requirements for site-based exposure and risk assessment (discussed in Section 2.2), a comprehensive, multimedia, multipathway pollutant exposure and risk assessment model (Multimedia Multipathway Simulation Processor - MMSP) is being developed. The MMSP is contained within a larger software system (FRAMES-HWIR Technology Software System) designed to automate the entire HWIR99 assessment strategy as described in Section 3.1. The greater FRAMES-HWIR Technology Software System is described in Section 3.4. Described in this section are the individual modules (i.e., sub-models) that make up the MMSP. The MMSP combines existing media-specific pollutant fate and transport models with newly developed models for simulating source release, fate and transport in a watershed, and exposure of human and ecological receptors via multiple pathways. Figure 3.11 shows the various modules and their relative position within the MMSP. A summary description of each of the sub-models (modules) that make up the MMSP is provided here. This summary includes a description of, 1) relevant comments received in response to the 1995 HWIR proposal, 2) requirements and alternative approaches for HWIR99, 3) the module itself, and 4) limitations associated with the module design.

3.2.1 Source Modules (Land Application Unit, Waste Pile, and Landfill)

3.2.1.1 Purpose

Source modules were developed for land application units (LAUs), waste piles (WPs), and landfills (LFs) to provide estimates of annual average surface soil constituent concentrations and constituent mass emission rates to air and groundwater. Additionally, LAU and WP source models have been combined with a watershed model to provide estimates of constituent mass flux rates from runoff and erosion to a downslope waterbody, as well as surface soil constituent concentrations in downslope buffer areas. Because the LAU and WP are considered in a watershed context, they are also referred to as "land-based" sources. The fundamental algorithms used for the LAU, WP, and LF are similar and these source models are discussed together here for this reason. An exception to this similarity is that the landfill is assumed to not be subject to stormwater runoff and erosion, and is not considered in a watershed context.

3.2.1.2 Summary of Major Comments from 1995 Proposal

The major comments that are relevant to the LAU, WP, and LF source models are summarized below.

- Lack of a true multi-pathway approach -- Both the US EPA Science Advisory Board (SAB) and the Public Commenters were critical of the single most limiting pathway anaylsis used in HWIR 95. Both concluded that a true, simultaneous, multipathway analysis is required.

- Mass balance violations -- Here, too, the SAB and Public Commenters were in agreement. Both commented that a mass balance approach is necessary for the HWIR analysis, and was lacking in the HWIR95 analysis.

- Lack of validation -- The SAB was critical of the lack of effort to validate the model components of the HWIR 95 analysis.

- Need to model waste constituent concentrations (C_s) in soil as a function of time and depth. -- In HWIR95, constituent concentrations in soil (for the LAU) were assumed uniform in a given depth

of soil, and were incremented only with the addition of constituent mass, with no decrement in C_S due to volatilization losses, and no upper limit on C_S. SAB was critical of this modeling approach due to its lack of mass balance and also due to its lack of ability to recognize a C_S sufficiently large as to be indicative of the presence of a non-aqueous phase liquid (NAPL). Public commenters were also critical of this approach, and noted the importance of modeling C_S as a function of time and depth given the need for estimates of surface soil concentrations (for calculation of mass losses due to dust emissions and erosion), which could be significantly different from depth-averaged constituent concentrations, particularly for volatile constituents that are depleted from surface soils rapidly.

- Need to consider other removal processes -- Public Commenters were critical of the lack of consideration of first order biological and chemical degradation in HWIR 95.

- Simplistic treatment of partition coefficients -- SAB expressed concern that HWIR 95 made extensive use of partition coefficients (i.e., K_d, soil-water partition coefficients) without adequate treatment of the factors that can affect K_d, such as characteristics of the chemical, the medium, and the method of measurement.

3.2.1.3 Requirements for HWIR99 and Approaches Considered

Based on the needs for HWIR99 and the comments received on the HWIR95 proposal, the following features were identified as the major requirements of the land-based source emission models for HWIR99 :

- Simultaneous estimates of constituent mass losses through different pathways should be provided to allow a true, multi-pathway, exposure/risk estimate,
- Constituent mass balance should be maintained,
- Constituent concentrations in the medium of interest (waste or soil) should be estimated as function of time and depth,
- Constituent mass loss processes simultaneously modeled should include:
  - ♦ 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,
  - ♦ first-order losses, including:
    - abiotic and bio-degradation
    - 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 (LAU and WP only), and
    - surface run-off of aqueous phase constituent mass (LAU and WP only),
- Waste additions/removals should be accounted for to simulate active facilities,
- Contaminant concentrations in soil (or waste) that are sufficiently high as to be indicative of the presence of NAPL should be flagged, and
- All constituent flux rates and contaminant concentrations should be long-term (annual) averages.

A soil column model was developed to describe the dynamics of constituent mass fate and transport within non-wastewater WMU's and, optionally, in the unsaturated soil below. Because it is applied in all the WMU source emission models developed, it is referred to as the Generic Soil Column

Model. Governing equations are similar to those used by Jury et al. (1983, 1990) and Shan and Stevens (1995). However, the analytical solution techniques used by these authors were not applicable to the source emission models primarily because of the need to consider the periodic addition of constituent mass to each WMU and enhanced constituent mass loss rates in the surface soil (e.g., due to runoff, erosion, wind and mechanical processes). For HWIR99, a new quasi-analytical solution technique was developed that is computationally efficient and sufficiently flexible to allow consideration of the unique design and operational aspects of each WMU under consideration. An alternative would have been to develop a standard numerical solution. While a numerical solution technique would likely provide more accurate contaminant concentration and mass flux estimates, it was determined that the significant computational savings afforded by the newly-developed solution technique outweighs the increase in accuracy obtainable by a numerical solution technique. A formal comparison has been proposed as a science support activity.

The source emission models developed address most of the SAB's and CMA's concerns directly by satisfying the requirements listed above. In addition, although the newly developed Generic Soil Column Model, upon which the source emission models are based, is not capable of explicitly modeling contaminant fate and transport in the presence of NAPLs, calculated contaminant concentrations in soil are checked to determine if they are greater than a calculated theoretical upper limit without NAPL. If this occurs, it is noted in an output file. This is not expected to be a significant limitation in applying the model to develop HWIR exit levels. It is expected that in most circumstances exit levels will be sufficiently low that the presence of NAPL would be precluded.

With regard to partition coefficients, the widely-used assumption of linear equilibrium partitioning of constituent mass between the solid and aqueous phases is used for both inorganic and organic contaminants in both soil (for the LAU) and waste (for the landfill and waste pile). For organic contaminants, K_d is determined using the *foc* x K_{oc} relationship, where *foc* is the organic carbon fraction in soil (or waste) and K_{oc} is the equilibrium partition coefficient normalized to organic carbon. For inorganic contaminants, a model such as MINTEQ will be used to calculate a K_d in soil (or waste) as a function of the temperature and pH of the transport medium.

Efforts to validate the model will be limited by the availability of data for long-term (annual), simultaneous emission fluxes from and contaminant concentrations in the WMU's of interest. Comparisons of model results with those of existing models (Jury et al. 1990) for simplified contamination scenarios will be performed.

3.2.1.4 Module Description

A generic soil column model was developed to describe the dynamics of constituent mass fate and transport within non-wastewater WMUs. An overview of the model has been provided above in Section 3. Major assumptions of the model are:

- Partitioning to three phases: solid, liquid, gas.
- Reversible, linear partitioning between solid and liquid phases.
- Equilibrium partitioning between liquid and gaseous phases according to Henry's Law.
- Material in the soil column (including bulk waste) can be approximated as unconsolidated, homogeneous, porous media.
- Transformation processes are first-order losses.
- Boundary conditions are zero concentration for the upper boundary (soil/air interface) and a zero

concentration gradient for the lower boundary (WMU bottom/vadose zone interface).

3.2.1.5 Limitations

- Simplified partitioning assumed for metals (the coupled relationship between Kd and the metal concentration is not integral to the model).
- The governing equations are not applicable in the presence of non-aqueous phase liquid (NAPL). This is not expected to be a significant limitation for HWIR purposes, i.e. exit concentrations would be expected to be far below NAPL concentrations. (NAPL presence is checked-for internally by the model.)
- The model simulates a single contaminant at a time, i.e. it does not simulate reaction products. (With further development, however, the existing algorithms could be extended to chains of daughter products.)

3.2.2 Source Modules (Tanks and Surface Impoundments)

3.2.2.1 Purpose

The surface impoundment (SI) and aerated tank (AT) model simulates gaseous emissions of chemicals due to volatilization. In addition, for the SI, a leaky liner is assumed and leachate fluxes (flow and chemical load) are simulated. Flow and chemical loads in treated effluent are also simulated for both sources, but these outputs are not considered as part of the HWIR multi-media pathways.

3.2.2.2 Summary of Major Comments from 1995 Proposal

The following comments were generic to all source models, and have been listed and discussed previously in the LAU, WP, and LF section.

- Lack of a true multi-pathway approach -- Both the US EPA SAB and the Chemical Manufacturers Association (CMA) were critical of the single most limiting pathway anaylsis used in HWIR 95. Both concluded that a true, simultaneous, multipathway analysis is required.

- Mass balance violations -- Here, too, the SAB and CMA were in agreement. Both commented that a mass balance approach is necessary for the HWIR analysis and was lacking in the HWIR95 analysis.

- Lack of validation -- The SAB was critical of the lack of effort to validate the model components of the HWIR 95 analysis.

- Need to consider other removal processes -- CMA was critical of the lack of consideration of first order biological and chemical degradation in HWIR 95.

- Simplistic treatment of partition coefficients -- SAB expressed concern that HWIR 95 made extensive use of partition coefficients (i.e., K_d, soil-water partition coefficients) without adequate treatment of the factors that can affect K_d, such as characteristics of the chemical, the medium, and the method of measurement.

The primary comment from SAB specific to tanks and SI was the comment regarding biodegradation.

Most of the specific comments for tanks and SI came from EPA ORD and from State regulators. These are summarized below:

- need to include biodegradation; also some SI are facultative (have both aerobic and anaerobic degradation);
- need to include solids settling and partitioning to suspended solids; need to estimate impact of sediment accumulation on leaching rate and mass balance;
- need to include temperature effects on operating conditions/reaction rates;
- overflow/run-on releases generally impractical and inconsistent with SI model;
- well-mixed flow model may be inappropriate for quiescent SIs.

3.2.2.3 Requirements for HWIR99 and Approaches Considered

The primary requirements for the tank and SI models were to provide accurate estimates of volatile emissions, while including other loss mechanisms in a mass balance solution. Specifically, the model needed to include:

- biodegradation;
- partitioning to sediment;
- more rigorous modeling of leaching losses
  - to model the effects of sediment accumulation on the infiltration rate
  - to eliminate the disconnect between the SI leaching rate estimates and the groundwater leaching rate estimates;
- abiotic loss mechanisms (i.e., hydrolysis); and
- temperature effects on partitioning and reaction rates.

Additionally, the HWIR99 model needed to be both flexible (it needed to model not only aerated tanks and quiescent SI, but also quiescent tanks and aerated SI) and provide a quick solution algorithm.

To include sediment accumulation, a two compartment model was selected. The liquid compartment included losses by emissions, biodegradation (assumed aerobic), hydrolysis, and sedimentation. The sediment compartment included losses by biodegradation (assumed anaerobic); hydrolysis, leaching, and sediment resuspension.

The emission modeling equations used in HWIR95 to estimate the gas and liquid phase mass transfer coefficients for both quiescent and turbulent sources were again selected for HWIR99 as no comments were received regarding their use, and these equations are used throughout other EPA offices (e.g., in CHEMDAT8 and WATER8 models). Documentation of these equations can be found in the Chapter 6 of the CHEMDAT8/WATER8 model documentation, which is available at:

http://www.epa.gov/ttn/chief/software.html.

The well-mixed, steady-state assumption were also used again, although the HWIR99 uses a pseudo-steady state solution and updates for sediment accumulation to yield a time dependent solution.

The well-mixed, steady-state assumption was employed because it is generally applicable to many tank and SI applications, and it provides a direct analytical solution. Additionally, a plug-flow model would predict an uneven sediment accumulation which cannot be readily handled by the leaching model.

Three general models were considered to estimate biodegradation losses. These were a simple, first-order biodegradation (first-order reaction in contaminant concentration only); a complex, first-order biodegradation (first-order reaction in both contaminant concentration and biomass concentration); and Monod biodegradation kinetics (mixed-order reaction rate in contaminant concentration with first-order biomass concentration). The Monod model was not used because the regulatory contaminant concentrations are generally in the range where first-order reaction rate is applicable, and because there is a general lack of data to support the use of the Monod biodegradation rate model, which requires two rate constants for each contaminant. The complex, first-order biodegradation model was selected for the liquid compartment as the biomass concentration in liquid can vary widely from tank to tank or SI to SI. The first-order biodegradation rate model was selected for the sediment compartment due to its simplicity and the smaller fluctuations expected in the active biomass population within the sediment compartment.

Leaching losses were estimated using the EPACMTP model. This model was selected because it could model the effect of sediment accumulation, and because this model is used for the groundwater modeling component. Thus, there is no longer a disconnect between the SI and groundwater modules.

There were very few models available to predict sedimentation and resuspension rates. Several different theoretical sedimentation models were developed, and the sediment accumulation and sediment mixing rates (sedimentation and resuspension rates) were compared for various SI and accumulated sediment thicknesses. These results were compared to expected sediment behavior in terms of sediment removal efficiency and general trends of the parameters. A new sedimentation model was subsequently developed. This model employs the characteristics of the SI or tank, as well as the mean particle size and particle size distribution of the suspended solids to estimate the sedimentation, resuspension and accumulation ("burial") rates using equations for the terminal velocity of spheres.

The model includes temperature-dependent variations for diffusivity and Henry's law (volatile) partitioning, viscosity, biodegradation, and other key chemical properties that may impact the fate of the contaminant in the tank or SI.

3.2.2.4 Module Description

The AT and SI models are essentially the same model due to similarities in their governing equations. Their differences arise only from shutting down certain processes (e.g., no leaching for the AT). The general model consists of steady-state mass balance equations for two state variables (chemical, solids) in two compartments (water column, sediments). The AT or SI is considered as a completely stirred tank reactor (CSTR), i.e. no concentration gradients exist in the water column or sediments. Transport is by bulk advective flow through the unit, with leaching considered for the SI. Fate processes for the liquid compartment are settling, resuspension, volatilization, hydrolysis, biodegradation, and solid/liquid partitioning. The sediment compartment considers settling, resuspension, burial, hydrolysis, biodegradation, and solid/liquid partitioning. For AT units, settling is considered to occur only in the quiescent zones. Although steady-state, sediment accumulation (equal to the burial rate) is tracked on an annual basis.

3.2.2.5 Limitations

- Simplified partitioning assumed for metals (the coupled relationship between Kd and the metal concentration is not integral to the model).
- The model simulates a single contaminant at a time, i.e. it does not simulate reaction products. (With further development, however, the existing algorithms could be extended to chains of daughter products.)
- The SI and AT sources are modeled as CSTRs. This is a simplification of the actual fate and transport processes.
- Dynamics of varying loading and environmental conditions are not modeled. (A pseudo-dynamic approach is used in which instantaneous steady-state conditions vary on a monthly basis monthly in response to varying conditions.)

3.2.3 Atmospheric Module

3.2.3.1 Purpose

With respect to the atmospheric medium, the purpose of the modeling effort is to provide an annual average estimate of air concentration of dispersed constituents, and annual deposition rate estimates for vapors and particles at various receptor points over distances not to exceed 50km. The pollutants are assumed to be in the form of volatilized gases or fugitive dust. The atmospheric module simulates the transport and diffusion of the pollutant. The simulated air concentrations are used to estimate bio-uptake from plants and human exposures due to direct inhalation. Deposition rates are used to determine chemical loadings to watershed soils, farm crop areas, and surface waters.

3.2.3.2 Summary of Major Comments from 1995 Proposal

There were no major comments that were specific to the air modeling. The following general comments could apply:

- conservation of mass must be accounted-for or maintained
- concerns about the ability to address episodic events such as intense rainfall
- QA of data and methodology

3.2.3.3 Requirements for HWIR99 and Approaches Considered

There are several different approaches that could be taken to provide the concentration and deposition estimates needed for HWIR99. These different approaches represent different levels of complexity both in the physics contained in the models and in the computational aspects. The decision that had to be made is what is the appropriate level of sophistication for HWIR99, keeping in mind that the most appropriate approach may not be the most sophisticated or complex approach. Consideration must be given to the runtime of the models, since HWIR99 requires development of numerous constituent-specific waste levels applicable to nationally-distributed WMUs within a Monte Carlo simulation framework.

Air modeling platforms range in complexity of science from regional-scale Eulerian models to simple, local-scale, box models. Currently available Eulerian models (CMAQ) do not provide estimates at a fine enough grid scale for use in HWIR99. Another option would be a puff model (e.g. CALPUFF). While puff models can provide estimates of concentration and deposition at the scales of interest, they are more applicable in applications where a 3-D wind field appropriately characterizes the transport and

dispersion of the pollutant. A wind field would be important in modeling complex interactions with terrain. Puff models also are useful for modeling calm wind conditions and plume fumigation. Since these conditions generally tend to be more site-specific, and the approach for HWIR99 is regionally site-based, these factors were not expected to be of significance in HWIR99. The traditional approach for modeling the types of sources included in HWIR99 is the steady-state Gaussian plume model (e.g. ISC3). Gaussian plume models provide hourly or longer term estimates of concentration and deposition at user-specified locations. The lowest level of sophistication is the box model, which assumes a constant concentration/deposition within the user-defined box. These models tend to be sensitive to the size of the chosen box and do not provide any spatial resolution in the estimates.

3.2.3.4 Module Description

The air module consists of a preprocessor, model and postprocessor. The preprocessor reads the system input files and prepares the needed input files for the air model. Additionally, the preprocessor determines if the air model needs to be run or if results from a previous run may be used. This is simply an optimization step. The postprocessor reads the output files created by the air model and write the results to the appropriate system results files.

The air model selected for use in HWIR99 is the Industrial Source Complex - Short Term (ISCST3) model. ISCST3 is a steady-state, Gaussian plume model. The model provides estimates of pollutant 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 was modified to sample from a file of hourly meteorological data at regular intervals and thus only models a fraction of the hours for the period of record (e.g. 30 years). This change enables the model to execute more quickly, while producing long-term averages comparable to those obtained from the full data set. ISCST3 will be run using normalized emissions in conjunction with the sampled meteorological data, and will be annualized by multiplying the normalized annual-average concentration and annual deposition predictions by an annual emission rate. Annual-averages will then be divided by 365.25 to provide predictions in the required daily average units.

3.2.3.5 Limitations

One of the largest areas of uncertainty in the air modeling related to the needs of HWIR is the deposition of gases. There are currently no air models that contain algorithms specifically designed to model the dry deposition of VOC's and SVOC's. Previous modeling exercises used a transfer coefficient to model the dry deposition of gases. The concern with this approach was that deposition would be calculated outside of the model, which precluded the consideration of the deposition in the amount of material depleted from the plume. This approach presents challenges in trying to preserve the conservation of mass. To calculate the wet deposition of gases, chemical-specific scavenging coefficients should be used. However, these values are not readily available. An alternative approach is to select a single scavenging coefficient for all gases that is based on approximating the gases as very small particles. This approach may lead to underprediction of wet deposition for some gases and overprediction for others.

3.2.4 Unsaturated Zone Module

3.2.4.1 Purpose

The unsaturated zone module simulates the migration of water and a contaminant between the top of the unsaturated zone and the water table. The module provides estimates of the annual average contaminant mass flux from the bottom of the waste management unit (WMU) to the water table. Water table contaminant mass fluxes are used as input by the saturated zone module to simulate contaminant fate and transport in the saturated zone.

3.2.4.2 Summary of Major Comments from 1995 Proposal

Comments on the 1995 HWIR Proposal addressed the lack of incorporation of biodegradation and transformation of contaminants into the methodology. The unsaturated zone module incorporates both of these degradation processes.

3.2.4.3 Requirements for HWIR99 and Approaches Considered

A single approach for simulating water flow and contaminant transport in the unsaturated zone was implemented in both the scientific and computational versions of the unsaturated zone module. This approach, described in the next section, meets the primary criteria for the module. The methodology is both scientifically rigorous and computationally efficient.

3.2.4.4 Module Description

The approach selected for the unsaturated zone was to adopt EPA's Composite Model for Leachate Migration and Transformation Products (EPACMTP) modeling approach. Flow in the unsaturated zone was assumed to be steady-state, one-dimensional, and vertical from underneath the source (WMU) towards the water table. The flow in the unsaturated zone is predominantly gravity-driven, and therefore the vertical flow component accounts for all of the fluid flux between the source and the water table.

The contaminant is transported in the unsaturated zone by advection and dispersion. The unsaturated zone was assumed to be initially contaminant-free and that contaminants migrate vertically downwards. The unsaturated zone module can simulate both steady-state and transient transport, with single or multiple species chain decay reactions and linear or nonlinear sorption. The annual average mass fluxes at the water table are determined using a fast, semi-analytic solution. The computational burden associated with the unsaturated zone module is relatively small.

3.2.4.5 Limitations

The unsaturated zone module accounts for water and contaminant mass fluxes from the land surface to water table given a steady state flow condition, and hence, only serves to provide inputs to the saturated zone module. Partitioning to the air phase present in the unsaturated zone is not considered in the one dimensional analysis. Therefore, it is assumed that there is no mass transfer between the soil vapor and air above the soil, yielding a conservative estimate of the mass entering the groundwater. Also, transient flow effects are assumed negligible given the usually long time scale of sub-surface contaminant migration.

3.2.5 Saturated Zone Module

3.2.5.1 Purpose

The purpose of the saturated zone module is to provide estimates of annual average concentrations of contaminants at one or more water supply wells, and releases into a single, hydraulically-connected, intercepting (gaining) stream. Dissolved contaminants entering the system at the water table directly beneath the source (the waste management unit, WMU) are estimated by the unsaturated zone module. The annual average contaminant concentrations at the wells are used to estimate risks to human receptors due to groundwater pathways. The module uses the solution approaches developed for the EPA's Composite Model for Leachate Migration with transformation Products (EPACMTP).

3.2.5.2 Summary of Major Comments from 1995 Proposal

Comments on the 1995 HWIR proposal addressed the lack of use of biodegradation and transformation of contaminants into the methodology. The saturated zone module incorporates both of these degradation processes. A database of anaerobic biodegradation rate constants for organic chemicals is currently under development for implementation using the Monte Carlo procedure.

3.2.5.3 Requirements for HWIR99 and Approaches Considered

There are two approaches for determining annual average well and intercepting stream concentrations corresponding to the requirements of scientific and computational versions of the saturated zone module. The scientific module utilizes fully three dimensional numerical solutions for flow and transport for rigorous calculation of contaminant concentration estimates at receptor wells and to the stream.

The computational version uses the same approach for flow as the science module. The transient transport simulation utilizes a quasi-three dimensional formulation also implemented in the EPA's Composite Model for Leachate Migration with Transformation Products (EPACMTP): numerical in either a vertical plane, aligned with the regional groundwater flow direction (for relatively thick aquifers), or a depth-averaged areal plane (for relatively thin aquifers). If the vertical plane is used, the third dimension is added analytically. The result is a compact and efficient saturated zone flow and transport simulator to meet the execution requirements for HWIR99.

In an effort to further improve the computational efficiency of the saturated zone module, a one-dimensional analytical flow solution, coupled with an alternative quasi-three dimensional approach for transport, is currently under development as a potential alternative to the above approach for the computational version of the module.

3.2.5.4 Description of Module

The saturated zone module is designed to simulate flow in an unconfined aquifer with approximately uniform saturated thickness. The concept is that of regional flow in the horizontal direction, with vertical influx from the overlying unsaturated zone and waste disposal facility. The bottom of the aquifer is assumed to be impermeable. Flow in the saturated zone is assumed to be steady-state to approximate long-term flow conditions. The module accounts for infiltration from the bottom of a waste

management unit (WMU) and recharge to the aquifer from outside the source area.

Contaminant transport in the saturated zone is affected by advection, hydrodynamic dispersion, and degradation. The aquifer is assumed to be initially contaminant-free. Contaminants entering the aquifer only from the unsaturated zone immediately underneath the waste disposal facility are modeled as a rectangular, horizontal, plane source. The module can simulate both steady-state and transient three-dimensional transport in the aquifer. For steady-state transport, the contaminant mass flux entering at the water table must be constant. For the transient case, the flux at the water table may vary as a function of time. The module can consider the transport of a single species or multiple species, chain-decay, reactions, and linear sorption.

3.2.5.5 Limitations

The saturated zone module does not account for contaminant mass flux sources outside the boundary of the WMU. Vertical anisotropy of the hydraulic conductivity field can be modeled in the module, however, porous medium heterogeneity is not currently incorporated.

3.2.6 Watershed Module

3.2.6.1 Purpose

The Watershed Module addresses the following objectives:

- Simulates chemical loadings in surface runoff and erosion that will enter waterbodies as a result of indirect contamination (aerial deposition)
- Simulate regional flows and solids loads entering waterbodies
- Simulate chemical concentrations in surficial soils resulting from aerial deposition in the vicinity of the WMU. These concentrations are inputs to the exposure modules.

3.2.6.2 Summary of Major Comments from 1995 Proposal

- Overland pathway resulting from soil erosion not physically based.
- The implementation of the USLE and other equations used to calculate soil erosion resulted in higher concentrations at the receptor than in the source.

3.2.6.3 Requirements for HWIR99 and Approaches Considered

Many of the HWIR95 comments on watershed modeling related to the manner in which the USLE was implemented to transport eroded soil and chemical loads from a source area to downslope receptor areas and waterbodies. The HWIR95 approach eroded soil and chemical from the source and deposited these loads on downslope land areas, essentially in proportion to their surface areas relative to that of the source area. No physically based transport was considered, i.e. runoff and erosion loads were not hydraulically "routed" among consecutively adjoing downslope areas. This non-physically based implementation of the USLE has been modified for HWIR99. The source and adjoining land areas (upslope and downslope) are conceptualized in a holistic watershed perspective, with runoff and erosion proceeding from upslope to downslope with explicit consideration of deposition, resuspension, and

possible burial of eroded soil and chemical as one proceeds downslope.

In HWIR99, two different "watersheds" are conceptualized. The first is a so-called "local" watershed, which represents a relatively small watershed that contains the land-based source (LAU or WP) and its contiguous upslope and downslope land areas. Runoff and erosion from watershed areas that are not along the runoff flow path containing the source area are not considered in this local watershed construct. The conceptual model for this local watershed (also called an "extended source") is described in the preceding paragraph, i.e. a series of contiguous land areas among which runoff flows and loads are routed. This local watershed model is, in fact, the LAU and WP source models described elsewhere. The "local watershed" source models simulate not only air and groundwater fluxes from the WMU land area itself, but overland transport of runoff, soil, and associated chemical loads from upslope to downslope in a watershed context. The purpose of the local watershed construct, aside from simulating direct source emissions to air and groundwater, is to generate downslope surficial soil concentrations in buffer areas (with possible receptors), and to generate chemical loads entering the downslope waterbody directly from runoff and erosion from the WMU.

The second type of "watershed" is a generally larger land area than the local, or extended source, watershed type. These watersheds, in general, are not sheet-flow-only watersheds (i.e., "hillsides"), but are watersheds in the more general use of the term, i.e. drainage basins consisting of stream systems and their associated subbasins. The area covered by all such watersheds would comprise the overall WMU area, and the surrounding 2 kilometer buffer area. It is anticipated that this overall area of interest would be comprised of on the order of 5 to 10 such watersheds.

3.2.6.4 Module Description

The Watershed Module consists of a collection of submodels that, individually or collectively, simulates rainfall/runoff, soil erosion, groundwater recharge, and chemical fate and transport in both the runoff and the soil column. Rainfall/runoff is simulated on a daily basis (which is then rolled-up to annual average) using the Soil Conservation Service's Curve Number method. Soil erosion is estimated, also on a daily storm event-specific basis, using the (modified) Universal Soil Loss Equation (USLE) methodology. Chemical fate and transport in runoff and at depth in the soil column are simulated using the same Generic Soil Column model as described for the LAU/WP/LF model.

3.2.6.5 Limitations

- A watershed is considered to be homogeneous with respect to aerial deposition and resulting soil concentrations. Thus, "hot spots" of high localized deposition will be diluted by spatial averaging into the larger watershed containing that hot spot.
- A watershed is considered homogeneous with respect to factors affecting runoff and erosion, e.g. slopes, flow lengths, soil types and properties. Attempts have been made to develop good watershed-average estimates of those parameters that are amenable to averaging (some soil properties cannot be "averaged"); nonetheless, intra-watershed variability will not be captured.
- Contaminant fate and transport calculations are made on a more-or-less annual average basis (the algorithmic time step is not necessarily one year but changes in accordance with numerical stability criteria), although surface fate and transport processes are occurring on an episodic (approximately daily) scale. Although the model is capable of daily simulations, the

approximately annual time step was driven by run-time considerations. Consequently, intra-annual variability and short-term exposures from spikes or hot spots will not be captured.

3.2.7 Surface Water Module

3.2.7.1 Description of Module Purpose

The purpose of the aquatic module is to provide annual-average estimates of total and dissolved chemical concentration in the water column and underlying sediments at various receptor points within or near the affected watershed. Loadings are received from several modules, including the atmosphere, extended sources, regional watershed, and groundwater. Concentrations are used by the aquatic food web module and the human and ecological exposure modules.

3.2.7.2 Summary of Major Comments from 1995 Proposal

The 1995 proposal contained a simple water module. No significant comments were made criticizing the model structure.

3.2.7.3 Requirements for HWIR99 and Approaches Considered

The simulation module must incorporate a defensible set of transport and transformation algorithms that are driven by easily accessible data, but must be efficient enough to use for a national assessment within a Monte-Carlo framework. The source loadings are assumed to be a sequence of yearly-average fluxes of a single compound.

All assessment and scientific support models should be public domain software that can be freely adapted and used by EPA, its contractors, and the public.

The assessment models must be scientifically defensible, but simple enough to execute a single site within seconds (a 10 second run repeated 1000 times for 200 chemicals would take 556 hours). They should be consistent in sophistication and data requirements with other modules being incorporated into HWIR99.

The scientific support models should incorporate state-of-the-art process equations and allow dynamic solutions and spatial heterogeneity. They should be well-accepted models that are verified and tested against observational data if at all possible.

The water body models should be applicable to small water bodies, including streams, ponds, and lakes or reservoirs. They must simulate multiple chemicals, including parent compounds and reaction products. They must be able to handle loads from atmospheric deposition, runoff and erosion, and groundwater seepage. Transport/transfer processes must include advection, vertical diffusion, volatilization, deposition to the sediment bed, resuspension to the water column, and burial to deep sediments. Transformation processes should include hydrolysis and biodegradation as pseudo-first order reactions that are functions of relevant environmental properties such as pH.

Models at two levels of sophistication will be identified or developed -- assessment modules are

the primary focus of the effort, with scientific support models serving in a supporting role. The assessment modules will be linked with the other media and risk modules in a Monte-Carlo framework and run together to generate risk estimates for HWIR. The scientific support models can be run separately or linked to investigate more fully the relative importance of various processes at specific sites.

The assessment modules can be considered a subset of the scientific support models. These modules may be implemented independently, or they may actually use the scientific support software driven by a simpler input dataset invoking a subset of the equations. The scientific support models will be used to test the proper limits of the assessment modules and later to defend them in peer review.

The water body models will be applied to a one-dimensional reach of a small stream, to a well-mixed pond, and to simple configurations of small lakes (littoral, epilimnion, and hypolimnion segments). One or more sediment layers will be included. Sorption onto solids will be included using partition coefficients. For organic chemicals, correlations will relate measured octanol-water partition coefficients to organic carbon partition coefficients; the organic carbon content of solids will be used to obtain effective site-specific partition coefficients. Metals will be handled using partition coefficients that may vary with location in the water body. Derivation of appropriate partition coefficient values will be accomplished externally to the module. Solids derived from watershed erosion will be simulated using simple mass balance algorithms.

The assessment module will use a steady-state solution, driven by average annual loads and flows. Yearly-average environmental forcing functions, such as temperature and pH, will drive the chemical reactions. The scientific support model must be able to take monthly or yearly loadings and environmental functions (i.e. flow, temperature), and calculate time-variable concentrations. For stream simulations, it should be able to simulate pulse loadings using unsteady flow from a simple hydrodynamic model. The scientific support model will be used to identify those compounds that do not reach steady-state in a short period of time, and to develop appropriate assessment strategies. Depending on the run-time constraints of the HWIR assessment strategy, the scientific support model may be incorporated into the assessment software for use with a limited number of compounds.

Four options considered for the HWIR water body module were: (1) use the 1995 HWIR analytical equations; (2) develop a simple compartment model; (3) adapt the EXAMS compartment model; or (4) use the WASP5 compartment model (scientific support activities only). The team has chosen option 3 for the assessment model. EXAMS will be adapted to handle a simple solids balance given monthly or seasonal loadings from the watershed. Three networks will be defined to represent a stream reach, a pond, and a small lake.

EXAMS will be further adapted for use as a scientific support model. Linkage will be provided to a simple hydrodynamic model to properly handle stream dynamics. Dynamic simulations cnupling EXAMS with the terrestrial loading and stream hydrodynamics models will be conducted and compared with the simpler, time-averaged simulations to be used by the assessment model.

3.2.7.4 Description of Module

EXAMSII 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

error analyses of the probable aquatic fate of synthetic organic chemicals (Burns et al. 1992; Burns 1997). EXAMS combines chemical loadings, transport, and transformations 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 fate, persistence, and potential ecosystem exposure.

EXAMS is a computer-based system for installing and running chemical simulation studies with models of aquatic ecosystems. EXAMS' environmental models are maintained in a file composed of concise ("canonical") descriptions of aquatic systems. Each waterbody is represented 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 transport and transformation process equations, EXAMS compiles an 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 equations are used for sorption and ionization reactions. Kinetic equations are used for volatilization, hydrolysis (acid, base, and neutral), biodegradation (water column and sediments), photolysis, oxidation, and reduction. EXAMS will use 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.

EXAMS can be run interactively, or as a batch program. For HWIR, the interactive features will not be used. In addition, much of the tabular output will be suppressed. As currently envisioned, HWIR will not consider transformations due to photolysis, oxidation, and reduction. Transformation rate constants for hydrolysis and biodegradation will be calculated by the general chemical database and used directly by EXAMS.

At present, EXAMS does not simulate a solids balance. Solids concentrations are specified as input data. ($SUSED_{j,t}$ is the water column suspended sediment concentration; $PCTWA_{j,t}$ and $BULKD_{j,t}$ are used to derive the sediment solids concentration; $BNMAS_{j,t}$ and $CHL_{j,t}$ give the benthic and water column

biotic solids concentrations). The effects of settling and resuspension on chemical fate are accounted for in a bulk sediment-water exchange term.

An option will be added to EXAMS to simulate biotic and abiotic solids in the water column linked with sediment solids in underlying sediment layers. Abiotic solids enter the water column via external loading and resuspension from the sediments, and are subject to advection, dispersion, and settling. Biotic solids are created in the water column through primary productivity and are subject to advection, dispersion, settling, and mortality. Bed sediment solids can be resuspended, buried to lower layers, or mineralized. Assuming that benthic solids concentrations are constant over time, the burial velocity can be determined as a function of specified values for settling, resuspension, and mineralization, along with calculated values for biotic and abiotic water column solids concentrations.

The contaminant fate algorithms in EXAMS already include sorption to suspended solids, biotic solids, and sediment solids. These will be modified to include particulate phase chemical settling, resuspension, and burial to lower sediment layers. When chemical settling and resuspension are simulated explicitly, the sediment-water exchange term will incorporate pore water diffusion only.

The new parameters to be added to EXAMS include primary productivity, phytoplankton mortality rate constant, abiotic and biotic settling velocity, sediment resuspension velocity, and sediment mineralization rate constant. These will be specified as arrays that vary in space and time. EXAMS arrays allow for monthly values along with the yearly-average. Following a review of the scientific literature, functions may be generated to internally calculate some of these parameters based on commonly-available environmental data such as wind speed and literature-derived constants, such as phytoplankton composition.

3.2.7.5 Limitations

To save computational time in the HWIR regulatory application, EXAMS will be run in steady-state mode using yearly-average loadings and flows. For most chemicals in streams, rivers, and small lakes, the steady-state assumption should be acceptable. For some highly-sorptive chemicals, however, this assumption will lead to some biases. Predicted yearly maximum concentrations for highly sorptive chemicals should be greater in steady-state simulations than in dynamic simulations. A set of dynamic simulations will be compared with the steady-state simulations to explore the extent of this conservative bias.

The new EXAMS solids algorithms allow the simulation of multiple solids size fractions. Unfortunately, there will be no direct information on the solids size fractions in the erosion load from the regional watershed. EXAMS will have to simulate total solids using a lumped settling rate, or else arbitrarily divide the total erosion among representative solids size fractions in order to use individual settling rates.

3.2.8 Aquatic Food Web (AqFW) Module

3.2.8.1 Purpose

The purpose of this module is to predict the constituent concentrations in aquatic biota in surface

water bodies near a waste management unit (WMU). Chemical constituents released from WMUs may reach surface waters via overland pathways (e.g., runoff, erosion), aerial deposition, or through a subsurface connection (i.e., surface water recharge from a contaminated underground aquifer). Once a constituent reaches a surface water body, the module determines appropriate bioaccumulation factors (BAFs) for the biota specified in the aquatic food web. The BAFs are used to predict concentrations in aquatic invertebrates and fish (at any time *t* for a specific water body of interest) that are used in turn as input for the human health (HumEx) and ecological exposure (EcoEx) modules.

3.2.8.2 Summary of Major Comments from 1995 Proposal

- Bioaccumulation models that simulate the uptake and accumulation of hydrophobic organics in aquatic biota have not been calibrated or validated over a sufficiently broad variety of aquatic systems.

3.2.8.3 Requirements for HWIR99 and Approaches Considered

The HWIR99 analysis required an aquatic food web module that:

- uses a weight-of-evidence approach to determine appropriate BAFs;
- is flexible enough to simulate both riverine and lacustrine systems;
- reflects the current state-of-the-science for modeling bioaccumulation in steady-state systems;
- is appropriate for a national/regional scale analysis; and
- is consistent with other recent Agency initiatives (e.g., the Great Lakes Water Quality Initiative - GLWQI).

Consequently, a comprehensive literature review was conducted to identify: (1) BAFs from field and laboratory studies; and (2) models that simulate uptake and accumulation in aquatic food webs. Only peer-reviewed models that rely on the well-established body of theory applicable to flowing systems (e.g., the RIVER/FISH model by Abbott et al. (1995)) and to pelagic and benthic aquatic ecosystems (e.g., Thomann et al. (1992) Campfens and Mackay (1997), and Morrison et al. (1997)) were considered.

3.2.8.4 Module Description

The key function of the AqFW module is to determine suitable bioaccumulation factors (BAFs) for chemical constituents and use these values to predict concentrations in the tissues of aquatic biota. Mechanistic models, regression equations, EPA analyses, and empirical data are used in a weight-of-evidence approach to determine the appropriate BAFs and, where possible, distributions of these factors. For convenience, the approach summarized below is organized around five types of HWIR constituents: hydrophobic organics, hydrophilic organics, ionizable organics, PAHs, and metals (including mercury).

Hydrophobic organics - Although a strict definition for hydrophobic organics has not appeared in the literature, consensus across a number of sources suggests that a cutoff of log K_{ow} 3.0 is a reasonable value. This is a particularly important distinction, since the modeling approach to be used to predict

biological uptake values for hydrophilic constituents[1] is different than that proposed for hydrophobic constituents. The methodology developed to predict BAFs for hydrophobic organic constituents (i.e., accumulation via gill uptake and food ingestion) is based on a steady-state bioaccumulation model developed by Dr. F.A.P.C. Gobas that was used to support the EPA Great Lakes Water Quality Initiative (Gobas 1993). The aquatic food web module developed for FRAMES utilizes the Gobas model to estimate BAFs that are specific to 18 major hydrologic regions in the conterminous United States. The intent is to delineate the distributions for water quality characteristics (e.g., temperature, dissolved and particulate organic carbon) that reflect variability within each hydrologic region. It is expected that, for most hydrologic regions, data on aquatic species characteristics (e.g., weight, lipid content) will be insufficient. Therefore, values for these characteristics will be based on national distributions for aquatic species characteristics divided into coldwater and warmwater species (i.e., the data across hydrologic regions will be pooled for coldwater and warmwater fish, respectively). For each model run for a hydrophobic constituent, the aquatic food web module will: (1) receive the dissolved water concentration and sediment concentration from the surface water module; (2) select a value from a region-specific distribution (as appropriate) for each input variable; and (3) generate a lipid-based BAF for the human and ecological exposure modules. The BAFs will be specific to the trophic levels that are most relevant to human or ecological receptors.

Hydrophilic organics - For hydrophilic organics, it is generally assumed that the dominant exposure route is via gill uptake (i.e., gill uptake >>> food/particle ingestion). The measure of biological uptake and accumulation associated with gill uptake is often termed the bioconcentration factor (BCF). For the proposed HWIR95, a number of regression equations based on log K_{ow} and/or aqueous solubility were identified in peer-reviewed literature and Agency guidance documents, and the most appropriate equation was used to predict the BCF. Sources of these equations include (but are not limited to) the following examples:

- *Assessment and Control of Bioconcentratable Contaminants in Surface Waters* (USEPA 1991)
- *Relationship between Water Solubility, Soil Sorption, Octanol-Water Partitioning, and Bioconcentation of Chemicals in Biota (Kenaga and Goring (1980) as cited in Lyman, et al. (1990))*
- *Estimating Bioconcentration Factors from Octanol-Water Partition Coefficient and Aqueous Solubility* (Isnard and Lambert 1988)
- *Measuring and Estimating the Bioconcentration Factor of Chemicals in Fish* (Veith et al. 1979)

In general, these regression equations have very high correlation coefficients ($r^2 > 0.9$), particularly for the groups of constituents for which they were developed. Predicted bioconcentration values were adjusted for the lipid content assumed for the HWIR analysis as described in USEPA (1991). Exhaustive research on empirical BCFs for hydrophilic compounds was not conducted since bioconcentration data from laboratory studies were used to support the

[1] Organic constituents with log K_{ow} values between 1 and 3 are considered weakly hydrophobic. For convenience, organics with log K_{ow} values below 3 will be considered hydrophilic in this discussion.

regression equations. Where possible, data suggesting that the constituent was metabolized *in vivo* were identified and a study-generated BCF was used to override the predicted value.[2] For HWIR99, the same approach for hydrophilic organics has been adopted.

Ionizable organics - Ionizable organics include a number of constituents whose fate are sensitive to pH. For example, the Ambient Water Quality Criterion for pentachlorophenol is calculated using an empirical equation that accounts for this effect. In the proposed HWIR95, biological uptake factors for these constituents were identified only from empirical studies; modeling approaches and regression equations were considered inappropriate. Moreover, simulating the fate and transport of ionizable organics was not possible because the pH-dependent partition coefficients were not available. For HWIR99, pH-dependent log K_{ow} values are being generated by ORD and, therefore, it is possible to utilize either the mechanistic BAF model or the regression equations for BCFs. However, ionizable organics behave differently in living tissues and, as a result, it may not be appropriate to use the technical approach developed for non-ionizable organics. This issue is still under investigation.

Polycyclic aromatic hydrocarbons - It is widely accepted that aquatic organisms (particularly fish) readily metabolize PAHs, and that BAFs predicted from log K_{ow} values greater than about 5.0 overestimate the bioaccumulation potential for this group of organic constituents. Thus, BAFs for PAHs in the proposed HWIR95 were identified from the literature, and an EPA report developed to support the Great Lakes Water Quality Initiative (*Derivation of Proposed Human Health and Wildlife Bioaccumulation Factors for the Great Lakes Initiative*, Stephan, 1993). Subsequent to HWIR95, additional analyses have been performed by OSW to investigate other data sources for PAH bioaccumulation factors as well as alternative methods for their derivation. After a comprehensive literature survey and review, it was determined that the empirical database on PAH bioaccumulation was insufficient to support defensible BAFs for most PAHs. We have developed two alternatives to estimate BAFs for PAHs. The first alternative involves the use of interval analysis (or fuzzy arithmetic) as described by Spencer and Beaulieu (1997). In brief, the interval analysis predicts a range of bioaccumulation factors associated with a given level of possibility. The second alternative requires metabolic rates for use in the Gobas model. Theoretically, the Gobas model should be able to predict appropriate BAFs at steady-state conditions, provided that the metabolic rates are available. These alternatives, of course, are not mutually exclusive and the most appropriate approach for PAHs will be determined after module results are examined.

Metals and mercury - Bioaccumulation factors for metals are estimated exclusively from empirical data. For mercury, BAFs identified in the *Mercury Report to Congress* (USEPA 1997) will be adopted for HWIR99. However, the relatively complex environmental behavior of metals in surface water with respect to bioaccumulation and water quality criteria is an important source of uncertainty. The effects and accumulation of essential metals change with concentration; thus, a single BCF ratio may be inappropriate. Based on this information, essential metals (e.g., Cu, Zn) are distinguished from nonessential metals (e.g., Cd, Pb) in developing appropriate BAFs and BCFs. See, for example:

- *Evaluation of Bioaccumulation Factors in Regulating Metals* (Chapman et al. 1996)
- *Rethinking Water Quality Standards for Metals Toxicity* (Renner 1997)

---

[2] Empirical data on metabolism by aquatic species is available for relatively few constituents.

- *The Importance of Trace Metal Speciation to Water Quality Criteria* (Allen and Hansen 1996)
- *Reassessment of Metals Criteria for Aquatic Life Protection* (Bergman and Dorward-King 1997)

3.2.8.5 Limitations

The module involves a weight-of-evidence approach that considers the appropriateness of simulation modeling and regression equations to derive suitable BAFs, as well as measured BAFs from field studies. Although the Gobas model (and other similar models) adapted for use in HWIR99 have been validated (e.g., for Lake Ontario), they have not been validated across all of the aquatic systems included in this analysis, particularly small streams (i.e., stream order 2 and 3). In addition, estimates of fish tissue concentrations are limited by the quality and quantity of data on bioaccumulation.

3.2.9 Farm Food Chain (FFC) Module

3.2.9.1. Purpose

The purpose of this module is to predict the concentrations of chemical constituents in plants, beef, and dairy products grown on farms or home gardens near a waste management unit (WMU). Constituents released from WMUs may reach home gardens and farms via overland transport within a local watershed (e.g., through sheet flow) and through aerial dispersion and deposition. This module is designed to accept media concentrations from the air, watershed, and surface water modules (at any time *t* for a specific area of interest) and simulate the uptake and concentration in crops and in cattle that feed on contaminated vegetation. The concentrations in various food items are used as input for the human health exposure module (HumEx).

3.2.9.2 Summary of Major Comments from 1995 Proposal

The major comments regarding farm food chain modeling included:

- The food chain model did not reflect the expertise of scientists in ORD.
- Input parameters for biotransfer factors were not consistent with published values.

3.2.9.3 Requirements for HWIR99 and Approaches Considered

Based on the comments received on HWIR95, it was determined that the FFC module should be completely consistent with the scientific standards established by ORD in the 1997 draft of the Indirect Exposure Methodology (IEM) and the companion Parameter Guidance Document, or PGD (also USEPA (1997)). In adopting the IEM and PGD, the FFC module is designed to predict contaminant concentrations in various plant categories (e.g., exposed fruit, root vegetables) consumed by both the farmer and home gardener as well as beef and dairy products consumed by the farmer receptor. This satisfies both of the major comments received regarding the HWIR95 module in that:

- it reflects the state-of-the-science practiced by Agency scientists in evaluating the farm

food chain exposure pathways, and

- parameter values for national analyses are provided in both the IEM and the PGD.

3.2.9.4 Module Description

The approach selected is described in detail in the Indirect Exposure Methodology drafted by ORD in 1997. The module estimates waste constituent concentrations in major plant categories consumed by humans, distinguishing between plants that are exposed to aerial deposition or vapor-phase uptake and those that are in some way protected from air-to-plant transfer. Consequently, plant concentrations are calculated for exposed vegetables, protected vegetables, exposed fruits, protected fruits, and root vegetables. In addition, the module predicts concentrations in forage grasses, silage, and grain, since these items are food stuffs for beef and dairy cattle. The module uses predicted concentrations in these items in conjunction with biotransfer factors to predict the concentration in beef and milk, respectively.

For most organic constituents, the module uses regression equations to relate simulated air and soil concentrations to plant tissue concentrations and, in turn, soil and plant concentrations to beef/milk concentrations (as described in the IEM (1997)). Steady-state and equilibrium are assumed between soil and roots, between soil and aerial parts, and between air and aerial parts. No flow between compartments is considered. A simple partition coefficient between the plant and an environmental medium (air or soil) is used to estimate the concentrations in vegetables and forage grasses. Each of the mechanisms considered for plant uptake is represented by a biotransfer factor and includes the following:

- root uptake and translocation;
- air-to-plant transfer of vapor-phase contaminants; and
- deposition of particle-bound contaminants on plant surfaces.

Similarly, biotransfer factors are developed for each of the mechanisms considered for uptake into beef and dairy cattle, including:

- uptake from ingestion of contaminated forage, silage, and grain;
- uptake from incidental ingestion of contaminated soil; and
- uptake from ingestion of contaminated surface water (e.g., local pond).

For all organic constituents except for dioxins (and congeners), selected PAHs, and several hydrophobic constituents that are well studied, biotransfer factors are predicted using the empirical relationships represented by the regression equations. For these “special” organic constituents, the module selects override values from the data files in the system that are specific to both the chemical and, in some cases, the category of plant or cattle (i.e., beef or dairy).

For metals, including mercury, plant uptake factors are derived from field data, including but not limited to values reported in EPA's sludge risk assessment work. Extensive literature reviews of both secondary and primary sources have been conducted on these constituents. As with the “special” organic constituents, the module selects override values from the data files in the system that are specific to the metal and, in some instances, the category of plant or animal. For example, Stevens (1991, 1992) provides biotransfer factors for beef and milk, respectively, for six metals assuming steady-state conditions.

3.2.9.5 Limitations

The module is not mechanistic in the sense that it does not represent the anatomical and physiological features of plants and their transport and transformation processes. Rather, the module is based on empirical relationships for selected groups of constituents and on laboratory- and field-generated biotransfer factors. The module provides a simple framework appropriate to the resolution required in HWIR99 analysis; however, it sacrifices the precision that a mechanistic model might offer. Biotransfer factors are used to represent major categories of plants (and animal tissues) without regard to site-based conditions such as soil type, plant species, application matrix, or environmental conditions (e.g., temperature). As a result, predicted concentrations in plants and beef/dairy products may be associated with substantial uncertainty. For example, the biotransfer factors for metals may vary over several orders of magnitude depending upon the study conditions. Additional uncertainty is introduced in using annual average concentrations to evaluate uptake over discrete growing seasons.

3.2.10 Terrestrial Food Web (TerFW) Module

3.2.10.1 Purpose

The purpose of this module is to estimate the concentrations in various food items consumed by terrestrial receptors, primarily birds and mammals. Constituents released from WMUs may reach terrestrial habitats via overland transport within a local watershed (e.g., through sheet flow) and through aerial dispersion and deposition. This module is designed to accept simulated media concentrations from the air, watershed, and surface water modules (at any time *t* for a specific area of interest) and simulate the uptake and concentration in plants, earthworms, other terrestrial invertebrates, and vertebrates. The concentrations in various food items are used in turn as input for the ecological exposure module (EcoEx).

3.2.10.2 Summary of Major Comments from 1995 Proposal

- Major comments specific to the terrestrial food web module were not received. However, a number of commenters suggested that ecological exposure concentrations estimated by the HWIR95 model were overly conservative.

3.2.10.3 Requirements for HWIR99 and Approaches Considered

The requirements for the terrestrial food web module for HWIR99 include:

- The TerFW should treat plant uptake using the same methods as those used in the FFC module. However, the vegetation consumed by wildlife should be matched to the plant categories for human consumption such that plant types are evaluated consistently.

- The TerFW should maintain the four major food categories for terrestrial receptors that were developed in the Agency's dioxin work for pulp and paper regulations.

- Because of the lack of data supporting biomagnification of constituents in terrestrial food chains, as well as the paucity of data on the movement of constituents through terrestrial food chains, the TerFW should not attempt to develop chains within the food web.

3.2.10.4 Description of Module

The TerFW module is used to derive suitable factors to represent uptake and accumulation in food items, and using media concentrations calculated in the multimedia modules (e.g., air, soil, surface water), estimates concentrations in prey and vegetation found in the terrestrial habitat. The module divides all food items (i.e., prey, plants) into four major categories: (1) plants, (2) earthworms, (3) soil invertebrates, and (4) vertebrates (see *Assessment of Risks from Exposure of Humans, Terrestrial and Avian Wildlife, and Aquatic Life to Dioxins and Furans from Disposal and Use of Sludge from Bleached Kraft and Sulfite Pulp and Paper Mills* - USEPA (1990)). Each major category is divided into several subcategories that reflect significant differences in the dietary habits of receptors (e.g., forage grasses and forbs would not be treated the same as nuts and berries).

For plants, the farm food chain module is modified slightly to predict concentrations in various types of vegetation eaten by herbivorous and omnivorous animals. For example, the forage category under the FFC module is used in the TerFW module to predict concentrations in ferns, forbs, grasses, monocot and dicot shoots, and shrubs. The exposed fruit category is used to predict concentrations in wild fruits as well as seeds and berries.

Generally speaking, mechanistic models and regression equations are lacking for terrestrial systems, particularly models that address variability in the environmental setting (e.g., differences in soil characteristics). Consequently, the biotransfer factors for the other three non-food categories of terrestrial food items are generally derived from laboratory and field studies.

In conjunction with the few available modeling tools available to estimate uptake and accumulation, a weight-of-evidence approach is used to predict or identify appropriate BAFs and biotransfer factors (BTFs) and, where possible, determine the range and distribution of these factors.[3] The Oak Ridge National Laboratory has developed regression analyses appropriate for HWIR99 to estimate bioaccumulation of metals and highly hydrophobic constituents in earthworms and in small mammals. These regression models are presented in:

- *Methods and Tools for Estimation of the Exposure of Terrestrial Wildlife to Contaminants.* Prepared by the Oak Ridge National Laboratory - Sample et al., 1997.
- *Development and Validation of Bioaccumulation Models for Earthworms.* Prepared by the Oak Ridge National Laboratory - Sample et al., 1998a.
- *Development and Validation of Bioaccumulation Models for Small Mammals.* Prepared by the Oak Ridge National Laboratory - Sample et al., 1998b.

Since the derivation of terrestrial uptake factors revolves around only two types of constituents

[3] Based on previous research, the data on biotransfer seldom support a regional approach that accounts for abiotic characteristics such as soil ph and fraction of organic carbon.

(organics and metals), the approach summarized below is organized around the non-plant categories of food items. As discussed above, methods used to predict plant concentrations in the TerFW module are essentially the same those used in the FFC module.

Bioaccumulation factors for earthworms - Certain groups of constituents (e.g., phenols) have been studied extensively in earthworm bioaccumulation studies. Measured correlations between soil and tissue concentrations in worms will be used when available. The data and modeling approach recommended by Sample et al., (1998a) will be used for the selected constituents included in that report (e.g., nine metals, PCBs, and TCDD). For all other constituents, secondary compilations and primary literatures sources are under review to identify suitable BAFs.

Bioaccumulation factors for invertebrates - Modeling approaches that are suitable to predict BAFs for soil invertebrates have not been identified. Consequently, empirical data will be required for all constituents and will be gleaned from the primary literature and the in-house ecotoxicological database maintained by OSW. The paucity of data on invertebrate uptake suggests that default factors and distributions may need to be developed for constituent classes.

Bioaccumulation factors for vertebrates - For small mammals, the data and modeling approach recommended by Sample et al., (1998b) will be used for the selected constituents included in that report (e.g., 14 metals, TCDF, and TCDD). For all other constituents and mammals, empirical data are used to estimate BAFs and (if possible) BAF distributions. Similarly, empirical data are being gathered for all other vertebrates (e.g., birds, reptiles) relevant to exposures in terrestrial habitats. As with other biological uptake factors, primary sources of data include OSW's in-house ecotoxicity database, secondary compendia of uptake factors, and primary literature search and review. As part of the data collection effort, EPA databases, such as ECOTOX, and other relevant databases, e.g., COMPUTOX, are being searched and evaluated.

3.2.10.5 Limitations

The same limitations noted for the FFC module also apply to the TerFW module with respect to predicting plant concentrations (e.g., an empirically-based approach). In addition, the lack of data on uptake and accumulation of constituents in other terrestrial food items introduces significant uncertainty into this module. In many cases, only a single point estimate may be available to determine the bioaccumulation potential in a given category. These limitations were explained in some detail in the proposed HWIR95; however, little progress has been made since that proposal in the data and science required to model chemical uptake and accumulation in terrestrial habitats.

3.2.11 Ecological Exposure (EcoEx) Module

3.2.11.1 Purpose

The purpose of the ecological exposure module is to: (1) identify the ecological region (using Bailey's scheme as defined in Bailey (1996) and Bailey et al. (1994) in which the waste management unit (WMU) is found; (2) assign representative habitats to the site that are consistent with both the ecological region and the site-based data on land-use patterns, wetlands, managed areas, etc.; (3) select appropriate receptors (including threatened and endangered species) for each representative habitat potentially

affected by the WMU, and; (4) estimate doses and/or medium concentrations to which these receptors are exposed through ingestion or via direct contact (at any time *t* for a discrete area of interest). The module requires concentrations predicted by the multimedia modules (e.g., watershed module) and concentrations in biota predicted by the uptake modules (e.g., TerFW) that are contained in the Global Results Files (GRFs). These results are used to pass applied doses to the risk module to calculate ecological hazard quotients.

3.2.11.2 Summary of Major Comments from 1995 Proposal

- The two generic ecosystems (terrestrial and freshwater) are insufficient to characterize the variability across ecosystems. This was considered one of the most significant limitations in the ecorisk methodology in HWIR95.

- A national assessment of ecological risks from waste management units is not defensible. Instead, ecological risks should be evaluated on a site-specific basis.

- The suite of ecological receptors is incomplete and should include other species (e.g., bats). Threatened and endangered species are not included among the suite of ecological receptors.

- Exposure estimates for ecological receptors are overly conservative because 100% of the diet is presumed to originate from the contaminated area.

3.2.11.3 Requirements for HWIR99 and Approaches Considered

The requirements for the EcoEx module for HWIR99 are as follows:

- The module should contain representative habitats that reflect the variability across terrestrial systems (e.g., grasslands, shrub lands), aquatic systems (e.g., ponds, and lakes), and wetlands (e.g., permanently flooded and intermittently flooded). However, marine and estuarine habitats are not included in the HWIR99 framework.

- The module should include a diverse array of ecological receptors that are linked to the ecological region and habitat type(s) within the 2 km radius of the WMU site.

- The module should be useful in estimating exposures to both representative receptors (i.e., common species) and threatened and endangered species.

- The module should account for spatial differences in constituent concentrations with respect to the home range and foraging areas of target species.

- The module should include food web exposures as well as exposures through ingestion of contaminated media. Inhalation exposures will not be evaluated.

3.2.11.4 Module Description

Under HWIR95, proposed ecological risk assessment procedures included an assessment module for generic terrestrial ecosystems and one for generic freshwater streams. The EcoEx module developed to support HWIR99 increases the resolution of the assessment beyond the generic ecosystem level to include a suite of representative habitats for terrestrial, aquatic, and wetland systems. In this context, the term "habitat" implies a level of detail and specificity that is meaningful for a particular WMU site (e.g., presence of wetlands), but does not require extensive biological inventory, field investigation, or classification beyond matching potential habitats with the ecological region and site characteristics (e.g., land use patterns). The HWIR99 habitats are intended to reflect the variability of ecological systems across the conterminous United States and provide a context for selection of appropriate ecological receptors at each site. The habitats include:

terrestrial habitats (includes intermittently flooded habitats)

- grasslands
- shrub/scrub
- forest
- managed (e.g., crop fields, timber reserves)

aquatic habitats

- rivers (order 5 and greater)
- streams (order 4 and below)
- lakes ($\geq$ 10 acres)
- ponds (< 10 acreas)

wetland habitats

- permanently flooded forest
- permanently flooded shrub/scrub
- permanently flooded grassland

Once representative habitats have been assigned, the ecological receptors assigned to each habitat become the focus of the site-based assessment. Each habitat is characterized by site-based data such as habitat boundaries (i.e., area and spatial orientation of habitat), nature of the habitat (e.g., a managed habitat area such as a wildlife refuge), the “common” species and communities associated with that habitat, and the presence of threatened or endangered species. This module now contains over 50 representative species of birds, mammals, amphibians, and reptiles, and more than 25 threatened and endangered species (including fish). In addition, simple food webs are constructed that indicate the major trophic levels and the functional groups (such as decomposers, herbivores, or filter feeders) expected in each habitat type. The food webs are crucial in identifying relevant exposure pathways of concern for each receptor.

For receptors that receive significant exposures through the food web, exposure factors (e.g., body weight), information on dietary preferences, and estimated concentrations in terrestrial and/or aquatic food items are used to predict the applied dose. For receptors with foraging areas that are smaller than the habitat area, the foraging area is assigned randomly to the habitat (i.e., the foraging area can be located anywhere within the habitat boundaries). Weighted concentrations within that area are calculated for both contaminated media and contaminated food items. For receptors with foraging areas that are larger than the habitat area, the applied dose is simply prorated as the fraction of the habitat that

comprises the foraging area.

The applied doses to birds and mammals in each of the habitats assigned to the site are stored in the GRF. The media concentrations in soil, surface water, and sediment for habitats were stored in the GRF previously as results from the multimedia modules. These results are simply "passed" on to the risk module.

3.2.11.5 Limitations

The module is a significant step forward in terms of representing the variability of ecological systems. However, there are several limitations to this approach relative to the comments received on HWIR95.

- Estuarine and marine systems have not been included in this module since the modeling framework is not designed to simulate these systems.
- The spatial resolution continues to be below the level of a site-specific assessment in that media concentrations are averaged over relatively large areas.
- Delineating habitat "boundaries" is somewhat artificial with regard to the behavioral patterns of many wildlife species. Hence, prorated exposures based on area ratios and weighted averages may be associated with significant uncertainty.
- Exposure concentrations are calculated based on annual average media concentrations using data on dietary preferences that are often seasonal.

3.2.12 Human Exposure Module

3.2.12.1 Purpose

The human exposure module is designed to estimate the daily dose of contaminant for each human receptor type at each receptor location across a site. These data will be passed to the risk module for estimating risk or hazard quotient distributions across a receptor area associated with each waste management unit. The exposure module uses simulated media and food chain concentrations contained in the Global Results File of the FRAMES-HWIR system and distributions of the various exposure factors for each receptor type to calculate the applied dose for a receptor at a specified location. The locations of receptors are defined in the site layout file. Receptor types include adults, children and infants for each of the following: residents, home gardeners, beef and dairy farmers, and recreational fishers.

3.2.12.2 Summary of Major Comments from 1995 Proposal

The major comments regarding human exposure estimation included the following:

- Human exposures should include all relevant exposure pathways and exposure routes,

where appropriate. The most limiting pathway approach of HWIR95 was viewed as a major limitation of that analysis.

- The variability and uncertainty in exposures should be explicitly quantified where possible. This includes temporal and spatial variability, as well as, variability and uncertainty in exposure parameters.

3.2.12.3 Requirements for HWIR99 and Approaches Considered

The requirements of the human exposure module for HWIR99 include the following:

- The exposure module must include both oral and inhalation routes of exposure. The Agency considered the inclusion of dermal routes of exposure, but decided that derivation of health benchmarks for dermal toxicity derived from oral toxicity studies were not scientifically defensible and, therefore, decided not to include dermal routes of exposure.

- The human exposure module must be able to quantify spatial variability and temporal variability in exposure across a site.

- The human exposure module must be able to aggregate across exposure pathways and routes, when appropriate, and provide estimates of total exposure.

- The human exposure module must be able to explicitly address the variability and uncertainty in exposure factors for each receptor type.

3.2.12.4 Module Description

The module is a specific application of the exposure methodology presented in EPA's *Methodology for Assessing Health Risk Associated with Multiple Exposure Pathways to Combustor Emissions* (1997, draft). Fifteen types of receptors are considered in the module: an adult, child and infant for a resident scenario, home gardener scenario, beef farmer scenario, dairy farmer scenario, and recreational fisher scenario. The children in each receptor type include three age cohorts: 1-5, 6-12, and 13-19. The infant is less than one year old and is only evaluated for a specific set of constituents classified as dioxin-like compounds.

Each receptor may be exposed by inhaling and/or ingesting contaminants. Inhalation exposures include breathing outdoor air and breathing contaminants volatilizing from water while showering. Ingestion exposures include drinking contaminated ground water, eating contaminated fruits, vegetables, beef, dairy products, and fish ingestion. The receptors are differentiated by the pathways to which they are exposed (see below).

- Residents are exposed to some level of contaminant in the air (inhalation) and the soil (incidental ingestion). Some residents may be on drinking water wells that are also contaminated and, thus, ingest hazardous constituents in this water and use this contaminated water for showering. Those on public water supply systems are assumed to

have treated water that meets all relevant drinking water regulations.

- Home gardeners are residents who also grow some portion of their fruits and vegetables. The percent of the study population that are home gardeners is estimated from regional data presented in EPA's *Exposure Factors Handbook*.

- Farmers have the same exposure pathways as residents and gardeners with the additional exposure to either contaminated beef or contaminated dairy products (not both simultaneously).

- Fishers will be 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 recreational fishers and have elements of all of those risks described above, plus the risk of ingesting contaminated fish from local water bodies.

To represent the variability in exposure across a site, the exposure for each of these receptor types is estimated at numerous locations across a study area to capture spatial variability in exposure, and for every year throughout the modeling time frame to capture temporal variability. In addition, each receptor type has distributions for all exposure factors for each of the age groups. The location of receptors is based on census block and census block group data for the study area around a WMU. For each model iteration, a point is randomly selected within each census block in the study area All residents, home gardeners, and their children and infants will be evaluated at these locations. A typical study area may have between 100 and 200 census blocks. An area will also be randomly selected within the farmland in each census block group. Beef and/or dairy farmers and their children and infants will be evaluated at these locations. A typical study area may have 10 to 20 census block groups. Only census block groups with a farm population will contain farms. Based on data contained in the *National Survey of Fishing, Hunting, and Wildlife Associated Recreation*, the percent of each of the above receptors classified as fishers will have additional exposures due to ingestion of fish caught locally.

For each model iteration, one and only one value for each exposure parameter is used along with the simulated media concentrations at selected locations in estimating exposures. The values are randomly selected from the distributions for the exposure parameters. The distributions for the exposure parameters are developed by statistically fitting data available in literature. Means, standard deviations, and percentile data cited in the Exposure Factors Handbooks were used as a basis for fitting distributions. The best-fitting model (gamma, lognormal, or Weibull) was determined for each parameter for each age group and receptor types.

3.2.12.5 Limitations

- Dermal exposures are not considered. This may underestimate the total exposure and risk.

- The uncertainty associated with the actual location of the WMU and receptors presents uncertainty in the overall exposure estimates.

3.2.13 Risk Module

3.2.13.1 Purpose

The risk module is designed to compare exposure estimates to human health and/or ecological effects benchmarks to provide an overall quantitative characterization of risk to human and ecological receptors across a site. These data will be passed to the HWIR - FRAMES Exit Level Processor for combining this risk information across all sites and waste management units. For human health, the risk module will provide a population-weighted individual risk for each receptor type at each exposure location across a site. Similarly, for ecological risk the estimated exposure at each ecological habitat location for all relevant species will be compared to relevant ecological effects benchmarks. A temporal processor is used to identify the maximum risk associated with a specified exposure duration over the entire modeling period.

3.2.13.2 Summary of Major Comments from 1995 Proposal

The major comments regarding risk estimation included the following:

- Human health risk should include all relevant exposure pathways and represent an aggregate risk across pathways and exposure routes where appropriate.
- The use of no effects levels to develop estimates of ecological risk is overly conservative.
- The absence of ecological benchmarks has been equated with the absence of ecological risk for HWIR constituents that were not included in the ecological risk assessment.
- Ecological risks should not be evaluated by inference from data on individual effects (e.g., reproductive effects). Ecological risks should be evaluated for entire communities and ecosystems.
- The variability and uncertainty in the risk estimates should be explicitly quantified where possible.
- Health benchmarks for dermal routes of exposure which are based on oral toxicity data should be reviewed in terms of similar toxicokinetics.

3.2.13.3 Requirements for HWIR99 and Approaches Considered

The requirements of the risk module for HWIR99 include the following:

- The risk module must include cancer and noncancer health effects for humans for both oral and inhalation routes of exposure. The Agency considered the inclusion of dermal routes of exposure, but decided that derivation of health effects benchmarks for dermal toxicity derived from oral toxicity studies were not scientifically defensible and, therefore, decided not to include dermal routes of exposure.
- The risk module must include the flexibility to use ecological effects benchmarks at

levels of conservatism appropriate for both "common" species and threatened and endangered species.

- The risk module must be able to quantify spatial and temporal variability in exposure across a site.

- The risk module must be able to aggregate across exposure routes, when appropriate, and provide estimates of risk based on total exposure.

- The risk module must provide a population weight to each receptor-specific, individual risk estimate. The population weighting is then used to estimate the distribution of risk across all receptors at a site.

3.2.13.4 Module Description

The risk module combines outputs from the human health and ecological exposure modules with the appropriate health effects benchmarks to obtain receptor-specific risks or hazard quotients for each location being evaluated around a WMU. The exact spatial locations for each receptor are specified in the site layout file, and the total oral and total inhalation exposures are obtained from the Global Results File (GRF). All exposure data in the GRF are expressed either as an average daily dose (mg/kg-day) over each year for carcinogens and oral noncarcinogens, or as an average annual ambient concentration for inhalation of noncarcinogens. Each year in the modeling time frame has values for average daily exposures. For noncarcinogens and for ecological risks, the risk module finds the year with the highest hazard quotient for each receptor at each location. For carcinogens that have the same target organs via oral and inhalation exposures, the module finds the highest combined risk for any 9-year exposure duration for each receptor at each location. For chemicals in which the human health effects differ depending on the route of exposure, the module calculates the maximum as described above for each exposure route separately. Since ecological risks are estimated for either ingestion (e.g., birds, mammals) or direct contact and ingestion (e.g., soil community, aquatic biota), it is not necessary to sum exposures across multiple routes of exposure.

For human health, the risk module uses census data and a variety of supplementary sources to identify the receptor types, and their locations around a WMU. Census block data is used to determine the number of residents, by age group, in each census block within the 2-km radius of the WMU, and where they are located in proximity to the WMU. The census block group data are used to determine the number of people on farms, by age group, and their general location with respect to the WMU. These data are further refined using county level Census of Agriculture data to determine the percent of farms in a county that are either beef or dairy farms. The percent of the population considered recreational fishers is determined based on data from the *National Survey of Fishing, Hunting, and Wildlife Associated Recreation.* The percent of the population having home gardens uses region specific data. The appropriate population weight is applied to each estimate of individual risk for each receptor type and each location across the 2 km study area around a WMU. The weighted risks are then aggregated to determine the estimated distribution of risk at each WMU for each iteration. These data are then sent to the exit level processor for aggregation across all WMUs of a given type and across all iterations for that WMU type.

For ecological receptors, the receptors assigned to each habitat are presumed to exist at the site. Although population-level effects benchmarks have been developed for pilot constituents, OSW has decided that these values will be used to support and corroborate benchmarks used for inference of population effects, including endpoints on reproduction, developmental toxicity, and survival. The ecological effects benchmarks used to evaluate these receptors will include *de minimis* or low effects levels for common species and communities. The risk estimates for each receptor are recorded at the site for "common" species (e.g., raccoon). These data are then sent to the exit level processor for aggregation across all WMUs of a given type, across all iterations for that WMU type, and presented according to receptor category (e.g., common mammalian species; avian species; fish species). These data will also include information on habitat area sizes to provide an additional tool to interpret the ecological significance of potential ecological effects across the conterminous United States.

3.2.13.5 Limitations

The risk module is largely a function of the other modules in the system, and thus any of the uncertainties in the individual modules will be carried through to the risk estimates. Of particular note are two issues that have a strong effect on the characterization of human health risk. The first is the defining of the area of interest to a radial distance of 2km from the WMU boundary. If the boundary were set at 500 meters there would be a much different risk distribution.. Also, situations could exist where highly contaminated media do not present exposures to any receptors. For example, conditions could exist where the ground water is highly contaminated but, since no one uses it, it exhibits no actual risk. Similar situations could exist for any of the media and exposure pathways. Second, by using a population weighting scheme, the analysis is highly dependent on the location of actual receptors with respect to the WMU. The uncertainty associated with the actual location of the WMU and receptors presents uncertainty in the overall risk estimates.

With respect to the characterization of human non-carcinogenic hazards and ecological risk, there is an inherent limitation in using the hazard quotient (HQ) as the risk metric for adverse effects. First, because the HQ is a binary function, it is not amenable to interpretation of risk. An HQ above 1 indicates the potential for adverse effects and, conversely, an HQ below 1 is interpreted as below a level of concern. As a result, it is not possible to determine the significance of damages at HQ values above 1; it is only possible to determine that, given the modeling framework, the potential for adverse effects exists. Second, although the module evaluates risks to species populations (by endpoint inference) and communities (by statistical inference), it does not provide a measure of the ecological risks to the habitat or larger scale ecosystems as a whole. Thus, this type of risk characterization does not provide insight into complex ecosystem dynamics. The result of these two limitations is that the estimates of ecological risk are associated with some uncertainty that, given available tools and the current state-of-the-science, is not quantifiable.

3.3 Assessment Data

This section provides an overview of the HWIR99 data collection effort, including data groups, collection strategies, quality assurance/quality control, and transfer of data into the modeling system. A comprehensive treatment of the data collection effort is reported in "Data Collection Plan for the Hazardous Waste Identification Rule Multimedia, Multipathway Risk Assessment Model (HWIR99) - Draft February 1998". The data necessary to satisfy the needs of the multimedia, multipathway models

described in the following sections are grouped as follows:

1. Site-based

    - Facility Location Data
    - Waste Management Unit (WMU) Data
    - Waste Properties Data
    - Meteorological Data
    - Land Use Data
    - Topographic Data (watersheds and elevations)
    - Waterbody and Water Quality Data
    - Soil Data
    - Aquifer Data
    - Human Receptor Type and Location
    - Ecological Receptor Type and Location
    - Farm Food Chain Data
    - Terrestrial and Aquatic Food Web Data
    - Human Exposure Factors
    - Ecological Exposure Data

2. Human Health Effects Benchmarks

3. Ecological Effects Benchmarks

4. Waste Constituent Properties.

In collecting, organizing, and accessing the data necessary for conducting the revised HWIR Risk Assessment, a number of important strategies are planned, including

- A tiered approach is planned for compiling the complete set of data required for performing the site-based risk assessments.
- GIS-based, automated data collection will be utilized to characterize the physical and environmental characteristics of sites.
- QA/QC procedures are planned to ensure the quality and tractability of data.
- An extensive effort to compile chemical-specific property data is planned. Chemical property modeling, literature searches, and scientific judgement will be combined to facilitate the construction of a centralized database containing chemical-specific data.

The following sections provide a summary level of detail of the essential features of the data collection efforts related to 1) site-based data; 2) human health effects benchmarks; 3) ecological health effects benchmarks; and 4) chemical property data.

3.3.1 Site-based Data

The revised HWIR Risk Assessment is based on a multimedia multipathway assessment of exposures and risks to human and ecological receptors living in the proximity of Subtitle D facilities. To

perform such an assessment requires extensive data, not all of which is available for each site. For HWIR99, three data collection approaches are included in the plan, in order of preference, they are;

- Site-specific, where input data are collected at each facility/site location.
- Regional, where the nation is divided into regions of similar characteristics, data are collected to characterize variability within each region, and sites assigned to regions.
- National, where distributions or fixed values are collected for inputs that characterize the nation as a whole.

These three approaches represent a tiered protocol for collecting the necessary data. The assessment strategy, as presented in Section 3.1, is site-based, as opposed to site-specific. The use of the phrase site-based directly reflects the nature of the assessment data. The preference is to use only data representative of each individual site. Because it is impossible to satisfy this preference, a protocol must be established for assigning values to model parameters that are not known for any particular site. The data collection strategy devised is tiered and progresses from site-specific data, to data sampled from regional or national statistical distributions.

Table 3.3 shows these parameterization approaches by data type. The selection of data collection approach was based on the preference shown described above, data availability, and level of effort for data collection. Several of these data types are defined by data source and collection process and are required by multiple HWIR99 model components. Table 3.4 illustrates the crosswalk between model components and these common data types. The remaining data types are each only used by a single model component.

The strategy for collecting data to support the HWIR99 analysis includes both automated and manual collection methodologies.

- Automated methods utilize electronic processing of data utilizing geographic information systems (GIS) technology and a combination of GIS and conventional electronic databases.
- Manual techniques utilize desktop analysis, such as literature review and analysis.

Data availability, accuracy, sample coverage, and available resources were considered in developing collection methodologies for particular data types, along with experience gained during EPA's data collection pilot study.

3.3.1.1 Spatial Framework

The HWIR99 risk analysis strategy emphasizes the use of site modeling to provide spatial distributions of contaminants in a prespecified radius of interest around industrial D facilities with land-based waste management units (WMUs). To support this strategy, one of the goals of the data collection effort is to provide a spatial frame of reference around each facility. This will be accomplished by utilizing Geographic Information System (GIS) technology (ArcInfo software) to create several key spatial data layers for each site, as shown in Figure 3.12. They are:

- human areas of concern, defined by U.S. Census and land use data, that will be used to average exposure concentrations in various media and estimate risks to the receptors within each area.

- ecological areas of concern, defined by land use and other ecologically relevant data, that perform the same function as the human areas for ecological receptors.

- watersheds, delineated using digital elevation models (DEMs) of topography, that provide the input data and output spatial framework necessary to model contaminant erosion and overland transport in the land application unit, waste pile, and watershed models.

- waterbodies (lakes and streams), defined by the Reach datafiles, that provide the input data and output spatial framework necessary to model contaminant fate and transport in streams and lakes.

In the GIS, each of these spatial data layers is composed of 2-D polygons, with the exception of streams which are defined by 1D vectors (stream reaches). These polygon coverages will be exported directly to the modeling system (described in Section 3.4).

The spatial data layers can be extended to a prespecified distance beyond the radius of interest to ensure that the radius is fully covered in terms of model inputs and to allow for possible varying of facility location during the Monte Carlo process to account for location error.

The base grid (or x-y coordinate system) also can serve as the basis for air and ground water model outputs. Each of these models will produce contaminant concentrations (and deposition rates for the air model) only in terms of distance and direction from the WMU, so an additional spatial framework (e.g., polygon coverage) is not appropriate.

3.3.1.2 Data Storage and Processing

Requirements for converting the collected data to the form and units necessary for model inputs, along with procedures for deriving inputs from related data are discussed in detail in the "Data Collection Plan for the Hazardous Waste Identification Rule Multimedia, Multipathway Risk Assessment Model (HWIR99) - Draft February 1998". A data processor will be required to store the collected data, to automatically perform conversions, and prepare input files suitable for use by the modeling system.

Regular (daily) backups of all data files will be conducted and maintained to protect against data loss. Detailed design of this database and data processor needs to be conducted; its development is not covered in this plan.

3.3.1.3 QA/QC and Record-Keeping

Details of QA/QC procedures for each module-specific data collection effort are described in "Data Collection Plan for the Hazardous Waste Identification Rule Multimedia, Multipathway Risk Assessment Model (HWIR99)". In addition to these, there are certain approaches that are common to all activities in this effort, which are discussed in this section. This may or may not fit a particular data type, depending on final arrangements for data collection. Prior to data collection, for each data type, a basic QA/QC protocol will be developed and given to all staff working on this project to ensure that they are aware of these requirements. Any necessary deviations from these must be discussed with and approved by the appropriate work task leader.

All data that are manually entered into the inputs database from a hard copy source will be extracted and entered independently by two different staff members, after a senior staff member has reviewed the data source and highlighted the data that should be entered. A comparison program will be used to identify discrepancies between the two data entries, and discrepancies will be resolved before the data are loaded into the data base. Other QA/QC and record-keeping procedures will include:

- Electronic data forms will be used and will include the name of the staff member entering data and the date of the entry.

- Formal files, similar to a docket, will be maintained for all parts of this project. These will be used to track data sources, data entry, and changes to data, for instance, and will include copies of all hard copy data sources.

- Metadata will be maintained electronically for all data collected or generated in this project.

For the automated pulling of data from electronic sources, the data extraction system will require thorough validation before use (general guidelines will be developed, but details may be up to the best professional judgement of the person in charge of that task, and should be described in that section of the plan). After initial system validation, about 10% of all data will be checked manually to ensure that the system is functioning properly.

Since this effort will depend on data from a wide variety of sources, it is anticipated that there will be instances of data that are of unacceptable quality. Approaches for spotting such errors and inconsistencies are described under each data type. If and when these instances are identified, they will be brought to the attention of the task leader for resolution. If data for the same site from another source are available and acceptable, they will be used instead. If not, it may be possible to estimate data based on another similar site. If not, it may be necessary to select a different site. All problems of this type and their resolution will be carefully and thoroughly documented in the project files.

Similar to automatic data collection, the HWIR99 input data processor system will be validated and about 10% of all data will be checked manually to ensure that the system is functioning properly.

3.3.1.4 Methodology and Data Collection

The data collection activities in support of the HWIR99 risk analysis can be divided into three categories

- Development, in which data collection methodologies and procedures are designed, tested, reviewed, and approved. This is largely an up-front effort and is relatively insensitive to the number of sites involved.

- Collection, during which the data are collected and compiled from various sources.

- Processing, which involves readying the data for input to the modeling system.

Details of this topic are included in "Data Collection Plan for the Hazardous Waste Identification

Rule Multimedia, Multipathway Risk Assessment Model (HWIR99) - Draft February 1998"

3.3.1.5 Case Studies

Case studies will be conducted for a limited number (e.g., 5 - 10) Industrial D sites to provide information on the accuracy of the data collection methodologies outlined in this document. These case studies will involve three components:

- Desktop methods, such as manual delineation of watersheds using USGS topographic quadrangle maps

- Site visits, using global positioning satellite (GPS) technology to obtain accurate facility locations and to verify features and conditions of interest around the site through windshield surveys

- State office visits, to collect available permit information on facility location; WMU location, design, and operation; and hydrogeology (where available).

Table 3.5 summarizes the information to be collected during these case studies and compares it to the information collected during the larger, 200-site, data collection effort. Actual details of the Case study methodology are not yet developed.

3.3.2 Human Health Effects Benchmarks

There has been identified a list of approximately 460 waste constituents of potential concern for HWIR99. As in HWIR95, the EPA will use as the primary sources of toxicity benchmarks, those derived by the Agency (i.e., reference dose, reference concentration, oral and inhalation cancer slope factors). These are available in the Integrated Risk Information System (IRIS) and the Health Effects Summary Tables (HEAST). Approximately 260 of the 460 have at least one Agency-derived benchmark; approximately 200 constituents currently lack any benchmark.

EPA is developing a tiered methodology to develop toxicity values for constituents currently lacking any of the necessary benchmarks. The methodology, which will undergo a separate peer review, is described in *Conceptual Approach To Establishing Interim Health Benchmarks for HWIR Constituents*. The approach selected to estimate an interim benchmark is constituent-specific and is a function of the available toxicity data. For chemicals with an existing toxicity data set describing a dose-response relationship, the approach will be essentially the same as that used in the development of benchmarks derived by the Agency. For the remaining constituents, possible approaches include the use of quantitative structure-activity relationships (QSAR) and adjustments to account for constituent-specific properties and mode of toxicity by chemical class.

EPA has collected available toxicity information from many sources including ATSDR, IARC, WHO, NTP, and CalEPA. EPA will also evaluate peer-reviewed toxicity studies submitted by commentors on HWIR95 and other Federal and state agencies data bases to supplement the IRIS and HEAST benchmarks. Those constituents for which the EPA will develop interim benchmarks has yet to be determined.

3.3.3 Ecological Health Effects Benchmarks

The Agency has identified approximately 460 waste constituents for consideration of ecological impacts under HWIR. In HWIR95, the Agency generated ecological effects benchmarks for 47 constituents based on a prioritization scheme to identify those chemicals that are most likely to have adverse effects at concentrations lower than acceptable levels for human receptors and the availability of effects data for the constituents. The data for these benchmarks came from sources such as the Ambient Water Quality Criteria documents, the Great Lakes Initiative, PHYTOTOX, TERRETOX, and AQUIRE, and other on-line sources. The principal shortcoming noted in HWIR95 was that the reviewers could not identify any criteria for choosing the chemicals for which ecological effects benchmarks were developed.

For HWIR99, EPA is developing a methodology for determining whether constituents have adequate data to develop benchmarks. The methodology will address both the number of receptor types in a habitat for which data are available, as well as the quality of the data for each receptor type. Similar to HWIR95, the methodology will examine endpoints that are indicative of effects at the population or higher level. Unlike HWIR95, however, the Agency will not be attempting to draw conclusions about effects at the ecosytem level, which requires analysis of the abiotic as well as biotic environment. The methodology will seek to match regional habitats with appropriate receptors, and will use scaling methodologies to estimate effects benchmarks for receptor types lacking data. In addition, the methodology will lay out criteria for assigning qualitative criteria that describes the quality of data supporting each benchmark. The methodology will be peer reviewed by internal Agency scientists and external scientists. The number of chemicals for which ecological benchmarks will be developed is dependent on the availability of ecological data and the minimum criteria outlined in the methodology.

The data sources for the effects benchmarks are the same sources outlined in HWIR95, which are some of the most comprehensive secondary sources of ecological benchmarks. However, EPA has conducted additional literature searches to find articles published subsequent to HWIR95 and to collect some of the key primary literature.

3.3.4 Chemical Property Data

All HWIR modules will obtain chemical-specific data as needed from a central HWIR chemical database. A central database promotes consistent use of chemical-specific data among the various modules, and allows for convenient management of these data It is recognized that all of the chemical-specific data needs cannot be satisfied with measured values. The environmental conditions within which the contaminants find themselves are simply to varied and have not been studied sufficiently to enable the exclusive use of measured values. Thus, other means of developing the required data must be used (e.g., chemical modeling, expert judgment leading to simplifying yet environmentally protective assumptions).

The HWIR database is composed of four sections covering basic properties of organic chemicals, basic properties of metals and inorganics, transformation reactions of organic chemicals, and exposure and risk parameters. These sections are presented separately below.

3.3.4.1 Basic Properties of Organic Chemicals

Several fundamental organic chemical properties are found in this section of the HWIR database. These properties and their units are listed in the accompanying Table 3.6. Many of these properties vary with temperature, and some vary with pH. The property values are calculated for different temperatures using the SPARC expert system, and then are fit to an descriptive temperature function. The HWIR database stores the parameters of the temperature function for each parameter. When an HWIR module queries the database for chemical properties, these parameters are used to calculate appropriate chemical property values for the given temperature and pH.

SPARC Models

An in-depth description of SPARC procedures is beyond the scope of the discussion of this database project for the Office of Solid Waste (OSW) (see Karickhoff et al. (1991) and Hilal et al. (1993, 1994a, 1994b, 1995)). Reactivity assessment and computational algorithms are patterned after those presented by Dewar and Dougherty (1975) but similar descriptions have been developed by many others. The basic philosophy is not to compute any chemical property from "first principles". Rather, it is to utilize directly the extensive knowledge base of organic chemistry. Organic chemists have established the types of structural groups or atomic arrays that impart certain types of reactivity and have described, in "mechanistic" terms, the effects on reactivity of other structural constituents appended to the site of reaction. To encode this knowledge base, a classification scheme was developed that defines the role of structural constituents in effecting or modifying reactivity. Furthermore, models have been developed that quantify the various "mechanistic" descriptions commonly utilized in structure-reactivity analysis, such as induction, resonance, and field effects. SPARC execution involves the classification of molecular structures (relative to a particular reactivity of interest) and the selection and execution of appropriate "mechanistic" models to quantify reactivity.

For example, for ionization

$$pK_a = (pK_a)_c + \delta_p (pK_a)_c \quad \textbf{(26)}$$

where $(pK_a)_c$ describes the ionization behavior of the reaction center and $\delta_p (pK_a)_c$ is the change in ionization behavior brought about by the appended 'perturber' structure. SPARC computes reactivity perturbations, $\delta_p (pK_a)_c$, that are then used to "correct" the ionization behavior of the reaction center for the compound in question in terms of potential perturbation mechanisms.

$$\delta_p (pK_a)_c = \delta_{ele} pK_a + \delta_{res} pK_a + \delta_{sol} pK_a + \ldots \quad \textbf{(27)}$$

where $\delta_{ele} pK_a$, $\delta_{res} pK_a$, and $\delta_{sol} pK_a$ describe electrostatic, resonance and differential solvation effects respectively.

SPARC Physical Models

For all physical processes (e.g., vapor pressure, activity coefficient, partition coefficient, etc.), SPARC uses one master equation to calculate a characteristic process parameters:

$$\Delta G_{process} = \Delta G_{interaction} + \Delta G_{monomer} \quad \textbf{(28)}$$

where $\Delta G_{monomer}$ describes entropy changes associated with mixing, volume changes, or changes in internal (vibrational, rotational) energies going from the initial state to the final state. $\Delta G_{monomer}$ depends only on the phase change involved and in the present application is presumed to depend only on solute/solvent volumes in each phase. $\Delta G_{interaction}$ describes the change in the intermolecular interactions in the initial state and final state. For example, for Henry's constant the interaction term describes the difference in the intermolecular interactions in the gas phase versus those in the liquid phase. The interactions in the liquid phase are modeled explicitly, interactions in the gas phase are ignored, and molecular interactions in the crystalline phase are extrapolated from the subcooled liquid state using the melting point.

The intermolecular interactions in the liquid phase are expressed as a summation over all the intramolecular interaction forces between the molecules:

$$\Delta G_{interaction} = \Delta G_{dispersion} + \Delta G_{induction} + \Delta G_{dipole} + \Delta G_{H-bonding} \quad \textbf{(29)}$$

Each of these interactions is expressed in terms of a limited set of molecular-level descriptors (density-based volume, molecular polarizability, molecular dipole, and H-bonding parameters) which in turn are calculated from molecular structure.

SPARC presently predicts, for a large number of nonpolymeric organic molecules, ionization pKa's and numerous physical properties such as distribution coefficients between immiscible solvents, solubilities, vapor pressure, density, boiling point etc. The ultimate goal for SPARC is to model the chemical and physical behavior of molecules to predict chemical reactivity parameters and physical properties for the universe of organic molecules strictly from molecular structure.

OSW Algorithms

The algorithms presented below were used as models for fitting SPARC generated data for each of the properties included in this data base over the temperature range of 0°C to 60°C, in increments of 5°C. The coefficients given in the sample data base are those derived from this process. From the above discussion it is apparent that the SPARC model does not use these algorithms to estimate chemical properties. The SPARC model consists of a set of core models describing intra/inter molecular interactions that are linked by the appropriate thermodynamic relationships to provide estimates of reactivity parameters under the desired conditions (temperature, pH, etc.). Temperature dependence is intrinsic to each core interaction model as opposed to algorithmically described at the property level. However, using these algorithms to generate coefficients in the data base is the most practical method to incorporate SPARC generated data in light of the fact that OSW's models cannot link directly into the SPARC models.

General Model

For consistency and technical balance, the temperature dependence of all physical/chemical process parameters was represented as log-linear functions of 1/T (i.e., linear functions on a free energy basis). For all properties (except molar volume, gas diffusion, and liquid density), the following temperature dependence model will be employed.

$$\log P_p = A_p + \frac{B_p}{T} \quad (30)$$

where A_p and B_p are fitted coefficients for property p for the chemical of concern. These coefficients will be fitted and tabulated for every molecule and property as appropriate. As an example, for vapor pressure

$$\log VP = A_{VP} + \frac{B_{VP}}{T} \quad (31)$$

or equivalently

$$VP = 10^{\left(A_{VP} + \frac{B_{VP}}{T}\right)} \quad (32)$$

Besides their temperature dependencies, many physical/chemical properties also depend on pH. Consequently, there is also a need to adopt a consistent and technically balanced approach for estimating physical/chemical properties of chemicals as a function of pH. To accomplish this task one must be able to accurately calculate the ionization constants and fractions for chemicals in a consistent manner. The next section discusses this approach.

Ionization

As discussed above, ionization constants for HWIR chemicals are given by

$$pKa = A_{Ka} + \frac{B_{Ka}}{T} \quad (33)$$

When multiple ionizations are involved, however, separate coefficients are fitted for each ionization site. For example, the ionization constant for a chemical's first ionization site is denoted by

$$pKa(1) = A_{Ka(1)} + \frac{B_{Ka(1)}}{T} \quad (34)$$

For organic acids, the fraction f_n of the acid that exists as the neutral form is given by

$$f_n = \frac{1}{1 + \frac{Ka}{H^+}} = \frac{1}{1 + 10^{(pH - pKa)}} = \frac{1}{1 + 10^{\left[pH - \left(A_{Ka} + \frac{B_{Ka}}{T}\right)\right]}} \quad (35)$$

On the other hand, for acids with two acid ionization sites ($Ka(1)$, $Ka(2)$), the fraction of the acid in neutral form is given by

$$f_n = \frac{1}{1 + \frac{Ka(1)}{H^+} + \frac{Ka(1)Ka(2)}{(H^+)^2}}$$
$$= \frac{1}{1 + 10^{[pH - pKa(1)]} + 10^{[2pH - pKa(1) - pKa(2)]}} \quad (36)$$
$$= \frac{1}{1 + 10^{[pH - (A_{Ka(1)} + \frac{B_{Ka(1)}}{T})]} + 10^{[2pH - (A_{Ka(1)} + A_{Ka(2)} + \frac{B_{Ka(1)} + B_{Ka(2)}}{T})]}}$$

For bases, the fraction f_n of the base in the neutral form is given by

$$f_n = \frac{1}{1 + \frac{H^+}{Ka}} = \frac{1}{1 + 10^{(pKa - pH)}} = \frac{1}{1 + 10^{(A_{Ka} + \frac{B_{Ka}}{T} - pH)}} \quad (37)$$

For bases with two basic sites, the fraction of the base in the neutral form is

$$f_n = \frac{1}{1 + \frac{H^+}{Ka(1)} + \frac{(H^+)^2}{Ka(1)Ka(2)}}$$
$$= \frac{1}{1 + 10^{[pKa(1) - pH]} + 10^{[pKa(1) + pKa(2) - 2pH]}} \quad (38)$$
$$= \frac{1}{1 + 10^{(A_{Ka(1)} + \frac{B_{Ka(1)}}{T} - pH)} + 10^{(A_{Ka(1)} + A_{Ka(2)} + \frac{B_{Ka(1)} + B_{Ka(2)}}{T} - 2pH)}}$$

Henry's Law Constant

In general, the Henry's Constant of a chemical of concern can be calculated by

$$H = f_n H_n + f_i H_i \quad (39)$$

where f_n and f_i denote the fractions of the acid that exists as the neutral and ionized species, respectively. However, because one generally assumes that $H_i \rightarrow 0$, it then follows that

$$\log H = \log f_n + \log H_n = \log f_n + A_H + \frac{B_H}{T} \quad (40)$$

where

$$\log H_n = A_H + \frac{B_H}{T} \quad (41)$$

delineates the temperature dependence of Henry's Law constant for the neutral chemical. Consequently, for an organic acid with a single ionization site

$$\log H = -\log\left(1 + 10^{[pH-(A_{Ka}+\frac{B_{Ka}}{T})]}\right) + A_H + \frac{B_H}{T} \quad \textbf{(42)}$$

See Equation **(35)**.

Solubility and Kow

In general, the solubility and octanol water distribution coefficient for a chemical of concern is given by

$$S = f_n S_n + f_i S_i \quad \textbf{(43)}$$

$$K_{ow} = f_n (K_{ow})_n + f_i (K_{ow})_i \quad \textbf{(44)}$$

Unlike the Henry's Law constant, however, the contribution of the ionized species dose not necessarily vanish.

For non-ionizable compounds and the neutral species of an ionizable chemical the chemical's solubility is given by

$$\log S = A_S + \frac{B_S}{T} \quad \textbf{(45)}$$

For ionizable chemicals, however, SPARC does not calculate the solubility of the ionic species but rather applies a multiplier to the solubility of the neutral form to estimate the behavior of the ionized form. In particular,

$$\begin{aligned} S &= f_n S_n + (1 - f_n) M_i S_n \\ &= (f_n + 10^2(1 - f_n)) S_n \\ &= (10^2 - 99 f_n) S_n \end{aligned} \quad \textbf{(46)}$$

where M_i=10^2 is a universal multiplier that is assumed for all ionic species. When Equation ? is substituted into this expression, the combined temperature and pH dependence of the solubility of an ionizable chemical is given by

$$\log S = \log(10^2 - 99 f_n) + A_S + \frac{B_S}{T} \quad \textbf{(47)}$$

Note that when the calculated solubility exceeds 10^5 mg/L, the compound can be assumed miscible.

For non-ionizable compounds and the neutral species of an ionizable chemical the chemical's octanol water distribution coefficient is given by:

$$\log K_{ow} = A_{Kow} + \frac{B_{Kow}}{T} \quad (48)$$

Although SPARC can generate estimates of Kow for ions, we have opted for a simpler model—that being the assumption that ions do not partition into octanol. In this case

$$K_{ow} = f_n (K_{ow})_n \quad (49)$$

where

$$\log (K_{ow})_n = A_{Kow} + \frac{B_{Kow}}{T} \quad (50)$$

It therefore follows that

$$\log K_{ow} = \log f_n + \log (K_{ow})_n = \log f_n + A_{Kow} + \frac{B_{Kow}}{T} \quad (51)$$

where f_n is described previously.

Molar Volume, Gas Diffusion, and Density

For molar volume V and gas diffusion coefficient coefficient, D_f we will fit the following equations

$$V = A_V + B_V T \quad (52)$$

$$D_{f(air)} = A_{Df} T^{B_{Df}} \quad (53)$$

For density, the following equation is used

$$D_n = \frac{MW}{A_v + B_V T} \quad (54)$$

Sorption

Sorption of organic chemicals to organic solids is calculated by

$$K_S = f_n (K_S)_n + f_i (K_S)_i \quad (55)$$

Quantifying this equation, however, poses two fundamental problems. Firstly, the only predictive algorithms available for calculating sorption are for neutral species. Secondly, the solids characterization employed in these methodologies is inadequate to 'drive' these models. Therefore, we will calculate sorption based on our knowledge of the carbon-normalized sorption. This representation is consistent with the approach used for other properties.

Carbon-normalized sorption (K_{oc}) of an non-ionizable chemical or the neutral species of an ionizable chemical is related to its octanol water partitioning behavior by

$$\log (K_{oc})_n = \log K_{ow} - 0.32 \quad \textbf{(56)}$$

Because the temperature dependence for the sorption of neutral compound can be assumed to be that of *Kow*, it also follows that

$$\log (K_{oc})_n = A_{Kow} + \frac{B_{Kow}}{T} - 0.32 \quad \textbf{(57)}$$

To calculate the sorption of ionized chemicals, one can apply an appropriate multiplier M_i to the preceding equation. In particular,

$$(K_{oc})_i = M_i (K_{oc})_n \quad \textbf{(58)}$$

$$\log (K_{oc})_i = \log M_i + \log (K_{oc})_n \quad \textbf{(59)}$$

These multipliers are assumed to be dependent on ionic type and strength. In particular,

$$M_i = \begin{cases} M_{a1} = 10^{-2} & \textit{for monoanions} \\ M_{a2} = 10^{-4} & \textit{for dianions} \\ M_{c1} = 10 & \textit{for monocations} \\ M_{c2} = 10^{2} & \textit{for dications} \end{cases} \quad \textbf{(60)}$$

Water Diffusivity

Water diffusivity will be calculated by the following function

$$D_{f(H_2O)} = \frac{1.4\times10^{-4}}{\eta_w^{1.1}\ V^{0.6}} \quad \textbf{(61)}$$

where V is the chemical's molar volume and η is the viscosity of water (CRC 1990). The chemical's molar volume will be calculated using Equation **(52)** and the viscosity of water will be calculated using

$$\eta = A_\eta + T^{B_\eta} \quad \textbf{(62)}$$

(see the CRC (1990)). The resulting algorithm for water diffusivity is therefore

$$D_{f(H_2O)} = \frac{1.12\times10^{-22}}{T^{-7.33}\ (A_V + B_V\ T)^{0.6}} \quad \textbf{(63)}$$

3.3.4.2 Basic Properties of Metals and Inorganics

Several inorganic chemical properties are found in this section of the HWIR database. These properties and their units are listed in the accompanying Table 3.7. For each of these properties, the

HWIR database has slots for minimum, maximum, central tendency, and standard deviation. This structure should allow these properties to be treated as either fixed or random variables in a monte-carlo simulation.

Most of the inorganic chemical properties listed here are operational rather than fundamental. The solubilities and partition coefficients for metals are always dependent on the natural or waste treatment system in which they are found. Their values depend on many geochemical parameters that define the system, including pH, concentration of sorption sites, the affinity of the metal for the sorption sites, the DOC concentration, the concentration of major ions, and the concentration of other ligands in the system that complex with the metal. The variation of these parameters causes a wide range of partition coefficients and solubilities for each metal. The lack of site-specific parameter data at the HWIR sites leads to the statistical characterization of solubility and partition coefficients that is used herein. During each monte-carlo realization, property values will be drawn from the probability distributions defined by this data base.

The metals to be included in the database are Sb, As, Ba, Be, Cd, Cr, Co, Cu, Pb, Mo, Hg, Bi, Se, Ag, Tl, Sn, V, and Zn. If data are available for multiple oxidation states (i.e., As^{III}, As^{V}, Cr^{III}, Cr^{VI}, Se^{IV}, Se^{VI}), these will be treated as separate metals. Partition coefficients will also be collected for methyl mercury and cyanide.

Inorganic chemical property data will be generated in a two-tier approach. In the first tier, partition coefficients will be obtained from the scientific literature, from U.S. EPA reports and reports from other government and university sources, and from existing databases associated with exposure models. Electronic searches will be conducted using 20 national and international databases. Various estimating techniques will be used to derive partition coefficients as needed from reported metal concentrations in relevant media. The source of each partition coefficient collected or estimated will be documented. Where possible, the important geochemical parameters characterizing the natural or waste management system will also be documented. For those metals lacking literature or other values, best estimates based on available concentration data in relevant media, chemical similarities with other metals, and expert judgment will be used to estimate conservative, media-specific, partition coefficients.

In the second tier of analysis, the validity of the literature-derived partition coefficients will be explored by equilibrium speciation modeling. HWIR databases, the scientific literature, and EPA reports will be used to characterize the reactive surfaces in soils, sediments, suspended solids, and waste matrix materials. Pertinent surface reactions will be defined for the metals, and partition coefficients will be evaluated using the MINTEQA2 speciation model. This work should lead to a better understanding of the variation in partitioning due to variability in geochemical conditions and metals concentrations. This modeling in combination with expert geochemical judgment will be used to explore similarities in partitioning behavior among the metals of interest, and to establish reasonable bounds on partition coefficients where data are lacking. This analysis also will provide a check on the credibility of partition coefficients collected from the literature. It will identify the main geochemical variables that affect the partition coefficients and provide guidance for adjusting those coefficients, if necessary.

Partition coefficients and solubilities for groundwater are not included in this database. The HWIR groundwater module, developed over the past decade, includes a separate database that incorporates metals partitioning as a function of pH, redox conditions, and metals concentrations. This

database was regenerated using the latest version of MINTEQA2 along with background values of several relevant water quality parameters.

3.3.4.3 Transformation Reactions

The transformation reactions considered for the HWIR assessment included hydrolysis, aerobic biodegradation, anaerobic biodegradation, and biodegradation in activated media (e.g., activated sludge). The general approach to populating the chemical-specific data base for each of these processes is presented below. Our level of understanding of each of these transformation reactions varies substantially, and thus, so does our ability to populate the data base with rate constants for each of these reaction processes. Our intent in the design of chemical-specific data base was to be forward-looking and not limit its structure based on current knowledge of transformation reactions. For example, though our understanding of reduction in the environment has progressed to the point that we can identify the types of functional groups that will be susceptible to reduction in anaerobic systems, our limited knowledge of reaction mechanisms for such transformations is currently a barrier to the prediction of absolute rates, and how reaction rates will vary from one environmental system to the next. Due to an intensive research effort at NERL-Athens, we anticipate that we will have the capability to fully populate this part of the chemical-specific data base in the next 2-3 years.

Our understanding of hydrolysis reactions is quite advanced in comparison to the other transformation reactions. The prediction of hydrolysis rates, however, still requires the extrapolation of kinetics data that have been measured in the laboratory to transformations that occur in natural aquatic ecosystems. A unique aspect concerning the prediction of hydrolysis rates of organic chemicals is that, in the majority of cases, we can ignore the environmental system of interest except for hydrogen ion activity (pH).

Hydrolysis

A team of EPA scientists met numerous times to discuss hydrolysis rates and probable pathways of transformation for hydrolysis. The methods used to arrive at the reaction products were based primarily on the team's experience with similar compounds, their knowledge of the theory of these processes, and their understanding of structure-activity relationships. Literature searches were conducted afterwards to find needed hydrolysis rate data for the intermediate products of hydrolysis. If the literature failed to provide the required data, they were determined in the laboratory for some compounds.

In general, hydrolysis is a bond-making, bond-breaking process in which a molecule, RX, reacts with water forming a new R-O bond with the oxygen atom from water and cleaving an R-X bond in the original molecule. One possible pathway is the direct displacement of X^- with HO^-, i.e.,

$$RX + H_2O \longrightarrow ROH + HX \qquad \textbf{(64)}$$

The detailed mechanisms of hydrolytic processes are well defined and have been shown to involve the formation of intermediates such as protonated species, anions and carbonium ions, as well as combinations of these intermediates.

Generally, hydrolysis of organic compounds in water under pH-buffered conditions is first-order in the concentration of the organic species ([RX]), where the rate of hydrolysis (d[RX]/dt) is proportional to the concentration of pollutant RX:

$$\frac{d[\mathrm{RX}]}{dt} = -k_{obs}[\mathrm{RX}] \qquad \textbf{(65)}$$

where k_{obs} is the observed pseudo-first-order disappearance rate constant. The first-order dependence of the disappearance rate on [RX] is important, because it means that the half-life ($t_{1/2}$) associated with the preceding equation is independent of [RX]. Thus, the results obtained at a high RX concentration can be extrapolated to lower RX concentrations if other reaction conditions are held constant. The half-life of the reacting compound is given by

$$t_{1/2} = \frac{\ln 2}{k_{obs}} = \frac{0.693}{k_{obs}} \qquad \textbf{(66)}$$

where k_{obs} can include contributions from acid-catalyzed or base-mediated hydrolysis, or nucleophilic attack by water.

The overall hydrolysis rate constant is a summation of the the respective rate constants for acid, neutral and base hydrolysis. The following formula is used:

$$k_{hydrolysis} = k_a[H^+] + k_n + k_b\left(\frac{k_w}{[H+]}\right) \qquad \textbf{(67)}$$

where k_a and k_b are the specific acid and base second-order rate constants, respectively; and k_n is the neutral hydrolysis rate constant. In the data base, k_a, k_b, and k_n values are reported for the particular chemical at 25°C (+/-4°C). If $[H^+] = 10^{-pH}$ and $k_w = 10^{\frac{-6013.79}{T} - 23.6521\log T + 64.013 + pH}$ are now substituted into this equation and the entire expression is multiplied by $e^{\frac{E_a}{R}\left(\frac{T_2 - T_1}{T_2 T_1}\right)}$ to include temperature dependence, then

$$k_{hydrolysis} = e^{\frac{E_a}{R}\left(\frac{T_2 - T_1}{T_2 T_1}\right)}\left(k_a 10^{-pH} + k_n + k_b 10^{\frac{-6013.79}{T} - 23.6521\log T + 64.013 + pH}\right) \qquad \textbf{(68)}$$

where E_a represents the activation energy and R represents the universal gas constant (1.987 cal/mol K). The activation energy used in these calculations is assumed to be constant at 20,000 calories/mole. The temperatures, T_1 and T_2, are the standard temperature, 298.15 K, and the temperature at which the hydrolysis constant is desired, respectively.

Anaerobic and Aerobic Biodegradation

Rate constants for anaerobic and aerobic biodegradation were collected by searches of the BIOLOG file of the Environmental Fate Data Base compiled by the Syracuse Research Corporation (SRC) (Howard et al. 1986). The literature search was conducted by SRC personnel. Due to limited

resources, literature searches were conducted for a limited number of the HWIR chemicals. Chemicals were selected based on their occurrence in listed hazardous waste. The rate constants for anaerobic biodegradation are summarized in a report prepared by SRC for the American Petroleum Institute Consortium (Aronson and Howard 1997). The aerobic biodegradation rate constants will be summarized in a report prepared by SRC for NERL-Athens that is due in September of 1998.

The requirements for studies to be included in the aerobic biodegradation data base included (1) studies performed with soils, groundwater, aquifer materials, sediment, or surface water; and (2) studies conducted under aerobic conditions. Studies where the reaction system was seeded with microorganisms from other sources, e.g., sewage, pond sediment, and enrichment culture experiments were not included. These data will be reviewed by EPA scientists, and where sufficient data exists, the following rate constants for aerobic biodegradation will be provided to the chemical-specific data base: most likely rate constant, minimum rate constant, maximum rate constant, standard deviation and a distribution of rate constants.

The requirements for studies to be included in the anaerobic biodegradation data base included (1) the use of aquifer material, groundwater, or leachate (preferably from an anaerobic site, if stated); and (2) incubation under anaerobic conditions. Studies where the aquifer material was seeded with microorganisms from other sources, e.g., sewage, pond sediment, and enrichment culture experiments were not included.

Rate constants for anaerobic biodegradation were collected from eight types of groundwater studies: batch reactor, batch reactor with a groundwater inoculum, column studies, field studies, groundwater grab sample, groundwater inoculum, *in situ* microcosm and laboratory microcosm studies. For those published studies for which first-order rate constants were not available, but sufficient information was presented to calculate a value, the rate constant was calculated by SRC.

The first-order rate constants for anaerobic biodegradation collected by SRC were also reviewed by EPA scientists. Where sufficient data existed, the following rate constants for anaerobic biodegradation were provided for the chemical-specific data base: most likely rate constant, minimum rate constant, maximum rate constant, standard deviation and a distribution of rate constants). To achieve further resolution, rate constants for specific chemicals were grouped as a function of temperature ($T<15^{o}C$ and $T>15^{o}C$), pH ($pH<6$, $6<pH<8$ and $pH>8$), and redox conditions (e.g., sulphate-reducing and methanogenic).

3.4 Assessment Technology

The HWIR99 modeling system is designed to fully automate the assessment strategy as outlined in Section 3.1. As such, the HWIR99 modeling system reflects an integrated software system design consisting of: 1) a framework for organizing and executing the HWIR99 simulations; 2) a site definition processor for building the modeling input data files; 3) a set of core multimedia simulation modules; 4) a risk processor for establishing constituent-specific waste exit levels; and 5) a series of databases to build the HWIR99 site-based input files, store intermodule data during simulations, and store the final HWIR99 risk-based constituent-specific waste exit levels.

While much of the simulation software required for HWIR99 currently exists there remains a significant software development effort. The effort includes the following major design and development activities: 1) framework software; 2) global databases; 3) site definition processor; 4) constituent multimedia fate and transport module development and/or modification; and 5) risk-based exit level processor.

The purpose of this presentation is to describe the software systems design that meets the functional and testable requirements from the EPA for the FRAMES-HWIR Technology Software System. The requirements are outlined in *Requirements for the FRAMES-HWIR Technology Software System*. The design summarized here will be used to develop detailed specifications and test plan documents for the FRAMES-HWIR Technology Software System.

This presentation is organized around a description of the system design for the FRAMES-HWIR Technology Software System and the six principal processors contained within the software system.

- System Requirements and Design, Section 3.4.1
- System User Interface (SUI), Section 3.4.2
- Distribution Statistics Processor (DSP), Section 3.4.3
- Site Definition Processor (SDP), Section 3.4.4
- Computational Optimization Processor (COP), Section 3.4.5
- Multimedia, Multipathway Simulation Processor (MMSP), Section 3.4.6
- Exit Level Processor (ELP), Section 3.4.7

Included in Section 5.0 is a glossary containing definitions of key terms used throughout this presentation.

3.4.1 Summary of the FRAMES-HWIR Technology Software System Requirements

The FRAMES-HWIR Technology Software System will

1. be implementable on one or multiple stand-alone IBM-compatible personal computers (PC).
2. be developed to operate in and have applications compiled for a MS Windows'95 environment (32-bit).
3. be designed to run on a Pentium (586)-compatible computer with a 200 MHZ processing speed, 64 megabytes of RAM, and a 6-gigabyte hard drive or greater.
4. be designed with performance criteria emphasizing run-time efficiencies.
5. be an object-oriented system with each processor/module being developed for a specific purpose and linked through data specifications.
6. accommodate existing environmental models in a variety of programming languages (i.e., FORTRAN, C++, C). The System User Interface and processors will be programmed in Visual Basic and C++.
7. access the Regional and National Environmental Setting Distribution Statistics, Model Error Statistics, Site-Based Regional Statistics, National Statistics, Site Survey, MET (meteorological station data), and Chemical Constants databases.
8. produce the Site Definition Files, Site Simulation Files, Global Results Files, Risk Summary

Output File, and Protective Summary Output File.

9. use the Microsoft Access file format for the Regional and National Environmental Setting Distribution Statistics, Module Error Statistics, Site-Based Regional Statistics, National Statistics, Site Survey , MET, Chemical Constants databases, Risk Summary Output File, and Protective Summary Output File.
10. use a flat ASCII file format (sequence-independent) for the Site Definition Files, Site Simulation Files, and Global Results Files.
11. interact with the user through the System User Interface.
12. conduct a simulation or a series of simulations for waste constituent fate and transport on sampled waste management units (WMUs), and provide risk-based information for the determination of constituent concentration waste exit levels.
13. allow the user some control in accessing results and importing them to other applications for additional data analyses.
14. monitor and report Central Processing Unit (CPU) usage per major system component [e.g., processors and modules), and differentiate between Input/Output and data-processing within each processor/module].

The first 3 requirements are hardware and operating system requirements, and the last 11 are input and output requirements for databases and data files associated with the FRAMES-HWIR Technology Software System.

3.4.1.1 FRAMES-HWIR Technology Software System Components

The FRAMES-HWIR Technology Software System consists of a user interface and a series of processors within a system framework. Figure 3.13 shows the overall structure of the FRAMES-HWIR Technology Software System. The five processors within the system framework are as follows:

- Distribution Statistics Processor (DSP). This processor randomly samples from statistical distributions describing the variation of measurement mean and sampling error associated with the model variables. The DSP will select a particular mean or standard deviation from a distribution of means or standard deviations for a given variable. As mentioned previously, this functionality is being designed into the Technology Software system, but will not be utilized in the HWIR99 Risk Assessment due to a lack of required data.

- Site Definition Processor (SDP). This processor organizes all of the data for input to the Site Definition Files by accessing data files containing all the necessary information and executing a hierarchical protocol to read these data files and extract the required data; it also provides the preliminary simulation plan and control information to be used by the constituent Multimedia, Multipathway Simulation Processor.

- Computational Optimization Processor (COP). This processor assimilates the exposure and risk scenario contained in the Site Definition Files (from the SDP) and establishes, based on specific "rules," a modified scenario that is technically complete and computationally efficient. The computational rules are developed separately for the FRAMES-HWIR Technology Software System by EPA. These "rules" are used to eliminate source loss routes, transport and exposure pathways, and receptors to optimize the computational performance of the system. Any element

eliminated will be saved in the Site Simulation Files information for accountability later, but will not be part of the computational simulation.

- Multimedia, Multipathway Simulation Processor (MMSP). This processor implements the release, transformation, transport, exposure and risk/hazard assessment modeling protocol by choosing and linking the appropriate models to supply results to the Exit Level Processors; consists of a collection of individual software modules each representing a modeling-based approach to one of the fundamental elements of the risk assessment process. The MMSP is where the exposure and risk computations of the simulation are conducted.

- Exit Level Processor (ELP I and ELP II). These processors take the results of the MMSP individual site simulations and tabulate the information to discern levels of protection for decisions on the constituent waste exit criteria; ELP I produces the Risk Summary Output File; ELP II takes the Risk Summary Output File and generates the Protective Summary Output File. This site-based exposure and risk information is used to establish a national distribution of risks. The national distribution of risks, and all related data, forms the technical basis for EPA to select chemical-specific exit levels.

Note, all executable, database, data group, and data file names used in this report are descriptive names. These names are not meant to be the actual names employed in the software coding. The actual software names used in the coding will be defined during the development of the FRAMES-HWIR Technology Software System. The descriptive names in this report are used to provide a reference to the type of executables, data files, databases, or data groups employed.

3.4.1.2 FRAMES-HWIR Technology Software System Structure

The SUI, databases, data files, and processors that comprise the components of the FRAMES-HWIR Technology Software System and their respective interactions, linkages, and connections are presented in Figure 3.13. The circles in Figure 3.13 represent the processors that actually process the information that is read from databases and stored in data files. The boxes (e.g., Site-Based Database) associated with the DSP, SDP, and MMSP represent databases that are externally-populated (except for the Regional and National Statistics Database and Site Survey Database) and accessed by these processors. Vertically-elongated rectangles (e.g., Site Definition Files) represent data files that are populated by processors and can represent input data files to succeeding processors. Arrows indicate locations where data and information are transferred between processors and data files. The shaded boxes represent those processors, databases, and data files that are included in the FRAMES-HWIR Technology Software System design, but will not be implemented as part of the HWIR99 Assessment Strategy, as they are not specifically required. Although Figure 3.13 may imply that the databases and data files might be associated with one processor or other, they actually represent linkages between these processors.

Figure 3.14 presents the processors and the protocol for sequentially firing-off each processor as part of a two-stage Monte Carlo analysis. Horizontally-elongated rectangles (e.g., Outer and Inner loops) represent the protocol for sampling and analysis in the design of the HWIR99 Assessment Strategy. Each loop is briefly described as follows:

- Outer Loop. This loop is an iteration within the FRAMES-HWIR Technology Software System

that allows for the random selection of measurement and sampling errors associated with key risk assessment variables.

- Inner Loop. This loop is an iteration within the FRAMES-HWIR Technology Software System that loops through all sites or locations associated with the HWIR99 Assessment Strategy. This loop is also known as the site assessment loop.

- Source Loop. The source loop chooses a source type associated with the site/location.

- Chemical Loop. This loop is an iteration within the Inner Loop of the FRAMES-HWIR Technology Software System that ensures each waste constituent of interest for the source types is processed through the MMSP.

- Concentration of Waste Loop (C_w). The C_w loop sequentially goes through the pre-selected, defined waste concentrations for each chemical. The attributes and characteristics of each constituent influence the computational results associated with the possible release, migration, fate, and effects of that chemical.

The outer and inner loops are designed to implement a two-stage Monte Carlo approach. As noted in Figure 3.14, the outer loop will not be implemented as part of the FRAMES-HWIR99 Technology Software System, even though it has been designed into the system. As opposed to having sites randomly selected as part of the inner loop, the 200 sites associated with the Site-Based Database will be sequentially sampled for the FRAMES-HWIR99 Technology Software System runs.

3.4.2 System User Interface (SUI)

The SUI will connect, interact with, and direct the other processors housed in the FRAMES-HWIR Technology Software System, managing the overall execution of the software system. The interface will allow the user to do the following:

- define what mode of operation is to be conducted
- define the indices for the different loops associated with the HWIR99 Assessment Strategy
- start, stop, and resume simulations
- define where the results should be stored
- define what level of data storage is required (i.e., only required data, all data generated, or some level in between).

The SUI manages the different processors, warning/error files, data files, and databases through the use of user-interactive computer screens.

3.4.2.1 Summary of SUI Requirements

As outlined in *Requirements for the FRAMES-HWIR Technology Software System*, the SUI will

1. control the execution of the FRAMES-HWIR Technology Software System processors.
2. allow the FRAMES-HWIR Technology Software System to operate in several modes: a)

testing/debug; b) single-site; and c) production (automated).

a. Testing/Debugging mode requires the system to start, stop, resume, and report status at any processing point along a simulation to allow the developer or user to determine the status of the software or application.

b. Single-site mode requires that the system evaluate a site using a random or user-specified site location. This mode allows users to conduct "what if" analyses and case studies to compare with science-support model results.

c. Production mode will allow users to conduct the full-scale HWIR analysis with the sample set of sites that constitutes a production application. This mode requires the system to start, stop, and resume options, and to report the status for cases in which the production run is interrupted and not all the sites evaluated.

3. allow the user to select sites in several modes as follows,

   a. select some subset of a production application (e.g., sites 1 to 5; sites 6 to 10; sites 1, 4, 7, and 10; or sites 1 to "N")

   b. select all 200 "defined" sites.

   c. select "N" number of hypothetical sites, based on location from the Site Survey database for a waste management unit.

   d. select "N" number of sites with a combination of "defined" and hypothetical sites.

   e. select either a defined or hypothetical site.

4. have options to control which files from a simulation are stored and the amount of data to be stored. The Data Management Screen of the SUI will control the different levels of data storage related to components and modules with degrees of storage established that are understood by the various components/modules.

5. contain a File Management Screen of the SUI that identifies database location to be accessed and directories into which FRAMES-HWIR Technology Software System files are stored.

6. include as part of the System Management Screen the ability to allow the user to select indices for the distribution statistics loops to be executed for the simulation.

7. contain a System Status Screen that allows the user to determine the status of the simulations and allows the user to start, stop, and resume.

8. allow each FRAMES-HWIR Technology Software System processor to be independently tested.

3.4.2.2 SUI Structure

The SUI will be a Windows'95 menu-driven interface that collects information from the user and controls the activities associated with the simulation. There are three main screens associated with the SUI: 1) System Management Screen; 2) Data and File Management Screen; and 3) System Status Screen. These user interface screens are the main method of interaction between the user and the FRAMES-HWIR Technology Software System.

1. A System Management Screen allows the user to set the location of SUI data files. Any number greater than unity would store selected temporary files as permanent files. However, the SUI is not responsible for ensuring the linkage between "private" data files and an appropriate module; this is the responsibility of the individual module. The System Management Screen will be designed to have three modes of operation, where each mode of operation involves a simulation or a series of simulations defined by the user:

    a) testing/debugging -- Under the testing/debugging mode, the SUI provides the analyst with control options to start, stop, resume, or exit an analysis. "Start" initiates the simulation. "Stop" allows the user to stop the simulation following the successful completion of a particular processor; control reverts to the SUI. If the user has stopped the simulation after a designated processor, the user can resume the simulation using the "Resume" command. The user can also exit a simulation, following the successful completion of a particular processor, by implementing the "Exit" command.

    b) single site -- Under the single-site mode, the user will be able to simulate a single scenario. The user will also be able to control points where the simulation can be stopped, then resumed.

    c) production -- Under the production mode, the user cannot terminate the simulation, and therefore, a simulation proceeds to completion. A simulation represents the user-defined indices associated with the loops of the assessment. The default indices for the internal loops are the set for a complete simulation (e.g., M and N). Users will be able to select a subset of indices, including a single site.

2. A Data and File Management Screen allows the user to store files and manage the location of data. The level of stored information will also be controlled by the user and will have a value of 1 through 5, representing different levels and quantities of data that are to be stored for each iteration. A default value of unity (i.e., 1) stores the data required to successfully complete a simulation. A default value of 5 would store "all" of the files necessary to flow the information through the system.

3. A System Status Screen informs the user of the status of the system. The system will inform the user of the simulation mode, where they are in the analysis, and the status of the simulation. Warnings and errors would be displayed on this screen as well as CPU information per processor.

3.4.3 Distribution Statistics Processor (DSP)

The primary purpose of the DSP is to build databases containing all the probabilistic data reflecting

parameters included in the Regional and National Environmental Setting Distribution Statistics Databases. The DSP randomly selects a distribution out of potential distributions for each stochastic parameter, although the parameter distribution types will be constant. The DSP will 1) collect, collate, and analyze regional and national environmental data; 2) determine statistical properties from a regional or national perspective; and 3) populate databases from which random sampling can occur. The three components associated with the DSP are represented by the unshaded components in Figure 3.15.

3.4.3.1 Summary of DSP Requirements

The design of the DSP reflects the requirements outlined in the *Requirements for the FRAMES-HWIR Technology Software System*, which covers specifications on input and output, operating system, and accessory software and hardware, where appropriate. A summary of the requirements associated with DSP are as follows; the DSP will

1. read the Regional and National Environmental Setting Distribution Statistics databases.

2. populate the Regional and National Statistics databases with information that is a subset of the probabilistic data (i.e., randomly-sampled variable data), reflecting parameters included in the Regional and National Environmental Setting Distribution Statistics databases.

3. require the Regional Statistics and National Statistics databases to contain data groups that include, but are not limited to:
   Header
   Site Layout
   Source Data
   Air Data
   Vadose Zone Data
   Saturated Zone Data
   Watershed Data
   Waterbody Data
   Farm, Terrestrial Life, and Aquatic Foodchain Data
   Human and Ecological Receptor/Exposure Data
   Human and Ecological Risk Data

4. require the Regional Statistics and National Statistics databases to be accessible to the SDP.

5. conduct boundary condition and cross-correlation (e.g., positive definite) verification checks on the Regional and National Environmental Setting Distribution Statistics databases.

6. ensure that cross-correlated variables originate from the same data source (i.e., national, regional, or site-based).

7. report any processor-specific warnings or errors to the SUI.

8. be tested as a stand alone processor independent of the other FRAMES-HWIR Technology Software System processors.

3.4.3.2 Regional and National Environmental Setting Distribution Statistics Databases

The DSP reads the Regional and National Environmental Setting Distribution Statistics Databases. These databases are briefly discussed below:

1. Regional Environmental Setting Distribution Statistics Database. This database contains environmental data on a subset of environmental parameters for a given region or regions of the United States. Each region contains environmental data that describe the region's unique characteristics (e.g., geochemistry, geometry, hydrology, hydraulics, geology, hydrogeology, ecology). These data are collated and statistically-analyzed to develop statistical distributions of the means and variances of the stochastic variables as they vary within some range (e.g., maximum and minimum). Results (with the accompanying statistical information) are stored in this database, representing the error associated with the specific values used to describe the statistics (e.g., mean and variance). For example, if bulk density represented a stochastic variable for each waste unit at each site within the region, this file would provide the mean of the mean bulk densities in the sampled population. The Regional Environmental Setting Distribution Statistics Database also inherently reflects a conceptualization of a site, utilizing data collected for multiple sites over a region, and describes the environmental setting. For components of the site-based data sets for which regional-specific data are not available, the same sampling scheme from the national distribution, as performed in the generic conceptualization, will be performed. Cross-correlation between appropriate parameters in this database would be honored and carried-through the system.

2. National Environmental Setting Distribution Statistics Database. This database contains national distributions of environmental setting data. The data are similar to that contained in the Regional Environmental Setting Distribution Statistics Database. Cross-correlation between appropriate parameters in this database also would be honored and carried-through the system.

The databases contain individual parameters whose statistical distribution characteristics are themselves described with statistical distributions. For example, the maximum daytime temperature varies across the United States, and every region has its own unique distribution of maximum daytime temperatures. If all of the meteorological stations in the southeast are sampled on an hourly basis for 5 years, a distribution for maximum daytime temperature can be developed. The distribution may be of type "Normal" with a mean 81 deg F, standard deviation of 12 deg F, minimum of 52 deg F, and a maximum of 110 deg F. If data were collected at the same meteorological station in 5-year blocks, distributions of the individual parameters (i.e., mean, standard deviation, minimum, and maximum) could be generated. These distributions would reflect the sampling and measurement error associated with the variable, and this is what the Outer Loop attempts to capture. Typically, the statistical parameters of these distributions can be directly used in a Monte Carlo analysis. In reality though, there is error associated with each of the distribution parameters.

Region-specific variability can also factor into variations in the data. For example, daily maximum temperatures for any given year will differ as latitude changes. Therefore, regional and national databases will contain data describing the geographic boundaries of the regions (e.g., minimum and maximum latitude and longitude). The regional database will contain data for multiple regions, each defined with geographic boundaries. The national database will contain only one set of data, which

reflects the nation.

The file design for the Regional and National Environmental Setting Distribution Statistics Databases will be identical, except that there will be more entries associated with the regional data than the national data. The data in the two environmental setting distribution statistics databases will contain two data tables:

1. The first data table will contain the sequence-independent distribution information for each variable:

Data Set Name (string) (e.g., MET data)
Variable Name (string) (e.g., bulk density)
Indices (set of integers) (e.g., k-dimensional, based on module needs)
Units (string)
Type (choice of type) (e.g., integer, float, logical, character)
Distribution Type (choice of distribution) (e.g., normal, log-normal, uniform)
Minimum Value (float)
Maximum Value (float)
Central Tendency Distribution (CTD)
Distribution Type (choice of distribution)
Central Tendency (float)
Variance (float)
Minimum Value (float)
Maximum Value (float)
Variance Distribution (VD)
Distribution Type (choice of distribution)
Central Tendency (float)
Variance (float)
Minimum Value (float)
Maximum Value (float)
Cross Correlation between CTD and the VD (float)
Minimum Distribution (MinD)
Distribution type (choice of distribution)
Central Tendency (float)
Variance (float)
Minimum Value (float)
Maximum Value (float)
Cross Correlation between CTD and the MinD (float)
Maximum Distribution (MaxD)
Distribution Type (choice of distribution)
Central Tendency (float)
Variance (float)
Minimum Value (float)
Maximum Value (float)
Cross Correlation between CTD and the MaxD (float)

2. The second data table will contain the cross correlations between distributions of variables. Cross-correlation data items will be

Data Set Name (string)
Variable Name (string)
Indices (set of integers)
Variable Name (string)
Data Set Name (string)
Indices (set of integers)
Cross Correlation between the variables (float)

A cross correlation of unity will be assumed for a variable to itself. This is essentially a matrix of cross correlations between all variables in the database. This matrix can be checked for consistency by ensuring that the matrix is positive definite. Intuitively, a positive definite matrix will consistently correlate parameters "a" to "c," if "a" is correlated to "b," and "b" is correlated to "c." This ensures the transitive property of the correlation coefficients.

3.4.3.3 Regional and National Statistics Databases

The Regional and National Statistics Databases will be populated with the appropriate data by the DSP, based on sampling location, contaminants, and waste type. The Regional Statistics Database contains a subset of environmental data for a given region of the United States. This information was generated from the statistical analysis associated with the DSP for all stochastic variables, reflects a conceptualization of a sampling location utilizing data collected for multiple sampling locations over a region, and describes the environmental setting. The locations where data are collected and used to build the regional distribution may include locations not containing HWIR sites. For example, if a soil survey was done for a region, it probably would not have focused on Industrial Subtitle D facility "sites." The regional information contains the error associated with the specific values used to describe the statistics (e.g., mean and variance). For components of the location-based data sets for which regional-specific data are not available, the same sampling scheme from the national distribution, as performed in the generic conceptualization, will be performed. Cross correlation between appropriate parameters in this database would be honored and carried-through the system.

The National Statistics Database contains a subset of environmental data for the entire United States. This information was generated from the statistical analysis associated with the DSP for all stochastic variables. The database inherently reflects a conceptualization of a sampling location, utilizing data collected for multiple sampling locations across the nation, describes the environmental setting, and reflects the characteristics of the sampling location. The national information contains the error associated with the specific values used to describe the statistics (e.g., mean and variance).

Because the information is based on a composite of multiple sites, these data will represent a description of a "generic" site with characteristics associated with many sites. The generic site description is valuable if site-specific data are not available. These files do not necessarily contain data for all environmental parameters; rather, they contain data for a subset of the total list of parameters needed for a site risk assessment. A subset reflects key parameters for which data exist.

The data produced by the DSP will be a selection of a distribution from the set of distributions. The distribution information stored in the Regional and National Statistics Databases will have the following items:

Data Set Name (string)
Variable Name (string)
Indices (set of integers)
Units (string)
Type (choice of type)
Distribution Type (choice of distribution)
Central Tendency (float)
Variance (float)
Minimum Value (float)
Maximum Value (float)

An additional table of cross correlations will also be kept in the Regional and National Statistics Databases; these data will contain the following items:

Data Set Name (string)
Variable Name (string)
Indices (set of integers)
Variable Name (string)
Data Set Name (string)
Indices (set of integers)
Cross Correlation between the Variables (float)

During generation of the distribution for variables from the National Environmental Setting Distribution Statistics Database, cross correlations between central tendency and variance will be taken into account, as well as correlations between different variable distributions. The DSP will "verify" the appropriateness of data by testing the bounds against the minimum and maximum for the distribution. It will also verify that the cross correlation matrix of the variables is positive definite.

3.4.4 Site Definition Processor (SDP)

The purpose of the SDP is to develop and collate the data required to simulate the release, transport, exposure, and hazard/risk assessment to be eventually performed by the MMSP. This information may include attributes from national-, regional-, and/or site-based-setting data. Additional data that control the flow of information and account for model error are also included. Figure 3.16 illustrates those components of the FRAMES-HWIR Technology Software System that are associated with the SDP. The SDP consists of seven data files, providing information into a processor that creates a data file that meets all of the needs to implement the MMSP.

3.4.4.1 Summary of the SDP Requirements

The design of the SDP reflects the requirements outlined in the *Requirements for the FRAMES-HWIR Technology Software System*, which covers specifications on input and output, operating

system, and accessory software and hardware, where appropriate. A summary of the requirements associated with SDP are as follows. The SDP will

1. populate the Site Definition Files with all the data necessary to conduct the HWIR multimedia, multipathway exposure and risk assessment.

2. access the specified databases, including the Site-Based, sampled-Regional and National Statistics, Site Survey, and Model Error Statistics.

3 populate the Site Definition Files using a hierarchical scheme. When a simulation requires variable data, the actual value will be derived by randomly-sampling the Site-Based, then Regional Statistics, then National Statistics databases.

4. require the Site Definition Files to contain data groups that include, but are not limited to:
   Header
   Site Layout
   Source Data
   Air Data
   Vadose Zone Data
   Saturated Zone Data
   Watershed Data
   Waterbody Data
   Farm, Terrestrial Life, and Aquatic Foodchain Data
   Human and Ecological Receptor/Exposure Data
   Human and Ecological Risk Data

5. report any processor-specific warnings or errors to the SUI.

6. conduct boundary condition and Site Layout Data Group verification checks on the input databases (e.g., no streams in deserts).

7. allow and account for the cross-correlation between variables.

8. be testable independent of the other FRAMES-HWIR Technology Software System processors.

3.4.4.2 Databases Supplying Information to the SDP

Six databases can feed information into the SDP: Chemical Properties Database, Module Error Statistics Database, Site-Based Database, Regional and National Statistics Databases, and Site Survey Database. All of these databases remain static for the entire implementation, except for the Regional and National Statistics Databases, where a portion remains static. The portions of the Regional and National Statistics Databases that do change occur as part of the Outer Loop, and as a result of the implementation of the SDP (see Figure 3.16). Each database is described as follows:

1. Chemical Properties Database. This database includes: 1) all of the waste constituents required by the HWIR99 Assessment Strategy; and 2) physical and chemical properties required by the

MMSP. Some of the chemical properties may be a function of the site (e.g., temperature, pH) and will vary, depending on the location. When processing chemical data, the SDP will factor-in site location when defining the chemical properties.

2. Module Error Statistics Database. This database contains statistical information for quantifying the error associated with using analytically, semi-analytically, and empirically based models. These characterized errors may include, but are not necessarily limited to, differences with the more mechanistically-based numerical models that attempt to more accurately define the transformation, transport, fate, and effects of contaminants in the environment.

3. Site-Based Database. The Site-Based Data file includes site-specific information from the OSW HWIR site-based data collection effort. These data represent discrete values without statistics. Inherently built into this data file is site layout information, which reflects a conceptualization of a site, utilizing data specifically collected for the site to describe the layout of the physical waste units, environmental setting, and receptor distributions. This database contains the following information, when and where appropriate:

   Source data, including waste management unit and waste characteristics
   Air data
   Vadose zone data
   Saturated zone data
   Watershed data
   Surface water data
   Terrestrial foodchain data
   Aquatic foodchain data
   Human receptor/exposure data
   Ecological receptor/exposure data
   Human risk data
   Ecological risk data

4. Regional Statistics Database -- Static. This database contains 1) regional data generated from the DSP, and 2) regional information that remains static throughout the implementation of the HWIR99 Assessment Strategy. Regional data generated from the DSP was previously discussed in more detail in the DSP section of this report. The static data in the Regional Statistics Database include information that does not contain the error associated with the specific values used to describe the statistics (e.g., mean and variance), as with the numbers originating from the Regional Environmental Setting Distribution Statistics Database and stored in the non-static portion of the Regional Statistics Database. This database contains discrete values as well as parameters where the mean, variance, and range have been identified. Data with distributions and statistics pertaining to a site layout are also defined in this database. The site layout data reflect a conceptualization of a site, utilizing data specifically collected for the region to describe the layout of the physical waste units, environmental setting, and receptor distributions. This database will contain information similar to that outlined in the Site-Based Database, although its information may not be complete enough to fully implement a site simulation.

5. National Statistics Database -- Static. As with the Regional Statistics Database, the National

Statistics Database contains 1) national data generated from the DSP, and 2) national information that remains static throughout the implementation of the HWIR99 Assessment Strategy. National data generated from the DSP was discussed in more detail previously in the DSP section of this report. The static data in the National Statistics Database include information that does not contain the error associated with the specific values used to describe the statistics (e.g., mean and variance), as with the numbers originating from the National Environmental Setting Distribution Statistics Database and stored in the non-static portion of the National Statistics Database. This database contains discrete values as well as parameters where the mean, variance, and range have been identified. Data with distributions and statistics pertaining to a site layout are also defined in this database. The site layout data reflect a conceptualization of a site, utilizing data specifically collected for the region to describe the layout of the physical waste units, environmental setting, and receptor distributions. This database will contain information similar to that outlined in the Site-Based Database, and the information contained in this database will be able to fully implement a site simulation.

6. Site Survey Database. The EPA has collected data from over 2,700 different waste sites across the United States via the EPA OPPI Industrial D Survey. The OPPI Industrial D survey data are stored in the OSW OPPI Site Survey Database, as illustrated in Figure 3.16. Because this database contains some unnecessary information, the OPPI Processor will access the database, process the data, and place it in a format that is compatible with the other databases described above. This database will contain, but will not be limited to, location, waste management unit, and volume information.

The SDP represents the entry point for the Inner Loop in the FRAMES-HWIR Technology Software System. The Inner Loop represents a process (which may be random) for selecting a site. The SDP may be operated in one of four modes. The modes are described below:

1. Selects (and then holds static) and processes all 200 sites with its full complement of data (i.e., 1 to N, where N equals 200).

2. Randomly selects and builds "N" number of hypothetical sites, based on location and the generic site layout information.

3. Randomly selects and builds "N" number of hypothetical sites, from a combination of "defined" (i.e., Site Bases Data) and hypothetical sites, based on location and the site layout information.

4. Randomly selects and builds a single hybrid site from a combination of "defined" (i.e., Site Bases Data) and hypothetical sites, based on location and the site layout information.

Figure 3.17 illustrates the Inner Loop and the additional loops and processors that are impacted by the Inner Loop. The source type, chemical, and waste concentration (C_w) loops are contained inside the Inner Loop and are not randomly chosen, but sequentially stepped-through.

3.4.5 Computational Optimization Processor (COP)

The primary purpose of the COP is to streamline simulation of source release, multimedia fate

and transport, exposure, and risk for the FRAMES-HWIR Technology Software System. The streamlining is focused on computational issues and is intended to minimize the number of modules and simulations executed by the MMSP to improve run-time performance.

The COP acts as a filter on the simulation being conducted by reviewing the combinations of chemicals, source type, transport and exposure pathways and receptor types. This filtering process is conducted by use of predefined algorithms or "rules." These "rules" will key off sensitive variables for a given site scenario to determine if the site or pathway will result in *de minimis* impacts. The filtering will be conducted by site, source type, waste concentration category, environmental medium, and exposure pathway, eliminating transport pathways, exposure routes, and/or human and ecological receptors whose inclusion would result in *de minimis* impacts. For example, the atmospheric transport module and any related exposure pathways would not need to be executed for nonvolatile compounds buried in a landfill. A set of "rules" will be developed that will allow decisions of this type to be made based on the reading of the Site Definition Files. The EPA will develop these "rules" independent of the FRAMES-HWIR Technology Software System. These rules will be applied throughout the COP. Thus, the COP 1) reads the comprehensive Site Definition Files, 2) applies the computational efficiency rules, and 3) produces the Site Simulation Files which represents the file that is actually read by the various modules within the MMSP or changes nothing if the computational efficiency rules indicate that the normal sequence of modules to be executed for the simulation are appropriate. The COP does not modify Site Layout or any other Data Groups associated with the Site Definition Files. Figure 3.18 shows a detailed diagram of the Site Simulation Files created by the COP and the COP's operations.

3.4.5.1 Summary of the COP Requirements

Any design should reflect the requirements outlined in *Requirements for the FRAMES-HWIR Technology Software System*. These documents cover specifications on input and output, operating system, and accessory software and hardware, where appropriate. The COP will

1. read the Site Definition Files and modify them, as necessary . The modified Site Definition Files are renamed the Site Simulation Files.
2. require the Site Simulation Files to have a structure identical to that of the Site Definition Files.
3. require the Site Simulation Files to contain data groups that include, but are not limited to:
   Header
   Site Layout
   Source Data
   Air Data
   Vadose Zone Data
   Saturated Zone Data
   Watershed Data
   Waterbody Data
   Farm, Terrestrial Life, and Aquatic Foodchain Data
   Human and Ecological Receptor/Exposure Data
   Human and Ecological Risk Data

4. apply computational efficiency rules (to be determined by EPA) to Site Definition Files when transferring data to the Site Simulation Files.

5. be used to determine the execution sequence of the MMSP (through the SUI).

6. report any processor-specific warnings or errors to the SUI.

7. conduct boundary condition and data checks in pre-processor verification checks on the Site Definition Files

8. be tested as a stand alone processor, independent of the other FRAMES-HWIR Technology Software System processors.

3.4.6 Multimedia Multipathway Simulation Processor (MMSP)

The MMSP is a framework that uses information from the SUI to manage the modules to conduct multimedia multipathway exposure and risk assessment analyses for the FRAMES-HWIR Technology Software System. The MMSP manages the sequential execution of the required modules for each simulation. The modules reflect the individual components of the risk assessment process. A module is defined as a model and necessary pre/post processors. Figure 3.19 illustrates where the MMSP fits within the FRAMES-HWIR Technology Software System.

3.4.6.1 Summary of MMSP Requirements

Any design should reflect the requirements outlined in *Requirements for the FRAMES-HWIR Technology Software System*. These documents cover specifications on input and output, operating system, and accessory software and hardware, where appropriate. The MMSP will

1. execute the sequence and manage the flow of data through the various computational modules.
2. represent the framework around the multimedia, multipathway exposure and risk assessment capability required for the HWIR assessment.
3. have the following modules included in the MMSP for HWIR:
   - Source Modules (Surface Impoundment, Land Application Unit, Waste Pile, Landfill, Aerated Tank)
   - Fate and Transport Modules (Air, Vadose Zone, Saturated Zone, Watershed, Waterbody)
   - Foodchain Modules (Terrestrial Life, Farm, and Aquatic)
   - Human Exposure and Risk Modules
   - Ecological Exposure/Risk Module
4. perform a simulation that is represented by a multimedia, multipathway source, transport, transformation, exposure, and risk assessment .
5. receive input from the COP through the Site Simulation Files or receive input from the SDP through the Site Definition Files if the COP doesn't make any changes to the data group data.
6. be responsible for providing information necessary to perform input and output (e.g., provide the name of the data file) for the different modules.
7. define specifications that link the modules into a simulation for the HWIR assessment.
8. provide the input to the ELP in an appropriate format through the Global Results Files.
9. be designed to allow for the storing of appropriate files used in the exposure and risk assessment per simulation.
10. have the capability of storing varying degrees of data, depending on the user's needs (defined by

user through the SUI's Data Management Screen).

11. process errors that cause modules to abnormally terminate. The MMSP will recognize the occurrence of such errors and execute explicit protocols (e.g., terminate simulation and transfer control to the System Status Screen of the SUI).
12. report any processor-specific warnings or errors to the SUI.
13. be tested as a stand alone processor, independent of the other FRAMES-HWIR Technology Software System processors.

3.4.6.2 Module Requirements

The modules reflecting the individual components of the risk assessment process reflect the sequential processing of risk assessment. A module is defined as a set of pre- and post- processors and a model. Figure 3.20 indicates the general interactions between these module types within the MMSP. The following module types are included in the HWIR99 Assessment Strategy:

- Source Modules (Surface Impoundment, Land Application Unit, Waste Pile, Landfill, Aerated Tank)
- Fate and Transport Modules (Air, Vadose Zone, Saturated Zone, Watershed, Waterbody)
- Foodchain Modules (Terrestrial Life, Farm, and Aquatic)
- Human Exposure and Risk Modules
- Ecological Exposure/Risk Module

Modules representing each of the risk assessment steps will be formulated outside of the FRAMES-HWIR Technology Software System development. The MMSP and the FRAMES-HWIR Technology Software System assume that all the modules 1) have been unit tested, 2) have undergone quality assurance and quality control by the module developers, and 3) will access all databases and data files required without guidance from the MMSP. The modules should operate as "black boxes" in the MMSP and should not require the MMSP to provide information on how to execute.

It is anticipated that different levels of data storage associated with simulations, addressing varying degrees in quantity (e.g., temporary versus permanent file), could be implemented in the MMSP. The module is responsible for the data storage level (defined by the user through the SUI). If a module is given a data storage level greater than unity (e.g., 2-5), then the module is responsible for determining what files are to be saved. If a file is left in temporary space for data storage state greater than unity (i.e., >1), then that file will be copied into permanent space.

Module errors and warnings are reported to the MMSP, which in turn reports them to the SUI via an output file that is created by the module. Because it may be difficult to change each module to correctly detect errors, when invoked, a module will immediately write the error message to an error file and open a warning file. If a "detectable" error occurs when the code executes, the information in the error file is updated, and the module terminates. If a module detects a warning, information about that warning is written to a warning file. If the algorithm successfully continues through to the end, the error file is deleted, and the warning file is closed. The MMSP will echo module warnings and errors to the SUI, as well as any warnings and errors that occur within the MMSP.

Each module will be given the location of the inputs data it requires. The module is expected to

read these files, using the subroutines in the shared DLL (Dynamic Link Library). If a module needs MET data, that module is expected to read that format by methods designed and implemented by EPA. The MET Database is in a flat ASCII format determined by EPA and will be populated by EPA. Modules are expected write their outputs to a given location. The module is expected to write these files using the subroutines in the shared DLL. The specification of the Global Result Files will dictate the output variables that are expected to be written out by the module.

Pre- and post-processors are expected to be designed, implemented, and tested by the module developers. The MMSP design and implementation stops at the specified Site Definition Files, Site Simulation Files, and Global Result Files. The module developers are expected to reformat and re-order data to meet the specific needs of their module. Shared subroutines designed and developed by Pacific Northwest National Laboratory will be the mechanisms used by the files to efficiently implement the reformatting and re-ordering. The reformatting and re-ordering can be done in one of three ways:

1. Develop pre- or post-processors without modifying the legacy code.
2. Modify the code to directly read specified files using the shared subroutines.
3. Use a combination of processors and code modifications.

If pre- or post-processors are created for a module, a "batch" file will be also be delivered as part of the module. This "batch" file will serve as the single entry point for execution of that module. Modules are expected to not consume ALL of the memory, disk, and time resources available to the FRAMES-HWIR Technology Software System. The current resource assumptions are a computer with 200-MHZ processing speed, 64 megabytes of RAM, and a 6-gigabyte hard drive or greater.

3.4.7 Exit Level Processor (ELP)

The primary purposes of the ELP are to process risk-based information generated from the MMSP and develop datasets that will be used to create chemical-specific, waste exit-level outputs. The HWIR waste exit levels, in simplest terms, define a chemical-specific waste stream concentration level that, if exceeded, defines that entire waste stream as hazardous and, thus, requires strict Subtitle C disposal. Waste containing concentrations below the exit level may "exit" a Strict Subtitle C disposal system and be disposed-of in Industrial Subtitle D units. Figure 3.21 illustrates where the ELP fits within the SUI. The simplest output of the ELP is a list of waste constituent-specific exit levels. However, because so many factors influence the actual concentration determined as an exit level, the ELP will output additional information that describes the dimensions of the exit level. This additional output will be a database that others can query in different ways to arrive at other possible exit levels.

3.4.7.1 Summary of ELP Requirements

Any design should reflect the requirements outlined in *Requirements for the FRAMES-HWIR Technology Software System*. These documents cover specifications on input and output, operating system, and accessory software and hardware, where appropriate.

The ELP I will:

1. be designed to process risk data in the Global Results Files generated from the MMSP
2. create the Risk Summary Output File.
3. require the Risk Summary Output File to contain risk information per site, per waste management unit, per chemical, per human and ecological receptor, per measure of risk.
4. process a limited number of pre-specified "roll-up" protocols defined by EPA (e.g., find and save only the maximum impact and its time).
5. allow the Risk Summary Output File to be queried by the user to conduct additional analyses outside the FRAMES-HWIR Technology Software System.
6. report any processor-specific warnings or errors to the SUI.
7. be tested as a stand alone processor, independent of the other FRAMES-HWIR Technology Software System processors.

The ELP II will:

1. access the Risk Summary Output File (Microsoft Access format).
2. create the Protective Summary Output File that describes the dimensions of the exit level in such a way that the results can be analyzed by users to assist in decisions regarding exit criteria for contaminants. EPA is responsible for summarizing (e.g., plotting) the level of "protection" achieved.
3. allow users to redefine risk trigger levels through the SUI.
4. report any processor-specific warnings or errors to the SUI.
5. be tested as a stand alone processor, independent of the other FRAMES-HWIR Technology Software System processors.

3.4.7.2 ELP Implementation

The ELP has two processors, as illustrated by Figure 3.22, in addition to a Risk Summary Output File and a Protective Summary Output File. The ELP I retrieves the information from the Global Results Files and processes it, as presented in Figure 3.23. The ELP I is executed for every Outer Loop (statistical iteration) and each Inner Loop (site or location) to produce a matrix of results. The results are maximum risk/HQ values and associated time by source type, chemical, concentration in the waste (C_w), and receptor. These results are stored in the Risk Summary Output File (RSOF). The ELP II retrieves the data from the RSOF and sums and analyzes the data in a number of different ways, as illustrated in Figure 3.24, and stores the results of the analysis in the Protective Summary Output File (PSOF).

The y axis associated with the matrix presented in Figure 3.22 refers to the Inner Loop, that is, the number of randomly- selected sites, indexing from one to "N." The columns (as indexed across the top of the matrix) refer to the "Outer Loop," that is, the number statistical sampling iterations, identifying and implementing discrete deterministic input files (saved in the Site Simulation Files), indexed from one to "M." Each deterministic run produces a risk that is arrayed to the Inner and Outer Loops. For each column, the percentage of the risk values that are below a predetermined safe limit (e.g., 10^{-6}) are summed and stored along the bottom of the matrix. This summation represents a level of protection.

3.5 Science Support Activities

The HWIR99 assessment approach must be based upon sound science and engineering (i.e., modeling). In general, each element/step of the assessment approach should be selected based on a thorough understanding of 1) the HWIR99 regulation-based needs, and 2) the relevant science and available modeling technology. There are many instances, however, where, due to a combination of incomplete technical knowledge and HWIR99 constraints (i.e., resources and schedule), it is not possible to select an absolute and definitive approach. For example, a decision must be made concerning which exposure pathways to simulate. While it would be preferred to process only exposure pathways that are "significant", with respect to their relative impact on risk, it is not possible, at this time, to devise a protocol to rank individual pathways with respect to their contribution to total risk. When decisions of this nature exist in the development of the HWIR99 assessment strategy the approach to be taken will be twofold. First, a technical team will make a decision as to which approach to take in the near term (i.e., HWIR99 time frame). This decision will be based on combined knowledge and experience. Secondly, the technical team will design a study that will, separate from the main HWIR99 technical assessment developmental effort, provide additional information and data relevant to the particular issue. Going back to the example concerning the selection of exposure pathways, the decision is to include numerous pathways in the assessment approach. In addition, a special study will be conducted (using perhaps a case study approach with models outside the HWIR99 modeling system) with the objective of developing the technical understanding necessary to specify a pathway ranking scheme.

The following represents a short list of issues and activities designed to support the HWIR technical assessment. It is expected that as HWIR99 unfolds additional science support activities will be identified. One of the primary intents in designing the FRAMES-HWIR Software system is to provide a base technology within which assessments can be conducted and science-based modeling experiments can be conducted. Section 3.5.1 presents science support activities related to the HWIR Source Module. Section 3.5.2 describes an Intermedia Transport activity, Section 3.5.3 presents support activities related to the Air Module, Section 3.5.4 presents Groundwater Module activities, and Section 3.5.5 presents activities related to the Surface Water Module.

3.5.1 Science Support Activities Related to HWIR Source Module

3.5.1.1 Source Module Activity #1

Title: Benchmarking analysis of the generic soil column model quasi-analytical solution technique

A. Current HWIR Approach.

A computationally-efficient, quasi-analytical solution technique used in the Generic Soil Column Model, upon which the landfill (LF), waste pile (WP), and land application unit (LAU) source models are based. This is assumed to provide fairly accurate estimates of *long-term* (i.e., annual average) contaminant fate and transport behavior (i.e., volatilization and leaching fluxes and depth-averaged contaminant concentrations) relative to a more rigorous, but computationally- expensive numerical solution of the same set of governing equations and initial and boundary conditions.

B: List of HWIR Modules Involved . Sources (LF, WP, and LAU)

C. Potential HWIR Approach Limitations.

The computationally-efficient Generic Soil Column Model may be inaccurate to some degree relative to a computationally-expensive numerical solution of the same set of governing equations and initial and boundary conditions for some contaminants and some physical/chemical settings.

D. Science Support Activity

Objective. To benchmark the annual-average results of the Generic Soil Column Model against those of a numerical solution of the same set of governing equations and initial and boundary conditions for a wide variety contaminants and physical/chemical settings. In addition, since several analytical solutions to the same set of governing equations, but different boundary conditions, are available, the results of the Generic Soil Column Model will also be compared to these.

Technical Summary. The governing equation used in the Generic Soil Column Model to describe contaminant fate and transport in a homogeneous, unconsolidated porous medium or soil is:

$$\frac{\partial C_T}{\partial t} = D_E \frac{\partial^2 C_T}{\partial z^2} - V_E \frac{\partial C_T}{\partial z} - k C_T \qquad \textbf{(69)}$$

where t is time (d), z is depth from the surface (m), C_T(g/m^3) is the total contaminant concentration in soil, D_E is the effective diffusivity (m2/d), V_E (m/d) is the effective convection velocity, and k (1/d) is the effective first order loss rate. A novel, computationally-efficient, quasi-analytical solution technique was developed for use in HWIR that is a step-wise solution of the three components of equation 1 on a numerical grid disaggregation of the soil column. Contaminant concentration within any individual grid layer is assumed uniform. Initial conditions in the soil column can be specified by the model user, but are limited by the degree of resolution provided by the specified grid. The boundary condition at the surface ($z = 0$) is $C_T = 0$. At the bottom of the modeled soil column, the boundary condition can be specified with use of a ratio (zero to one) between the total contaminant concentration below and above the lower boundary, where zero corresponds to a zero concentration boundary condition and one corresponds to a zero gradient boundary condition.

This paper proposes to develop and code a numerical solution of the same governing, initial, and boundary conditions and benchmark the results of the newly developed solution technique used in the Generic Soil Column Model to the numerical solution. In addition, the results of the Generic Soil Column Model for simple scenarios (i.e., initially contaminated layer in soil with no additional mass added) will be compared to results created using analytical solutions, as appropriate, for a QA/QC check.

Expected Benefit/Application. The results will contribute to the quantification of model error for the LAU, WP, and LF source models.

Contact and Organization: Robert Ambrose, EPA/ORD

3.5.1.2. Source Module Activity #2

Title: Evaluation of Land Treatment Source Unit Assumptions–Rainfall Assumptions

A. Current HWIR Approach

Dissolution of contaminants in land treatment units is driven by infiltrating rainwater and irrigation passing through the unit. The rate at which contaminants are carried to underlying vadose zones and aquifer depends upon the soil properties and recharge rates. Contaminants are also lost to the atmosphere through volatilization. The latter occurs in response to climatic and chemical factors. The proposed HWIR Land Treatment Unit Model uses averaged rainfall amounts to drive these processes.

B. List of HWIR Modules Involved. Sources (Land Treatment Unit), Vadose Zone, Aquifer

C. Potential HWIR Approach Limitations

Since rainfalls occur as discrete events, at any site there are individual rainfall events of higher intensity than averaged rainfall fluxes. Further, only rainfalls of certain volume and duration penetrate the vadose zone to create aquifer recharge. Water from these lesser rainfalls is initially retained in the vadose zone, then later evaporated or transpired. Therefore, contaminants that do reach the aquifer, may do so in relatively concentrated pulses. Since transient vadose zone transport is driven by nonlinear processes, the impact on the receiving aquifers of the pulses may not be replicated by the averaging. Advective-dispersive-sorptive transport in aquifers may, however, dampen the effect, depending on the specific receptor configuration and subsurface properties.

D. Science Support Activity

Objective. To assess the impact on ground water receptors of averaging rainfall and recharge events.

Technical Summary. The Transient Investigative Land Treatment (TILT) model will be used to evaluate the effect of various averaging assumptions concerning rainfall. TILT uses stochastically generated sequences of rainfall to simulate climate over long time periods. The Solar and Meteorological Surface Observation Network (SAMSON) database provides the necessary meteorological parameters for 239 stations in the U.S. that can be used to drive TILT simulations. The model is based upon a kinematic-dynamic approximation to the vadose zone flow and transport equations, which runs simulations of long duration efficiently. For example, a simulation of 30 years of rainfall for Athens, Georgia requires approximately 10 minutes on a Pentium100 PC. The Transient Source Gaussian Plume (TSGPLUME) model will be used to simulate contaminant transport to various receptors in the aquifer. TSGPLUME is designed to handle a time varying mass input at a source and calculate aquifer concentrations with an analytical solution. By simulating the land treatment unit with various assumptions, the relative impact on receptors can be assessed. Health effects will be considered by determining the impact, if any, on simulated long term and acute exposures via drinking water.

Expected Benefit/Application. The expected results of the project are the definition of relative model error at a variety of aquifer receptor locations. These will be beneficial to determine if significant differences exist between models with varying rainfall assumptions.

Contact and Organization: Jim Weaver, EPA/ORD

3.5.1.3. Source Module Activity #3

Title: Evaluation of Land Treatment Source Unit Assumptions–NAPLs

A. Current HWIR Approach

The proposed HWIR Land Treatment Unit Model allows contaminants to partition only among the sorbed and aqueous phases.

B. List of HWIR Modules Involved. Sources (Land Treatment Unit), Vadose Zone, Aquifer

C. Potential HWIR Approach Limitations.

The presence of NAPLs has an unknown effect on ground water receptor concentrations. Their impact depends upon their nature and abundance in the contaminant source, and the scenario that is modeled. A multi-component NAPL in a land treatment unit may, for example, reduce the rate of release of an organic contaminant to the vadose zone, because of hydrophobic partitioning phenomena. A consequence is that the release may last longer than if there had been no NAPL present. Under other circumstances, a NAPL could reach the water table because of its over abundance and lack of vadose zone retention capacity. Therefore, receptor risk may vary greatly because of the presence/absence of NAPL in a specific well. Thus the impact of NAPL under either long-term averaged or acute conditions is not easily predicted because of nonlinear transport phenomena and the variety of scenarios that can occur.

D. Science Support Activity

Objective. To assess the impact of land treatment unit NAPLs on ground water receptors.

Technical Summary. The Transient Investigative Land Treatment (TILT) model will be used to evaluate the effect of various types of immobile NAPLs under several release scenarios. Single and multi-component NAPL simulations will be compared against simulations that include only sorbed and aqueous phase wastes. The Transient Source Gaussian Plume (TSGPLUME) model will be used to simulate contaminant transport to various receptors in the aquifer. TSGPLUME is designed to handle a time-varying mass input at a source, and calculate aquifer concentrations with an analytical solution. Comparisons against the Hydrocarbon Spill Screening Model (HSSM) will be used to assess the impact of mobile NAPLs that are released from a similar land treatment unit.

Expected Benefit/Application. These results will provide information upon which to judge the importance of including NAPL in the analysis. The results will also illustrate the complexity of impacts of NAPLs under various scenarios, and show that there may or may not be an effect on exposure.

Contact and Organization: Jim Weaver, EPA/ORD

3.5.2 Science Support Activities Related to HWIR Intermedia Transport

3.5.2.1 Intermedia Transport Activity #1

Title: Evaluation of Re-emission Fluxes from Soil and Water to the Atmosphere

A. Current HWIR Approach.

The HWIR atmospheric model deposits pollutant mass to soil and water body surfaces. Subsequent volatilization losses of pollutants are modeled in the regional watershed and waterbody modules. These loss fluxes are not added back to the atmospheric model.

B. List of HWIR Modules Involved. Atmosphere (ISC3), Regional Watershed, Surface Water (EXAMS)

C. Potential HWIR Approach Limitations. The atmospheric model lacks a secondary source term for re-emission fluxes of volatile compounds. The design of the HWIR multimedia simulation software prevents feedback among modules. As a result, there will a mass imbalance, and downgradient atmospheric concentrations and deposition rates will be underestimated. The HWIR system will keep track of the "lost" mass and report its magnitude. It is not presently known how often the mass imbalance might be significant.

D. Science Support Activity

Objective. To assess the effects on atmospheric concentrations and deposition fluxes of ignoring the re-emission of volatile compounds from soils and surface waters.

Technical Summary. The effects of re-emission will be examined in two different ways on two example sites for two or three volatile and semivolatile compounds. The example sites should represent a dry and a humid location with nearby meteorological stations. The ISC3 model will be run for each pollutant, and average atmospheric concentrations and deposition fluxes will be reported. The regional watershed and waterbody modules will be run based on the average air concentrations and fluxes, and re-emission fluxes will be calculated. ISC3 will be rerun using the original source loadings along with the re-emission fluxes, and the new average atmospheric concentrations and deposition fluxes will be reported. The percent differences will be reported and analyzed for significance.

The second approach will be to set up and run the MEND-TOX compartmental multimedia model for the two example sites. While this model does not simulate spatial gradients, it does simulate feedback among media. The predicted concentrations and deposition fluxes from MEND-TOX will be benchmarked against those predicted by ISC3.

Expected Benefit/Application. This project should help define the model error in atmospheric exposure concentration and deposition calculations due to ignoring re-emission of volatile compounds.

Contact and Organization. Robert Ambrose and Donna Schwede, EPA/ORD

3.5.3 Science Support Activities Related to HWIR Air Module

3.5.3.1 Air Module Activity #1

Title: Evaluation of Effect of Combining Sources vs Modeling Separately on Air Concentrations and Deposition

A. Current HWIR Approach.

Due to runtime limitations in the HWIR system, individual sources associated with a particular WMU cannot be modeled. For example, in and near a land application unit, emissions are produced from wind erosion from the unit itself and also associated activities (e.g. spreading, tilling, compacting). Emissions and particle size distributions used in the modeling are generated from combining the contribution from individual sources.

B. List of HWIR Modules Involved. Air

C. Potential HWIR Approach Limitations.

Predicted impacts from the WMU may be sensitive to the location of individual sources, particularly close to the sources.

D. Science Support Activity

Objective. To assess the impact of combining emissions from individual sources on predicted downwind concentration and deposition.

Technical Summary. ISCST3 model runs will be made in which the emissions are combined and kept separate. A matrix of individual source types and sizes will then be developed and modeled using hourly meteorological data for a one year period from five meteorological sites. The meteorological sites will be selected to provide comparisons across different climates.

Expected Benefit/Application. This study will determine the error introduced in the air model results due to the necessity of using combined emissions estimates for WMUs.

Contact and Organization Donna Schwede, EPA/ORD

3.5.3.2 Air Module Activity #2

Title: Evaluation of Effect of the Use of Regional vs Site-Specific Values for Surface Characteristics on Air Concentrations and Deposition

A. Current HWIR Approach.

Due to limitations of the HWIR system, meteorological data will be processed using site characteristics of the airport from which the data are obtained. The characteristics of the locations where deposition

occurs are not accounted for.

B. List of HWIR Modules Involved. Air

C. Potential HWIR Approach Limitations. Deposition estimates depend on the surface characteristics of the deposition site. Site characteristics vary from site to site and land use varies in the vicinity of an individual site.

D. Science Support Activity

Objective. To assess the impact on concentration and deposition of using regional vs site- specific surface characteristics.

Technical Summary. ISCST3 model runs will be made using site-specific surface characteristics in place of the regional values. The sites used in the testing will be selected from the HWIR sites that were intensively characterized during the data collection process. Comparisons will be made between concentration and deposition estimates obtained from the various surface characteristic methods.

Expected Benefit/Application. This study will determine the error introduced in the air model results due to the necessity of using regional surface characteristics.

Contact and Organization Donna Schwede, EPA/ORD

3.5.4 Science Support Activities Related to HWIR Groundwater Module

3.5.4.1 Groundwater Module Activity #1

Title: Evaluation of Methods for Determining Anaerobic Biodegradation from Field Data

A. Current HWIR Approach

Data on anaerobic biodegradation rates are being summarized from published literature by consultants to a consortium of industry groups. The summarized rates were determined by a variety of procedures, based on evaluation of contaminant concentration data. A certain amount of error is introduced into these estimates simply from the various methods used for the analysis.

B. List of HWIR Components Involved. Ground Water

C. Potential HWIR Approach Limitations. Variability in the field-derived rates may be partially due to the methods used for their estimation. Use of the field rates without assessment of this error may lead to an overly wide distribution of true rates.

D. Science Support Activity

Objective. To assess the impact of various methods for estimating degradation rate constants from field

data.

Technical Summary. Data sets from two contaminant plumes will be used for testing at least four methods for estimating degradation rate constants from field data. The methods include one-dimensional, steady-state with regression analysis; two-dimensional steady-state; three-dimensional transient; and a natural tracer method. All of the rate constant determinations will be conducted with the Tools for Analysis of Contaminated Sites (TACS) software currently under development by ORD and Region 4. The two sites have contaminant plumes of differing configuration: long and thin vs. short and spreading. They also each have several organic contaminants and varying density of sampling data. Thus the sites provide test beds for the methods that illustrate some of the variability expected from around the country.

Expected Benefit/Application. The investigation will determine the error introduced in rate constant determination by using various estimation methods on well characterized sites. The results are expected to generate further insight into the industry-derived database as they will be useful in comparing against the reported variability in rate constants.

Contact and Organization Jim Weaver, EPA/ORD

3.5.5 Science Support Activities Related to HWIR Surface Water Module

3.5.5.1. Surface Water Module Activity #1

Title: Evaluation of Pollutant Dynamics in Water Body

A. Current HWIR Approach.

The HWIR MMSP will simulate a multi-year period following pollutant releases from each source. Pollutant loadings and flow rates will be averaged for each year in this series. The water body model, EXAMS, will be run in steady-state mode for each year in the series to obtain an estimate of the yearly-average concentrations at an exposure point.

B. List of HWIR Modules Involved . Sources (LAU, Waste Pile), Regional Watershed, Surface Water

C. Potential HWIR Approach Limitations. Runoff loadings occur as discrete events that are correlated with high stream flow, which dilutes the resulting instream concentrations. As a result, calculating an average yearly concentration as the mean of the daily loadings divided by the daily flows gives a different result than the steady-state result, which essentially divides the average yearly loading by the average yearly flow. Averaging the daily calculations is more realistic and can give a higher estimated exposure concentrations than the steady-state approach implemented here.

D. Science Support Activity

Objective. To assess the effects on surface water exposure concentration of averaging watershed loadings and flows.

Technical Summary. EXAMS or an equivalent model such as WASP will be linked with a dynamic watershed runoff model such as PRZM and run on two or three example sites to explore the nature and extent of the bias introduced by the steady-state approach. The sites should represent geographical diversity, including both humid and dry locations with nearby meteorological stations and streamflow gages. The watershed model will be driven by daily meteorological data for a period of at least 20 years and receive hypothetical atmospheric wetfall and dryfall loadings. Daily runoff and erosion loads to an adjacent watercourse will be predicted. The water body model will be run in dynamic mode using daily loads and stream flows, and predicted concentrations will be averaged yearly. EXAMS will then be run in steady-state mode for each year using yearly average loads and flows. The outputs will be compared for systematic bias, and possible remedies for bias will be explored, such as parameterizing yearly-average flows using harmonic means rather than arithmetic means.

Expected Benefit/Application. This project should help define the model error in water body exposure concentration due to the steady-state assumption. It may suggest some feasible actions that could minimize this error.

Contact and Organization Robert Ambrose, EPA/ORD

3.5.5.2 Surface Water Module Activity #2

Title: Evaluation of Nonlinear Sorption Isotherms in Surface Water Bodies

A. Current HWIR Approach.

The HWIR water body model, EXAMS, was developed specifically for organic chemicals. It uses a simple partition coefficient to describe sorption of metals to solids in the water column and in the underlying sediments.

B. List of HWIR Modules Involved . Surface Water

C. Potential HWIR Approach Limitations. Metals exhibit nonlinear sorption dynamics to solids in environmental media. As the concentration of a metal increases, the binding sites on solids become saturated and the effective partition coefficient decreases. As a result, predicted concentrations on solids and in the sediment may be too high, and dissolved concentrations in the water column may be too low.

D. Science Support Activity

Objective. To assess the effects on simulated surface water exposure concentrations of using linear partition coefficients for metals.

Technical Summary. EXAMS, or an equivalent model such as WASP, will be modified to handle nonlinear sorption isotherms and run on two or three example sites for two or three HWIR metals to explore the nature and extent of the bias introduced by the linear partitioning approach. The sites will represent different types of water bodies, such as shallow streams, deep turbid rivers, eutrophic lakes, and oligotrophic lakes. The metals will include a cationic form such as lead and an anionic form such as arsenic or chromium. EXAMS will be run on the example water bodies subject to a range of loadings

using the average partition coefficients being used by HWIR. MINTEQ will be parameterized and run to generate nonlinear isotherms for the chosen metals. These isotherms will be summarized in tabular or mathematical form, and used in the modified water body model to obtain new predicted concentrations. The output from the two water body models will be compared for systematic bias, and model error will be estimated.

Expected Benefit/Application. This project should help define the model error in simulated water body exposure concentration for metals due to the linear partitioning assumption.

Contact and Organization Robert Ambrose, EPA/ORD

3.6 Peer Review Plan

The strategy for peer review of HWIR99 is characterized as strategic peer review. No formal Science Advisory Board review is anticipated. The SAB reviewed the HWIR95 proposal and provided numerous recommendations for improving the assessment. These suggestions, as well as others forwarded by ORD and the public, have been assimilated and are reflected in this plan.

Background:

Some aspects of the HWIR methodology have been under development for a number of years, and date back to the Toxicity Characteristic (TC) Rule promulgated in 1990. That proposal focused on the groundwater / drinking-water exposure route to humans. In December of 1995 the Agency proposed, for the first time, a comprehensive, multimedia analysis that included both human and ecosystem multipathway exposures and impacts. This methodology came to be known as the Multiple Pathway Receptor Analysis (MPRA), or simply HWIR 95. One of the characteristics of the HWIR 95 methodology was that all identified exposure pathways were individually analyzed in a conservative way by utilizing conditions that would maximize the potential exposure via each respective path. During an extensive series of reviews of the 1995 proposal, the EPA Science Advisory Board (SAB) and others recommended the analysis be revised to consider all exposure pathways simultaneously, instead of only analyzing the most limiting pathway. The HWIR 95 approach allowed all pollutant mass present to be made available to each exposure pathway, rather than being appropriately allocated among the various paths. The SAB recommended the Agency abandon the HWIR 95 approach in favor of true multipathway calculations. The incorporation of this correction was / is one of the prominent forces driving the development of HWIR99.

In addition to the mass-balance issue, many other comments were received from the SAB, environmental groups, industry, academia and the stakeholder community during the review process of HWIR 95. These involved the human toxicity data used, the nature of the algorithms defining exposure paths, the inadequate representation of pathway chemical and biological transformation processes, the lack of data to support the ecological exposure analysis and model validation aspects and other issuer. Table 3.8 contains a condensed and paraphrased listing of some of the more important comments received during the HWIR95 review process. Many more issues were identified than are listed, and indeed many more were received than are being / can be addressed in the present HWIR99 development effort because of severe time, resource and scientific constraints. The list in Table 3.8 is reflective of the most important categories of comments.

The peer review approach outlined in Phases I and II below pertains to the HWIR99 methodology development. It is a follow-on to the HWIR95 review results, and has two overarching goals: 1) to determine how well the present HWIR99 research plan addresses the collection of issues raised in earlier reviews, and 2) to determine how appropriate the new modeling components produced actually are. These goals are the focuses of Phase I and Phase II of the overall peer review process outlined below.

Materials Offered for Review:

The HWIR99 development effort is being implemented via eight cooperative research teams addressing various needed improvements in the methodology. Together, these teams began by producing three early working drafts of documents covering research, assessment strategy and technology design aspects of the planned HWIR99 development effort. These working drafts were later revised, updated and merged to produce the present, stand alone, research/implementation plan. This plan will serve as the basis for the first part (Phase I) of the overall peer review.

In addition to the Phase I general review of the present document, which attempts to make clear the overall HWIR99 development and application approach, several of the major model development products (component modules) that are planned for development will be subjected to detailed peer review at later times as they materialize (Phase II). These will include: 1) the revised MINTEQ code and database, 2) the air module, 3) the surface water module, 4) the groundwater module, 5) the sources module, and 6) the ecological impact module.

Consistent with its research mission and cooperative role in the HWIR99 development effort, the Office of Research and Development (ORD) will coordinate the general peer review covering the research planning aspects (Phase I). Similarly, and consistent with their regulatory mission, the Office of Solid Waste (OSW) will coordinate Phase II of the review process, focusing on the actual regulatory support modeling components as they are produced. Eventually, the complete assemblage of the HWIR99 methodology and its outcomes will again be subjected to public scrutiny when it becomes a part of a formal regulatory proposal.

Phase I - ORD's Peer Review of the Research Plan

Phase I peer review will focus on a single document, the present research/implementation plan. The review will be coordinated by ORD via the Ecosystems Research Division (ERD) of the National Exposure Research Laboratory. This review will utilize the letter review format and will be implemented through a small group of independent peer reviewers, collectively having expertise covering all aspects of the HWIR99 development effort. An extended list of well qualified, potential peer reviewers has been assembled and submitted to the NERL/ERD's Peer Review Officer, who will act as a third party in making final selections from the list. Four or five reviewers will be selected, and asked to provide comments within one month of receipt of this research plan. To help assure that the review panel is able to view the research plan in proper context, a brief background document describing the history of HWIR and summarizing major points and concerns of the earlier reviews of HWIR95 will be provided them. In the accompanying charge statement, the review panel will be asked to judge whether or not the proposed HWIR99 research and development effort is on the right track. This will be accomplished through a set of questions on topics central to the overall regulatory support model development effort. Review

panelists will be asked to return their individual written responses within 30 days of receipt of the review package. Comments will be returned to the Peer Review Officer, who will consolidate the comments and transmit them to the HWIR99 research teams for address.

Phase II - OSW's Review of Products

Phase II peer review will deal with the detailed outcomes of various aspects of the model development and data collection efforts. As noted earlier in this research plan, the HWIR99 methodology will be housed in an open architecture, object-oriented modeling framework (FRAMES). The objects in this framework are the component modules where the basic fate, transport, exposure and risk assessment modeling calculations are to be accomplished. In responding to the previous reviews, many of these modules had to be slated for material change and / or newly developed. These modules are also quite complicated, and will require detailed, module-specific expertise on the part of reviewers. For this reason, and also because they are expected to materialize individually during the next several months, they will be submitted for review individually, and will be addressed by different review panels selected for their module-specific expertise. Unlike the general approach to be reviewed in Phase I, these modules are regarded as interim 'products' of the overall development effort, and they will constitute the building blocks eventually to be used to populate the HWIR99 modeling framework. Since they are 'objects' of the open architecture, their development can proceed with a certain degree of independence relative to the over-arching framework so long as framework specifications are adhered-to. Phase II of the review is intended as a mid-stream test of the scientific soundness of the HWIR99 modeling components. Since this deals with some of the actual outcomes to be utilized in a regulatory support effort, this phase of the peer review will be coordinated by OSW with ORD participation and support as needed.

The Phase II reviews will be implemented via a contractor. The OSW staff will provide the contractor with a reviewer charge statement, criteria for selecting reviewers, and a list of suggestions. The contractor will be charged with assembling review panels of 3 - 5 reviewers for each module, and for implementing the review process. Reviewers will provide individual responses to the written materials they will be provided on each of the respective modules. The OSW staff will consolidate the review comments for action by the appropriate HWIR99 research teams. Modules to be submitted in this phase of the peer review will include the following:

* MINTEQ code and database

* Air module

* Surface water module

* Groundwater module

* Sources module

* Ecological exposure module

* Human exposure module

* Farm foodchain Module

* Terrestrial foodweb module

* Aquatic foodweb module

* Watershed module

* Exposure parameters data distributions

Table 3.1 HWIR99 Multimedia Risk Assessment Dimensions.

CONTAMINANTS
- Organics (approx. 200)
- Metals (20)

SOURCE TYPES
- Landfill
- Land Application Unit
- Surface Impoundment
- Aerated Tank
- Waste Pile

SOURCE TERM CHARACTERISTICS
- Mass Balance
- Multimedia Partitioning
- Chemical Decay

SOURCE RELEASE MECHANISMS
- Erosion
- Volatilization
- Runoff
- Leaching
- Particle Resuspension

TRANSPORT MEDIA
- Atmosphere
- Soil
- Vadose zone
- Saturated zone
- Surface water

INTERMEDIA CONTAMINANT FLUXES

Source	-> Air (vol, resuspension)
Source	-> Vadose zone (leaching)
Source Surface soil	-> Local Watershed Soil (erosion, runoff)
Air	-> Watershed/Farm /Habitat Soil (wet/dry deposition)
Air	-> Surface water (wet/dry dep)
Air	-> Vegetation (dep/uptake)
Farm/Habitat Soil	-> Vegetation (root uptake)
Watershed Soil	-> Surface water (erosion, runoff)
Surface water	-> Aquatic organisms (uptake)
Surface water	-> Sediment (sedimentation)
Vadose zone	-> Groundwater (percolation)
Groundwater	-> Surface water
Soil	-> Vegetation (uptake, dep)
Vegetation, Soil, Water	-> Beef and dairy (uptake)

FATE PROCESSES
- Chemical/Biological Transformation (and associated products of transformation)
- Linear partitioning (water/air, water/soil, air/plant, water/biota)
- Nonlinear partitioning (metals in vadose zone)
- Chemical Reaction/Speciation

FOODCHAIN
- Human (Farm)
- Human (Aquatic)
- Ecological (Aquatic Habitat)
- Ecological (Terrestrial Habitat)

RECEPTORS

Human
- Resident (Adult & Child)
- Beef Farmer (Adult & Child)
- Dairy Farmer (Adult & Child)
- Home Gardener (Adult & Child)
- Recreational Fisher (Adult & Child)

AGE GROUPS FOR HUMAN RECEPTORS

Infant	< 1 year
Child-a	1- 5 years
Child-b	6 - 11 years
Child-c	12- 19 years
Adult	20+ years

Ecological

Mammals, Birds, Soil Communities, Terrestrial Plants, Aquatic Communities, Benthic Communities, Aquatic Plants, Amphibians, Herpes, and Reptiles.

EXPOSURE ROUTES
- Ingestion (plant, meat, milk, aquatic food, water, soil)
- Inhalation (gases, particulates)
- Direct Contact (soil, water)

HUMAN AND ECOLOGICAL RISK ENDPOINTS
- Human Cancer Risk
- Human Noncancer Hazard Quotient
- Ecological Population and Community Hazard Quotients

Table 3.2 Technical Requirements for HWIR99 Assessment.

- Follows risk paradigm (P);
- Based on foundation of current science and modeling state-of-the-art;
- Multimedia/Multipathway/Multireceptor-based exposures and risks (P);
- Mass balance approach;
- Site-based (i.e., actual geographic locations) to the extent data is available;
- Applicable for any waste (P);
- Applicable nationally (i.e., under all environmental conditions) (P);
- Fully referenced data sources;
- Considers human and ecological endpoints;
- Addresses major review comments of HWIR95 (P);
- Level of assessment detail is commensurate with available data and is consistent across components (e.g., fate and transport, exposure) of the assessment;
- Assessment provides a quantitative relationship between the wastestream concentration of chemical constituents and aggregate risk to human and ecological receptors (P);
- Assessment reflects risk-conservative assumptions where knowledge/technology are limited (P);
- Assessment must reflect QA/QC protocols and be reproducible;
- Consistent with other Program Office assessments and related technologies (i.e., data, models) (P);
- Captures uncertainty in exposure/risk due to sampling errors under conditions representing natural variation in environmental conditions (T);
- Modeling technology (i.e., software system) is capable of assimilating new science and component modules;
- Capable of full automation via PC-based computers; and
- Approach is verified and components have been compared with 1) other analytical solutions, 2) numerical models, and/or field data (T).

NOTE: (P) denotes criterion that has potential policy implications and (T) denotes criterion that may be difficult to address technically given resource and time constraints.

Table 3.3 HWIR99 parameterization approaches by data type.

Data type	Parameterization Approach		
	Site-Specific	Regional	National
facility location	●		
waste management unit (WMU)	●		●
waste property			●
meteorological		●	
land use	●		
topographic (watersheds and elevations)	●		
waterbody	●	●	●
water quality		●	
soil	●		
aquifer		●	●
human receptor type and location	●		
ecological receptor type and location	●		
farm food chain			●
terrestrial and aquatic food web		●	●
human exposure factor			●
ecological exposure		●	●
human health benchmark			●
ecological benchmark		●	●
chemical properties			●

Table 3.4 Input data type by HWIR99 model component.

Model Component	chemical-specific (property)	landuse	meteor-ological	soil	topo-graphic	waste management unit	waste property
Aerated Tank (source)	●		●			●	●
Landfill (source)	●	●	●	●		●	●
LAU (source)	●	●	●	●	●	●	●
Surf. Imp. (source)	●		●	●		●	●
Waste Pile (source)	●	●	●	●	●	●	●
Air (ISCST3)	●	●	●		●	●	
Waterbody (EXAMS)	●		●		●		
Watershed	●	●	●	●	●		
Groundwater	●			●			
Aquatic foodweb	●						
Farm Food Chain	●			●			
Terrestrial Food Web	●			●			
Ecological Exposure							
Human Exposure				●			
Ecological Risk	●						
Human Risk	●						

Table 3.3. Data Collection Activities for Sites Representing National Distribution and Case Studies

		Approach for Case Studies
Facility location	Ind. D facility match to Locational Reference Tables (LRT) (facility centroid, front gate, zip code centroid locations). Address-matching software for unmatched sites	GPS front gate, facility boundaries, WMUs; State office visits (facility maps, locations).
Waste management unit (WMU)	Ind. D Screening Survey data (WMU area, capacity, waste loading); national estimates based on model unit approach for other inputs.	State office visits (facility maps; WMU locations, dimensions, operation). Site visits confirm characteristics where WMUs are visible.
		Confirm landuse, details within GIRAS area coverages during site visits.
	Watershed delineation (area, flow length, slope, streams), elevations for air model, using GIS Digital Elevation Models (DEMs).	Desktop delineation of watersheds (area, flow length, slope, streams), elevations for air model on USGS topo. maps. Confirm general watershed characteristics, topographic features during site visits.
	other databases (RF1, WATSTORE)	Desktop location on topo. maps; manual data extraction (BASINs). During site visits GPS waterbody locations (streams, lakes, ponds); confirm general characteristics; add details on fishable.
	Hydrogeologic Database (regional analysis), national distributions for aquifer properties; assume water flows down hill, towards surface water.	Desktop data review and compilation from State office visits. hydrogeologic setting analysis. During site visits, ground-truth setting; detail on residential well use.
Human receptor information	U.S. Census data (area averages within radius of interest) and GIRAS land use data to define human areas of interest (GIS).	Ground truth area averages, farms, exposure pathways; provide additional detail on home gardeners, farmers, subsistence activities, MEI (GPS).
Ecological receptor information	GIRAS land use data, other data to delineate habitats and ecological areas of interest (GIS).	Ground truth habitats, exposure pathways.

Table 3.5 Data collection activities for sites representing National distribution and case studies.

Table 3.6 Physical/chemical properties for organic chemicals.

Properties	Units
name	-
CAS number	-
Smiles string	-
molecular weight	g/mole
air diffusivity	cm^2/sec
water diffusivity	cm^2/sec
molar volume	mL
density	g/mL
vapor pressure	torr
ionization constants	-
solubility	mg/L
Henry's Law constant	$atm\text{-}m^3/mole$
octanol-water partition coefficient	L_w/L_o
organic carbon partition coefficient	mL/g

Table 3.7 Physical/chemical properties for metals and inorganics.

Properties	Units
name	-
CAS number	-
molecular weight	g/mole
solubility in soil water	mg/L
partition coefficient, soil water-soil solids	L/kg
solubility in pore water	mg/L
partition coefficient, pore water-sediment	L/kg
solubility in surface water	mg/L
partition coefficient, surface water - suspended solids	L/kg
partition coefficient, surface water - DOC	L/kg
partition coefficient, leachate - waste matrix, landfill	L/kg
partition coefficient, leachate - waste matrix, waste pile	L/kg
partition coefficient, leachate - waste matrix, treatment lagoon	L/kg
partition coefficient, leachate - waste matrix, aerated tank	L/kg

Table 3.8 Principal Review Comments for HWIR95 Technical Assessment (General)

●Integration of Groundwater and MPRA: The groundwater pathway and MPRA approach represent fundamentally different approaches to exposure and risk assessment, and, as such, result in a technically-confusing and inconsistent rulemaking.

●MPRA Methodology: The MPRA does not represent a true multimedia approach, "... the proposed method of calculating exit criteria is actually based on individually calculating each of many exposure pathways. This approach fails to maintain mass balance and may lead to significant, but unknown, errors in the exposure estimates". This approach should be abandoned in favor of true multi-pathway calculations in which a receptor receives contaminants from a source via all pathways concurrently.

●Characterization of High-end Exposures: The approach for assigning high-end or central-tendency values to model paramters results in an inconsistent and unquantifiable representation of high-end exposures across human and ecological pathways. To ensure a consistent and uniform approach, the Agency should conduct a systematic examination of parameter sensitivity and consider implementation of Monte Carlo simulation for the purpose of quantifying the national distribution of exposures and risks.

●Ecological Assessment: The ecological analysis in HWIR is fundamentally flawed because lack of toxicity data has been implicitly equated with lack of adverse ecological effect throughout the analysis. The Agency should discard the proposed ecological risk screening procedure for selecting an initial subset of chemicals for ecological analysis, and instead require that a minimum data set be satisfied before ecological-based exit criteria are calculated.

●Validation: The total construct of the HWIR methodology has not been validated against actual data derived from laboratory or field experiments or observations. Substantial validation of the overall methodology and its components is essential to developing any degree of confidence in the scientific defensibility of the resulting exit criteria. Recognizing that this approach to validation is not feasible in the near term, an alternative is to consult readily-accessible, published sources of data for cases that permit comparisons with calculations based on relevant pathways or portions of pathways.

●Temporal Scale of Assessment: The assessment methodology does not address pollutant transport associated with episodic events, such as intense rainfall or wind storms. The significance, with respect to underestimation of exposure and risk to both human and ecological receptors, should be determined.

●Documentation: The documentation of the HWIR methodology for calculating exit criteria lacks clarity and organization. The HWIR documentation should be reorganized and rewritten for both clarity and ease of use. Further, the documentation, with respect to methodology, should distinguish clearly between scientific judgment and EPA policy decisions.

●Quality Assurance: The purpose of QA in this context is to ensure that the methodology for calculating exit criteria is implemented without error. Upon review of the HWIR methodology and specific example calculations, there is concern that QA issues have not been adequately addressed. The Agency should conduct a thorough examination of all aspects of QA prior to subsequent publication of exit criteria.

●Science Support: The Agency should actively seek the substantive participation, input, and peer review

of Agency scientists, and outside peer review groups as necessary, to contribute to and evaluate the overall design and individual elements of a revised methodology.

Table 3.9 Summary of variables used to describe the HWIR99 Risk Assessment Methodology.

$AMR_{befghikt}(C_w)$	The medium-specific aggregate risk for medium *i* associated over all exposure routes from chemical *e* for cohort *t* associated with representative receptor of type *h* in exposure area *g* of site *f* from waste concentration C_w in WMU type *b*
$APPR_{beht}(C_w, TR)$	The nationwide percent protection for all receptors in WMU type *b* for waste concentration C_w of chemical *e* and target risk *TR* during year *t*.
$APPS_{bet}(C_w, TR)$	The nationwide percent of sites that are protected for all receptors in WMU type *b* for waste concentration C_w of chemical *e* and target risk *TR* during year *t*.
$APXR_{bet}(C_w, TR)$	The percentage of the nationwide total receptors that exceed the target risk, *TR*.
$\boldsymbol{AR}_{bef}(C_w)$	Matrix of the aggregate risks ($AR_{befghkt}(C_w)$) for each cohort *t* associated with each representative receptor type *h* at each exposure area *g* of site *f* for a given waste concentration (C_w) of chemical *e* in WMU type *b*.
AR_{befght}	The receptor-specific aggregate risk for a receptor cohort *t* associated with representative receptor of type *h* in exposure area *g* at time *t* from chemical *e* at site *f* and waste concentration C_w in WMU type *b*
$ASIND_{beft}(C_w, TR)$	An indicator variable that is set to 1 if site *f* is protective for cohort/year *t* associated for waste concentration C_w of chemical *e* in WMU type *b*. Otherwise it is set to zero.
$C_{befgijkT}$	Annual concentration of constituent *e*, in contact medium over the exposure area associated with exposure route *k* and pathway *j* in exposure area *g* of site *f* in year *T* due to waste concentration C_w in WMU type *b*
C_W	Incoming waste concentration of given chemical
C_{wout}	Concentration of given chemical in the waste volume removed from the WMU
CDI_{befght}	Chronic daily intake for chemical *e*, at site *f*, over exposure area *g*, for species *h*, at time *t* (mg/L)
$CSCL_{eh}$	Chemical stressor concentration limit for chemical *e* and species *h* (mg/L)
d_{fgh}	Exposure duration (yrs) for cohort *t* associated with a representative receptor of receptor type *h* in exposure area *g* of site *f* in year *T*
EF_{fghikT}	Exposure frequency (days/yr) for cohort *t* associated with a representative receptor of receptor type *h* from media *i* associated with exposure route *k* in exposure area *g* of site *f* in year *T*
$\boldsymbol{ER}_{bef}(C_w)$	matrix of the exposure route specific risks ($ER_{befghkt}(C_w)$) for each exposure

route k for each cohort t associated with each representative receptor type h at each exposure area g of site f for a given waste concentration (C_w) of chemical e in WMU type b.

$ER_{befghkt}(C_w)$ The exposure route specific risk for a receptor cohort t associated with representative receptor of type h for exposure route k at time t, in exposure area g, for chemical e at site f for waste concentration C_w in WMU type b

I_{fghikT} Daily intake (kg/day) of contact medium i associated with exposure route k and pathway j by cohort t associated with a representative receptor of receptor type h in exposure area g of site f in year T

$M(t_0)$ Mass of given chemical at time t_0

M_{Total} Total mass of given chemical

$\mathbf{MR}_{bef}(C_w)$ Matrix of contact medium specific risks ($MR_{befghikt}(C_w)$) for each contact medium i which are the respective sums of pathway specific risks from nj(i,k) pathways connecting contact medium i and exposure route k for each cohort t associated with each representative receptor type h at each exposure area g of site f for a given waste concentration (C_w) of chemical e in WMU type b.

$MR_{befghikt}(C_w)$ The contact medium specific risk for media i associated with exposure route k from chemical e for cohort t associated with representative receptor type h in exposure area g of site f for waste concentration C_w in WMU type b.

$ng(f)$ Number of exposure areas in site f

$NXR_{befht}(C_w, TR)$ The number of receptors of type h in year t at site f that exceed the target risk, TR, for waste concentration C_w of chemical e in WMU type b.

$PPR_{beht}(C_w, TR)$ The nationwide percent protection for receptors of type h in year t for target risk, TR, for waste concentration C_w of chemical e in WMU type b.

$PPS_{beht}(C_w, TR)$ The nationwide percentage of sites that are protected for receptors of type h in year t for target risk, TR, for waste concentration C_w of chemical e in WMU type b.

$\mathbf{PR}_{bef}(C_w)$ Pathway Risk Matrix of baseline impacts for a given waste concentration C_w of chemical e in a WMU of type b for each site f

$PR_{befghijkt}(C_w)$ The pathway specific for chemical e at waste concentration $C_{w,}$ for an individual cohort t (that starts exposure at time t) associated with representative receptor type h for pathway j, involving exposure route k and contact medium i, in exposure area g, in WMU of type b in site f

$PXR_{behit}(C_w, TR)$	The percentage of nationwide receptors of type *h* over all sites that exceed the target risk, *TR*.
$PXS_{befhit}(C_w, TR)$	
$Q_m(t)$	Net rate with which waste mass of given chemical is changed in the unit
$Q_V(t)$	Net rate with which waste volume is changed in the unit
$RIND_{befghit}(C_w, TR)$	An indicator variable that is set to 1 if the risk to cohort/year *t* associated with a receptor of type *h* in exposure area *g* of site *f* for waste concentration C_w of chemical *e* in WMU type *b* exceeds the target risk level *TR*. Otherwise it is set to zero.
S_{WMU}	WMU's available storage capacity
$SIND_{befhit}(C_w, TR)$	An indicator variable that is set to 1 if site *f* is protective for cohort/year *t* associated with representative receptor of type *h* for waste concentration C_w of chemical *e* in WMU type *b*. Otherwise it is set to zero.
t	Time
t_{oplife}	Unit operating life
$TQ_{befghit}(C_w)$	Toxicity quotient for chemical *e*, at site *f*, over exposure area *g*, for species *h*, at time *t*
TR	Target risk
$V(t_0)$	Waste volume at time t_0
V_{Total}	Total unit volume
V_{Win}	Waste volume entering the WMU at time *t*
V_{Wout}	Waste volume removed from the WMU at time *t*
W_{fghT}	Body weight for cohort *t* associated with a representative receptor of receptor type *h* in exposure area *g* of site *f* in year *T*
$W_R(fgh)$	Weight for receptor type *h* in exposure area *g* in site *f* which is given by the number of receptors of type *h* in exposure area *g* in site *f*.
$W_S(f)$	Sampling weight for site *f*
β_{ehk}	Carcinogenic risk potency (and the inverse of the reference dose RfD for non-

	carcinogens) for exposure route *k* for chemical *e* for cohort *t* associated with individual receptor m of receptor type *h* $(mg/kg/day)^{-1}$
δ_d	Time step (1 year).
Δ_e	Averaging time for chemical *e* (yrs)
ρ_{HW}	Density of regulated (hazardous) waste.
ρ_{Wout}	Density of the waste volume removed from the WMU.

4.0 SCHEDULE

The time frame associated with this research and development plan plays a critical role in decisions related to the details of achieving the HWIR99 goals. The following is a summary of the key milestones related to the effort to revise the HWIR Risk Assessment.

April 1997	Completed negotiations and received schedule extension: a proposal by October 1999, final by April 2001
May 1997	Began model development process with ORD laboratories; set up eight HWIR development teams: **Sources, Atmospheric Fate and Transport, Groundwater Fate and Transport, Surface Water/Watershed Fate and Transport, Exposure Pathways and Receptors, Risk Characterization, Chemical and Biological Fate, and Steering/Integration.**
October 1997	**Working Draft** versions of research plan, assessment strategy, and software technology design completed
Nov 1997	**Computer specifications for model development completed** and distributed to the development teams
March 1998	**Initial regulatory options revised,** Draft **preamble and rule** sketched out
Mar-Jun 1998	**Preliminary data sets** completed (20-30 chemicals), testing of model components begins
Jul-Sept 1998	**Model components** completed, model integration begins
Nov 1998	**Integrated risk assessment model** completed, initial testing of system begins
Jan-Feb 1999	**Draft exit levels** for representative chemicals available, **preliminary cost/benefits information** available, lead regulatory options chosen
Feb-Mar 99	**Running and refining** the risk model, policy issues resolved
March 1999	**Final exit levels** and **reg options** chosen; **final Regulatory Impact Analysis** development begins
May 1999	**Draft rulemaking package** completed
mid-June 99	**Final package** submitted to Agency Workgroup for review
early July 99	Final Agency review completed (formerly known as **Workgroup closure**)
late July 1999	Package Submitted to **Office of Management and Budget (OMB) for review**

October 1999 Proposal **Signed**

April 2001 Final rule **Signed**

5.0 GLOSSARY

Contextual Dictionary for the HWIR Technology Development Effort

Aerated Tank Source Module—module within the Multimedia Multipathway Simulation Processor that models the release of contaminant from an aerated tank; for modeling purposes, the only environmental pathway assumed for this module for a contaminant to leave the waste is atmospheric (vapor only)

Aquatic Foodchain Module—foodchain module within the Multimedia Multipathway Simulation Processor that simulates contaminant movement through the water-based foodchain; receives input from the Waterbody Module; provides input to the Ecological Risk/Exposure Module and the Human Risk Module.

Assessment Strategy --represents a detailed description of the technical approach designed to generate the HWIR exit levels. The assessment strategy lays out, on paper, the individual technical components of the HWIR problem (i.e., development of exit levels) and the individual steps of the problem solution.

Assessment technology --represents the computer-based technology (i.e., software and hardware) that will automate the HWIR assessment strategy. Included here would be 1) a software system designed to manage execution of the assessment strategy, the technical algorithms (i.e., black box) for each module, the numerous types and large quantity of data required to conduct the HWIR simulations.

Assessment Data-- would include all chemical, site, source, exposure, and risk data required by the HWIR assessment.

Assessment execution-- includes the integration of the assessment strategy, assessment technology, and the assessment data for the purpose of developing an to perform the necessary simulations for developing HWIR99 exit levels.

chemical loop—iteration within the Inner Loop of the FRAMES-HWIR Technology Software System that ensures each chemical of interest for the source types is processed through the Multimedia Multipathway Simulation Processor

concentration (of waste)—concentration of chemicals associated with a representative sample of a generator's waste stream (denoted by C_w).

Computational Optimization Processor (COP)—the processor that assimilates the exposure and risk scenario as contained in the Site Definition Files and establishes, based on specific "rules," a modified scenario that is technically complete and computational efficient.

C_w loop—iteration within the Inner Loop of the FRAMES-HWIR Technology Software System that loops through each value for the concentration of waste for each chemical of interest for the source types and all site locations

database—a collection of data, external to FRAMES-HWIR Technology Software System, arranged for ease of retrieval by various computer programs

data group—collection of related variables (e.g., data describing site atmospheric conditions) within a database or data file

data file—a collection of data, generate by FRAMES-HWIR Technology Software System, arranged for ease of retrieval by various computer programs

design—*noun*: comprehensive description of what a piece of software will do and how it will do it; hence, a design document includes such a description. *Verb*: to initially identify what a piece of software will do and how it will do it; hence, we design a piece of software by writing down the description. In either case for the FRAMES-HWIR Technology Software System, design includes short-term as well as longer-term capabilities of the software.

Distribution Statistics Processor (DSP)—the processor that randomly samples from statistical distributions representing measurement and sampling error related to the statistics of parameters required by the models (e.g., distribution, mean, standard deviation, and range).

DLL—see Dynamic Link Library

Dynamic Link Library—a modular set of routines that comes with or can be added to a software system to simplify the interface between existing and new codes and provide a flexible and expandable storage format

Ecological Exposure/Risk Module—exposure and risk module within the Multimedia Multipathway Simulation Processor that calculates exposure and risk (hazard quotient) to ecological receptors; receives input from the Terrestrial Foodchain Module and the Aquatic Foodchain Module; provides input to the Global Results File.

regional/national environmental setting distribution statistics—databases containing stochastic parameters (a subset of the Site Definition Files data) whose stochastic characteristics are themselves described with statistical distributions; one database contains information on environmental parameters collected for specific regions of the country identified by latitude/longitude descriptions; the other contains information on environmental parameters at a national level; data are used by the Distribution Statistics Processor

executable—self-contained set of coded instructions designed to process and control a particular component of the FRAMES-HWIR Technology Software System, including modules and processors

Exit Level Processors (ELP I and ELP II)—processors that take the results of the Multimedia Multipathway Simulation Processor individual site simulations and tabulate information to discern levels of protection for decisions on the exit criteria for contamination; ELP I produces the Risk Summary Output File; ELP II takes the Risk Summary Output File and generates the Protective Summary Output File. This site-based exposure and risk information is used to establish a national distribution of risks. The national distribution of risks, and all related data, forms the technical basis for EPA to select chemical-specific exit levels.

Exposure and Risk Modules—modules within the Multimedia Multipathway Simulation Processor that

calculate risk numbers or hazard quotients for either human or ecological receptors; includes Human Exposure Module, Ecological Risk/Exposure Module, and Human Risk Module.

Farm Foodchain Module—foodchain module within the Multimedia Multipathway Simulation Processor that simulates contaminant movement through a farm-related foodchain; receives input from the Saturated Zone Module, Air Module, and Waterbody Module; provides input to the Human Exposure Module.

Fate and Transport Modules—modules within the Multimedia Multipathway Simulation Processor that simulate contaminant behavior through a sequence of environmental media; include Air Module, Watershed Module, Vadose Zone Module, Saturated Zone Module, and Waterbody Module

file—see data file

Foodchain Modules— modules within the Multimedia Multipathway Simulation Processor that simulate contaminant movement through a particular food web to humans or ecological receptors; include Farm Foodchain Module, Aquatic Foodchain Module, and Terrestrial Foodchain Module

FRAMES-HWIR Technology Software System—name of the technology being developed by the Pacific Northwest National Laboratory to automate the EPA's HWIR99 Assessment Strategy; FRAMES in this context stands for Framework for Risk Analysis in Multimedia Environmental Systems.

geographic reference point—a latitude and longitude used to locate a site geographically; the point will be translated into UTM coordinates to facilitate the locating of various physical entities (e.g., streams, receptors, etc.) at a site.

Global Results Files—collection of data groups populated by execution of appropriate models in the appropriate sequence in the Multimedia Multipathway Simulation Processor and used to provide input to the Exit Level Processors. There is a set of Global Results Files for each site; these files are stored in a common directory.

Human Exposure Module—exposure module within the Multimedia Multipathway Simulation Processor that models how humans might be exposed to contamination through various environmental pathways; receives input from Saturated Zone Module, Air Module, Waterbody Module, Farm Foodchain Module, and Aquatic Foodchain Module; provides input to Human Risk Module

Human Risk Module—risk module within the Multimedia Multipathway Simulation Processor that simulates human-health impact that might result from exposures by human receptors to contamination in environmental pathways; receives input from the Human Exposure Module; provides input to the Global Results File

HWIR --(Hazardous Waste Identification Rule)

HWIR95 --refers to the initial HWIR proposal for exit levels as presented in the Federal Register in December, 1995. The technical assessment methodology associated with this proposal was highly critisized and resulted in the Agency deciding to update the methodology and repropose exit levels.

HWIR99 --refers to the planned update of HWIR95.

HWIR99 Assessment Strategy—the approach used for EPA's initiative to assess hazardous waste sites for the potential to exit Industrial Subtitle D status for particular waste streams. The HWIR99 Assessment Strategy is documented in the draft report *A Preliminary Framework for Finite-Source Multimedia, Multipathway, and Multireceptor Risk Assessment* (3MRA).

implementation—resource- and scheduled-constrained translation of design into operating software system; for the FRAMES-HWIR Technology Software System, a staged process, with the first stage consisting of deciding what design capabilities can and will be implemented by 10/98, the second stage consisting of an intensive three months of coding to develop a prototype of the FRAMES-HWIR Technology System (February to April 1998), and the third stage consisting of extensive testing and modification (May through October 1998).

Inner Loop—iteration within the FRAMES-HWIR Technology Software System that loops through all sites or locations associated with the HWIR99 Assessment Strategy; also known as the site assessment loop

input/output specifications—detailed descriptions of data necessary to allow processors and modules within processors to transfer information effectively with each other

Land Application Unit Source Module—module within the Multimedia Multipathway Simulation Processor that models release of contaminant from a land application unit; for modeling purposes, includes atmospheric (vapor, particulates), leaching, and overland; utilizes two distinct models, one with input surface hydrology that will sample annual average values for infiltration, runoff, and evapotranspiration from regional distributions while estimating erosion on an annual average basis based on a random sampling of appropriate parameters; and one with simulated surface hydrology that will function at the source and reflect a precipitation event-based methodology using daily MET data and source surface cover data to simulate infiltration, runoff, evapotranspiration, and erosion.

Landfill Source Module—module with the Multimedia Multipathway Simulation Processor that models release of contaminant from a landfill; for modeling purposes, includes atmospheric (vapor, particulates), leaching, and overland; utilizes two distinct models, one with input surface hydrology that will sample annual average values for infiltration, runoff, and evapotranspiration from regional distributions while estimating erosion on an annual average basis based on a random sampling of appropriate parameters; and one with simulated surface hydrology that will function at the source and reflect a precipitation event-based methodology using daily MET data and source surface cover data to simulate infiltration, runoff, evapotranspiration, and erosion

legacy code or legacy model—models or programs developed before the FRAMES-HWIR Technology Software System development effort that will be used to implement some portion of the HWIR99 Assessment Strategy and may require modification for efficient use

location—the geographic reference point for a site in latitude/longitude coordinates (UTMs will also be used)

model—scientifically based computer calculations that simulate physical or physiological phenomena

module—components within the Multimedia Multipathway Simulation Processor that, when collectively viewed and applied to a site, represent the modeling system for conducting exposure and risk assessment. A module comprises some combination of model, pre-processor, post-processor, and module user interface. For the HWIR99 Assessment Strategy, modules include source modules, fate and transport modules, foodchain modules, and exposure and risk modules.

Multimedia Multipathway Simulation Processor—implements the release, transport, exposure and risk/hazard assessment modeling protocol by choosing and linking the appropriate models to supply results to the Exit Level Processors; consists of a collection of individual software modules each representing a modeling-based approach to one of the fundamental elements of the risk assessment process (see elements and modules).

Outer Loop—iteration within the FRAMES-HWIR Technology Software System that allows for the random selection of measurement and sampling errors associated with key risk assessment variable and. loops through parameter distributions considered in the Monte Carlo simulation.

output specifications—see input/output specifications

parameter—see variable

processor—one of six major programs within the FRAMES-HWIR Technology Software System (i.e., Distribution Statistics Processor, Site Definition Processor, Site Simulation Processor, Multimedia Multipathway Simulation Processor, and Exit Level Processors) that result in a series of changes to data or data groups to support the HWIR99 Assessment Strategy

program—a computer procedure for solving a problem, including collecting data, processing, and presenting results

regional/national data with statistics—databases containing individual parameters (a subset of the Site Definition Files data) whose statistical distribution characteristics are themselves described with statistical distributions; one database contains information on environmental parameters collected for specific regions of the country identified by latitude/longitude descriptions; the other contains information on environmental parameters at a national level; data are generated by the Distribution Statistics Processor

requirements—characteristics and behaviors that a piece of software must possess to function adequately for its intended purpose

run—see simulation

Saturated Zone Module—a fate and transport module within the Multimedia Multipathway Simulation Processor that models contaminant behavior through the saturated zone; receives input from the Vadose Zone Module; provides input to the Waterbody Module, Farm Foodchain Module, and Human Exposure Module

shared routine—computer program made available to other programs to use in conducting common tasks

shareware—see shared routine

simulation—a single execution of the Multimedia Multipathway Simulation Processor and associated processors in which the Multimedia Multipathway Simulation Processor executes the modules defined for that specific simulation.

site—for the purposes of the HWIR99 Assessment Strategy, a site is an Industrial Subtitle D facility with one or more waste management units within a bounded area of approximately 20 km^2.

Site Definition Files—collection of data groups that result from executing the Site Definition Processor; provides input to the Site Simulation Processor and represents a complete data set for implementation of the Multimedia Multipathway Simulation Processor

Site Definition Processor—the processor that organizes all data for input to Site Definition Files by accessing data files containing all the necessary information and executing a hierarchical protocol to read these data files and extract the required data; it also provides the preliminary simulation plan and control information that could be used by the Multimedia Multipathway Simulation Processor

Site Simulation File—collection of optimized data groups that result from execution of the Site Simulation Processor for input to the Multimedia Multipathway Simulation Processor

source loop—iteration within the FRAMES-HWIR Technology Software System and the Inner Loop that loops through all source types in a particular simulation

source modules—modules within the Multimedia Multipathway Simulation Processor that model behavior for a particular waste type: Land Application Unit, Landfill, Waste Pile, Aerated Tank, and Surface Impoundment

source type--the five different source types addressed by HWIR99: aerated tank (AT), waste pile (WP), land application unit (LAU), landfill (LF), and surface imboundment (SI).

static regional/national data—databases with information concerning environmental parameters similar to site-specific parameters but collected outside specific waste disposal facilities; one database contains information on environmental parameters collected for specific regions of the country identified by latitude/longitude descriptions; the other contains information on environmental parameters at a national level.

Surface Impoundment Source Module—module within the Multimedia Multipathway Simulation Processor that models release of contaminant from a surface impoundment; for modeling purposes, the only environmental pathways considered are atmospheric (vapor only) and leaching; provides input to the Air Module and the Vadose Zone Module.

System User Interface—the interface that connects, interacts with, and directs the other processors

housed in the FRAMES-HWIR Technology Software System, managing the overall execution of the software system

Terrestrial Foodchain Module—foodchain module within the Multimedia Multipathway Simulation Processor that simulates contaminant movement through the terrestrial foodchain to ecological receptors; receives input from the Air Module; provides input to the Ecological Risk/Exposure Module.

Vadose Zone Module—a fate and transport module within the Multimedia Multipathway Simulation Processor that models contaminant behavior in the subsurface above the groundwater; requires input from the Land Application Unit, Landfill, Waste Pile, and Surface Impoundment Source Modules; provides input to the Saturated Zone Module.

variable—an input or output value associated with calculations in a model or module

waste management unit (WMU)—a single source of contamination that could result in contaminant release to multiple environmental media; may include several of a single source type (for example, three aerated tanks in a grouping might be one waste management unit)

Waste Pile Source Module— module within the Multimedia Multipathway Simulation Processor that models release of contaminant from a waste pile; for modeling purposes includes atmospheric (vapor, particulate), leaching, and overland; utilizes two distinct models, one with input surface hydrology that will sample from regional distributions of annual average values for infiltration, runoff, and evapotranspiration, while estimating erosion on an annual average basis based on a random sampling of appropriate parameters; and one with simulated surface hydrology that will function at the source and reflect a precipitation event-based methodology using daily MET data and source surface cover data to simulate infiltration, runoff, evapotranspiration, and erosion; provides input to the Air Module, Waterbody Module, Vadose Zone Module, and Watershed Module.

Waterbody Module—a fate and transport module within the Multimedia, Multipathway Simulation Processor that models contaminant behavior in surface waters such as streams, lakes and ponds; receives input from the Saturated Zone Module, Air Module, and Watershed Module; provides input to the Aquatic Foodchain Module, Farm Foodchain Module, and Human Exposure Module.

Watershed Module—a fate and transport module within the Multimedia, Multipathway Simulation Processor that simulates contaminant movement within the interconnected creeks and rivers comprising a watershed; receives input from Land Application, Landfill, and Waste Pile Source Modules, and the Air Module; provides input to the Waterbody Module.

6.0 ACRONYMS

AqFW - aquatic food web module - the model selected to predict concentrations in aquatic biota for the 1999 HWIR proposal

AT - aerated tank

BAF - bioaccumulation factor

CALPUFF - ?

CMAQ - Community Models of Air Quality

COP - Computational Optimization Processor

CSTR - completely stirred tank reactor

DSP - Distribution Statistics Processor

EcoEX - Ecological Exposure Module - the model selected to estimate does and/or medium concentrations to the ecological receptors for the 1999 HWIR proposal

ELP - Exit Level Processor

EPACMTP - EPA's Composite Model for Leachate Migration with Transformation Products - the saturated zone model selected to support the 1999 HWIR proposal

EXAMS - Exposure Analysis Modeling Systems - the surface water model selected to support the 1999 HWIR proposal

FFC - Farm Food Chain model - the model selected to predict concentrations in plants, beef, and dairy products grown on farms or home gardens for the 1999 HWIR proposal

FRAMES - Framework for Risk Analysis in Multimedia Environmental Systems - a comprehensive environmental exposure and risk analysis software framework

HWIR - Hazardous Waste Identification Rule

HumEX - Human Exposure Module - the model selected to estimate does to the human receptors for the 1999 HWIR proposal

IEM - Indirect Exposure Methodology

ISCST3 - Industrial Source Complex - Short Term model - the air model selected to support the 1999 HWIR proposal

LAU - Land Application Unit

LF - Landfill

MMSP - Multimedia Multipathway Simulation Processor

MPRA - Multipathway Risk Assessment (the risk assessment used for the 1995 HWIR proposal)

3MRA - Multimedia Multipathway Multireceptor Risk Assessment (the risk assessment being developed for the 1999 HWIR proposal)

NAPL - Non-Aqueous Phase Liquid

ORD - Office of Research and Development

OSW - Office of Solid Waste

PGD - Parameter Guidance Document

SDP - Site Definition Processor

SI - Surface Impoundment

SAMSON - Solar and Meteorological Surface Observation Network database

SUI - System User Interface

SVOC - Semi-Volatile Organic Compounds

TerFW - Terrestrial Food Web Module - the model selected to predict concentrations in food items consumed by terrestrial receptors the 1999 HWIR proposal

TILT - Transient Investigative Land Treatment model

USLE - Universal Soil Loss Equation

VOC - Volitile Organic Compounds

WASP5 - Water Analysis Simulation Program

WP - Waste Pile

WMU - Waste Management Unit

REFERENCES

Abbott, J.D., S.W. Hinton, and D.L. Borton. 1995. Pilot scale validation of the river/fish bioaccumulation modeling program for nonpolar hydrophobic organic compounds using the model compounds 2,3,7,8-TCDD and 2,3,7,8-TCDF. *Environmental Toxicology and Chemistry* 14:1999-2012.

Allen, H.E. and D.J. Hansen. 1996. The importance of trace metal speciation to water quality criteria. *Water Environment Research* 68:42-54.

Aronson, D. and P. H. Howard. 1997. Anaerobic Biodegradation of Organic Chemicals in Groundwater: A Summary of Field and Laboratory Studies. Syracuse Research Center, North Syracuse, N.Y. 13212-2509. Report No. TR-97-0223F.

Bailey, R.G. 1996. Ecosystem Geography. Springer-Verlag, New York. ISBN 0-387-94354-4.

Bailey, R.G., P.E. Avers, T. King, W.H. McNab (eds.). 1994. Ecoregions and Subregions of the United States. Washington DC: USDA Forest Service. 1:7,500,000; colored with supplementary table of map unit descriptions, compiled and edited by W.H McNab and R.G. Bailey.

Bergman, H.L. and E.J. Dorward-King (eds.) 1997. Reassessment of metals criteria for aquatic life protection: priorities for research and implementation. *SETAC Pellston Workshop on Reassessment of Metals Criteria for Aquatic Life Protection;* 1996 Feb 10-14; Pensacola FL: SETAC Pr. 114 p.

Burns, L.A. 1997. Exposure Analysis Modeling System (EXAMS II), User's Guide for Version 2.97.5, EPA/600/R-97/047

Burns, L.A. et al., 1992. Exposure Analysis Modeling System (EXAMS): User Manual and System Documentation, EPA-600/3-82-023.

Campfens, J. and D. Mackay. 1997. Fugacity-based Model of PCB Bioaccumulation in Complex Aquatic Food Webs. *Environmental Science and Technology* 31:577-583.

Chapman, P.M., H.E. Allen, K. Godtfredsen, and M.N. Z'Graggen. 1996. Evaluation of bioaccumulation factors in regulating metals. *Environmental Science and Technology* 30:448A-452A.

CRC Handbook of Chemistry and Physics. 1989-1990. 70th Edition. CRC Press, Inc. Boca Raton, FL. Page F40.

Dewar, M.J.S., and R.C. Dougherty. 1975. The PMO Theory of Organic Chemistry. Plenum Press, New York, NY.

Gobas, F.A.P.C. 1993. A model for predicting the bioaccumulation of hydrophobic organic chemicals in aquatic food-webs: Application to Lake Ontario. *Ecol. Model.,* 69:1-17.

Hilal, S. H., L. A. Carreira, S. W. Karickhoff and C. M. Melton. 1993. Prediction of Electron Affinity by Computer. *Quant. Struc. Act. Rel* 12: 389.

Hilal, S. H., L. A. Carreira, S. W. Karickhoff and C. M. Melton. 1994a. Estimation of Gas Chromatographic Retention Times from Molecular Structure. *J. Chromatography* 662: 269.

Hilal, S. H., L. A. Carreira, C. M. Melton, G. L. Baughman and S. W. Karickhoff. 1994b. Estimation of Ionization Constants of Azo Dyes and Related Aromatic Amines: Environmental Implication. *J. Phys. Org. Chem.* 7:122.

Hilal, S. H., S. W. Karickhoff and L. A. Carreira. 1995. A Rigorous Test for SPARC's Chemical Reactivity Models: Estimation of More Than 4300 Ionization pKa's. *Quant. Struc. Act. Rel.* 14: 348.

Howard, P.H. et al. 1986. BIOLOG, BIODEG and FATE/EXPOS: New files on microbial degradation and toxicity as well as environmental fate/exposures of chemicals. Environ. Toxic. Chem. Vol. 5, pp. 977-988.

IEM. 1997. Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions; Update to Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions EPA/600/6-90/00. NCEA-0238. U.S . EPA, National Center for Environmental Assessment. Cincinatti, OH.

Isnard, P. and S. Lambert. 1988. Estimating bioconcentration factors from octanol-water partition coefficient and aqueous solubility. *Chemosphere* 17:21-34.

Jury, W. A., D. Russo, G. Streile, and E.A. Hesham. 1990. Evaluation of volatilization by organic chemicals residing below the soil surface. *W. Res. Res.*, 26:13-20.

Jury, W. A., W.F. Spencer, and W.J. Farmer. 1983. "Behavior Assessment Model for Trace Organics in Soil." *J. Environ. Qual.*, 12: 558-564.

Karickhoff, S. W., V. K. McDaniel, C. M. Melton, A. N. Vellino, D. E. Nute, and L. A. Carreira. 1991. Predicting Chemical Reactivity by Computer. *Environ. Toxicol. Chem.* 10:1405-1416.

Kenaga, E.E. and C.A. Goring. 1980. Relationship between Water Solubility, Soil Sorption, Octanol-Water Partitioning, and Concentration of Chemicals in Biota. *Aquatic Toxicology, ASTM STP 707.* J.G. Eaton, P.R. Parrish, and A.C. Hendricks, Eds., American Society for Testing and Materials, 1980, pp. 78-115.

Lyman, W.J., W.F. Reehl, D.H. Rosenblatt. 1990. Handbook of Chemical Property Estimation Methods. American Chemical Society, Washington D.C.

Morrison, H.A., F.A.P.C. Gobas, R. Lazar, D.M. Whittle, and G.D. Haffner. 1997. Development and Verification of a Benthic/Pelagic Food Web Bioaccumulation Model for PCB Congeners in Western Lake Erie. *Environ. Sci. Technol.*, 31:3267-3273.

Renner, R. 1997. Rethinking water quality standards for metals toxicity. *Environmental Science and Technology* 31:466A-468A.

SAB. 1995. US EPA's Science Advisory Board's Report on the Review of EPA's Composite Model for Leachate Migration with Transformation Products (EPACMTP). US EPA's Science Advisory Board, Washington D.C., 20460.

Sample, B. E., M. S. Aplin, R. A. Efroymson, G. W. Suter , II, and C. J. E Welsh. 1997. Methods and Tools for Estimation of the Exposure of Terrestrial Wildlife to Contaminants. ORNL/TM-13391. Oak Ridge, TN, Oak Ridge National Laboratory.

Sample, B. E., J. J. Beauchamp, R. A. Efroymson, and G. W. Suter , II. 1998a. Development and Validation of Bioaccumulation Models for Small Mammals. ES/ER/TM-219. Oak Ridge, TN, Oak Ridge National Laboratory.

Sample, B. E., J. J. Beauchamp, R. A. Efroymson,G. W. Suter , II, and T. L. Ashwood. 1998b. Development and Validation of Bioaccumulation Models for Earthworms. ES/ER/TM-220. Oak Ridge, TN, Oak Ridge National Laboratory.

Shan, C., and D.B. Stephens. 1995. An analytical solution for vertical transport of volatile chemicals in the vadose zone. *Journal of Contaminant Hydrology* 18: 259-277.

Spencer, M. and S. Beaulieu. 1997. Bioaccumulation Factors for Polycyclic Aromatic Hydrocarbons in Fish: Methods for Dealing with Uncertainty. Draft Report. Research Triangle Institute, RTI Project Number 6720-001.

Stephan, C. E. 1993. Derivation of Proposed Human Health and Wildlife Bioaccumulation Factors for the Great Lakes Initiative. PB93-154672. Springfield, VA, Office of Research and Development, U. S. Environmental Research Laboratory.

Stevens, J.B. 1991. Disposition of Toxic Metals in the Agricultural Food Chain. 1. Steady-state Bovine Milk Biotransfer Factors. *Environ. Sci. Technol*., 25:1289-1294.

Stevens, J.B. 1992. Disposition of Toxic Metals in the Agricultural Food Chain. 2. Steady-state Bovine Tissue Biotransfer Factors. *Environ. Sci. Technol*., 26:1915-1921.

Thomann, R.V., J.P. Connolly, and T.F. Parkerton. 1992. An equilibrium model of organic chemical accumulation in aquatic food webs with sediment interaction. *Environmental Toxicology and Chemistry* 11:615-629.

USEPA. 1986. National Survey of Industrial Facilities with Subtitle D Waste Management Units. U.S. EPA, Office of Solid Waste, Washington D.C. 20460.

USEPA. 1991. Assessment and Control of Bioconcentratable Contaminants in Surface Waters. Draft. U.S. EPA, Office of Water, Washington D.C. 20460.

USEPA. 1993. Wildlife Exposure Factors Hand Book. EPA/600/p-95/002 Fa, U.S. EPA, Office of Research and Development, Washington D.C. 20480.

USEPA. 1995. Identification and Listing of Hazardous Wastes: Hazardous Waste Identification Rule (HWIR): Proposed December 21. Federal Register, pp 66344 -66469, Washington, D.C. 20460.

USEPA. 1997a. Exposure Factors Hand Book. EPA/600/p-95/002 Fa, U.S. EPA, Office of Research and Development, Washington D.C. 20480.

USEPA. 1997b. Guiding Principles for Monte Carlo Analysis EPA/630/R-97/001.

USEPA. 1998. A Preliminary Framework for Finite-Source Multimedia, Multipathway, and Multireceptor Risk Assessment, **3MRA**. U.S. EPA, Office of Solid Waste, Washington D.C. 20460.

Veith, G.D., D.L. DeFoe, and B.V. Bergstedt. 1979. Measuring and estimating the bioconcentration factor of chemicals in fish. *Journal Fish.Res.Board of Canada* 36:1040-1048.