Demonstration of the Wildlife Ecological Assessment Program (WEAP)

December 2000

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G. Whelan
M.A. Pelton
R.Y. Taira
F. Rutz
G.M. Gelston

December 2000

Pacific Northwest National Laboratory

Richland, Washington 99352

Summary

The U.S. Army Research and Development Center, Waterways Experiment Station (WES), U.S. Corps of Engineers develops tools to help analysts assess the impacts of anthropogenic activities in the environment. As such, WES is developing the Army Risk Assessment Modeling System (ARAMS) to provide the Army with the capability to perform human and ecologically based risk/hazard assessment associated with past-practice and current activities at military installations. The intent of the system is to provide a platform from which a variety of assessments can be performed, utilizing screening level tools, science-support tools, site-specific databases, physicochemical databases, visualization, and Conceptual Site Model (CSM) guidance. The system is envisioned to help a risk analyst visualize an assessment from source, through multiple environmental media (e.g., groundwater, surface water, air, and land), to sensitive receptors of concern (e.g., humans and wildlife). Concurrently, WES is also sponsoring the development of the science-support-based Land-based Management System (LMS), which has many of the same goals of ARAMS, yet is taking a more detailed approach to each of the components of an integrated system. The linkage of ARAMS and LMS is a an ultimate goal of WES, such that utilization of the components in each system can be used by the other system to support assessment activities.

To help utilize current and existing state-of-the-art multimedia tools and to gain an appreciation for current technological advances, the Pacific Northwest National Laboratory (PNNL) is supporting WES and ARAMS by modifying and updating the Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) for inclusion as a component in ARAMS. FRAMES is a Windows-based software platform that provides an interactive user interface and, more importantly, specifications to allow a variety of DOS and Windows-based environmental codes to be integrated within a single framework. As a new component in ARAMS and FRAMES, PNNL has developed the Wildlife Ecological Assessment Program (WEAP), which is a software package that summarizes ecological health impacts to wildlife from exposures to chemical contaminants.

WEAP is an updated beta version of the FRequency ANalysis of COncentration (FRANCO) model, which was developed by PNNL for the U.S. Environmental Protection Agency (EPA) for regulatory and compliance purposes. WEAP is statistical package that 1) correlates duration of exposure to contaminant levels to help determine the impacts of the exposure to organisms and 2) bridges the gap between simulated chemical transport and fate modeling and ecological-risk assessment data that are available from laboratory studies. The WEAP statistical analysis accommodates different organisms as they relate to different contaminants, resulting in a flexible and versatile tool.

This document provides requirements, design, data-file specifications, test plan, and Quality Assurance/Quality Control (QA/QC) protocol for WEAP. The requirements identify the attributes of the system. The design describes how the system will be structured to meet those requirements. The specification presents the specific modifications to FRAMES to meet the requirements and design. The test plan ensures that the basic functionality listed in the requirements (black box testing) actually functions as designed, and QA/QC ensures that the software meets the client's needs.

Acknowledgments

Acronyms and Abbreviations

ARAMS	Army Risk Assessment Modeling System
BBF	Body Burden File
CCC	Criterion Continuous Concentration
CSM	Conceptual Site Model, simplified description of the environmental problem to be modeled
DES	DESCRIPTION file, containing all necessary information to link a module into FRAMES
DOS	Disk Operation System, basic operation system on the computer
EBF	Ecological Benchmark File
ED	Effective Dose
EHQ	Ecological Hazard Quotient
EPA	U.S. Environmental Protection Agency
ERED	Environmental Residue-Effects Database
FRAMES	Framework for Risk Analysis in Multimedia Environmental Systems
FRANCO	FRequency ANalysis of COncentration
FUI	Framework User Interface
GID	Global Input Data File, contains all of the input data to run modules
LC	Lethal Concentration
LD	Lethal Dose
LMS	Land-based Management System
MUI	Model-Specific User Interface
NOAEL	No Observable Adverse Effects Level
NOEL	No Observable Effects Level
OCRWM	Office of Civilian Radioactive Waste Management
PNNL	Pacific Northwest National Laboratory
QA/QC	Quality Assurance and Quality Control, processes that ensure the quality of the product
WCF	Water Concentration File, containing time-varying constituent concentrations
WEAP	Wildlife Ecological Assessment Program
WES	Waterways Experiment Station

Contents

Figures

Tables

1.0 INTRODUCTION

1.1 Objective

The objective is to develop ecological impacts model that can statistically compare simulated, modeled, or measured time-varying concentrations, doses, or body burdens to topological data. The Wildlife Ecological Assessment Program (WEAP) is a program that correlates simulated, modeled, or measured ecological contaminant levels (e.g., concentration, body burden, dose) with toxicological benchmarks and provides a statistical analysis of this comparison.

1.2 Definitions

- Requirement – Characteristic and behavior that a piece of software must possess to function adequately for its intended purpose. A good requirement is also testable. Sometimes called an attribute.

- Design – A design is a comprehensive description of how a piece of software will function (i.e., how it will meet its requirements).

- Specifications – Specifications are a detailed description of an interface to a computer program or set of subroutines such that another programmer could develop a program, which would make proper use to the subroutines.

- Model/Code – Loosely defined herein to represent the software product for simulating an aspect associated with the release, fate & transport, exposure, intake, or risk/hazard of chemicals released into the environment; however, a model/code can simulate any phenomena and is not limited to hazardous-waste-site assessments.

- Module – Model/Code and accompanying 1) pre- and post-processors for communicating with other models, databases, frameworks, etc. and 2) model-specific user interface (MUI).

- System or Framework – Loosely defines a grouping of models, modules, databases, processors, or combination.

- Testable – Refers to the property of having the capability to examine and interrogate, such that a clear and concise conclusion can be drawn.

2.0 REQUIREMENTS

Requirements are characteristics and behaviors that a piece of software must possess to function adequately for its intended purpose.

2.1 System Requirements

WEAP shall meet the following requirements when integrated into the Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) architecture:

1. WEAP shall be capable of connecting to a Surface Water Icon that produces a Water Concentration File (WCF), containing time-varying constituent concentrations.
2. WEAP shall be capable of connecting to an Eco Exposure Icon that produces a Body Burden File (BBF).
3. WEAP shall be located under the Ecological Effects Icon.
4. WEAP shall connect to an Eco Benchmarks Icon that produces an Ecological Benchmark File(EBF).

2.2. Input Requirements

WEAP shall meet the following input requirements:

1. WEAP shall be capable of accessing and reading a WCF, which contains a time series of water concentrations (i.e., concentration versus time).

2. WEAP shall be capable of accessing and reading an ecological BBF, which contains a time series of body burden or doses containing units of mg/kg (i.e., dose/body burden versus time). . . . . 3 . WEAP shall be capable of accessing and reading an EBF, which contains ecological benchmark information, as described by an EBF Dictionary (EBF.DIC) file. A Dictionary file describes the parameters and the characteristics of the parameters (e.g., name, value, definition, units, etc.).

2.3 Output Requirements

WEAP shall produce two types of output each for time-varying concentrations and/or doses/body burdens. The two forms of outputs are as follows:

1. When consuming information from a WCF, WEAP shall produce a table, computing acute (e.g., #96-hr) and chronic exposures (e.g., >96-hr), for the percentage of time that a time series of concentrations, doses, or body burdens are

    a. below an acceptable limit (e.g., Chronic Limit, Criterion Continuous Concentration [CCC], No Observable Effects Level [NOEL], No Observable Adverse Effects Level [NOAEL], etc.)
    b. above an unacceptable limit (e.g., exposure duration curves associated with Lethal Concentration for 50% mortality [LC-50], Lethal Dose for 50% mortality [LD-50], Effective Dose at 50% [ED-50], etc.)

      c.   in between acceptable and unacceptable limits.

This table will result in a maximum of six values.

2. When consuming information from a WCF, WEAP shall produce a table reporting the Probability of Exceedence, based on the Period of Record (i.e., assumed equal to the Exposure Duration) versus Concentration: probability that concentration will be equal to or greater than a selected value.

3. When consuming a BBF, WEAP shall produce a table reporting the Ecological Hazard Quotient (EHQ) versus time. The EHQ is defined as the ratio of the body burden to the benchmark dose.

4. When consuming an BBF, WEAP shall produce a table reporting the Probability of Exceedence, based on the Period of Record (i.e., assumed equal to the Exposure Duration) versus EHQ: probability that an EHQ will be equal to or greater than a selected value.

5. When consuming an BBF, WEAP shall produce a table reporting the Probability of Exceedence, based on the Period of Record (i.e., assumed equal to the Exposure Duration) versus Dose or Body Burden: probability that dose/body burden will be equal to or greater than a selected value.

2.4 Scientific Requirements

Development and implementation of the system assumes that the WEAP model must operate within FRAMES under Windows-95 or higher.

3.0 DESIGN

Design elements are strategies for meeting requirements. This section reviews the design associated with meeting the requirements outlined in Section 2.0.

3.1 System Design

WEAP is located under the Eco Effects Icon and is designed to connect to Eco Benchmarks, Surface Water, and/or Eco Exposure Icons.

3.2 Input Design

WEAP is designed to consume data contained in a WCF, BBF, or EBF. The specifications associated with a WCF are documented in Whelan et al. (1997) and updated in http://mepas.pnl.gov:2080/earth/earth.htm. The BBF and EBF, which are not yet system-specified files, are documented in Appendices A and B.

3.3 Output Design

3.3.1 Percentage of Time a Lifeform is Associated with an Ecological Health Impact Region

WEAP statistically analyzes time-varying water-column concentrations and compares these results to ecological benchmarks to determine health impacts to selected lifeforms. WEAP tabularizes the percentage of time that a lifeform is associated with an ecological health impact region for a given chemical, based on 1) time-varying water-column concentrations, 2) an impact-toxicity benchmark curve (e.g., percent mortality LC curve), and 3) lower acceptable limit curve.

Tables 3.1 through 3.3 and Figures 3.1 and 3.2 illustrate the procedure used to produce Table 3.4 and Figure 3.3, which contain an illustrative example of the output results. The illustrative example compares time-varying water-column concentrations (see Table 3.1 and Figure 3.1), to which a lifeform might be exposed through respiration, to ecological toxicity benchmarks in the form of a LC curve at 50% mortality (i.e., LC-50) and a Chronic Limit concentration curve (see Table 3.2 and Figure 3.2). The LC-50 curve defines the duration of exposure at a given chemical concentration that produces an effect of 50% mortality. The Chronic Limit curve defines the maximum concentration below which the ecological health impacts, if any, are deemed acceptable, regardless of the duration of exposure. Although this illustrative example uses LC-50 and Chronic Limit curves, any toxicity benchmarks can be used (e.g., body burden or dose).

Table 3.3 provides the duration of exposure that equals or exceeds a given concentration, which is correlated to the information in Table 3.1 and Figure 3.1. For specified concentrations, the total duration associated with the concentration is determined. For example, over an exposure duration of 100 d, as illustrated in Figure 3.1, which represents the Period of Record, the lifeform is exposed to concentrations equal to or greater than 0 mg/L. Over an exposure duration of 66 d, the lifeform is exposed to concentrations equal to or greater than 30 mg/L. The tabulated data in Table 3.3 are plotted in Figure 3.2 as the solid line. The percentage of time

3.1

that a given concentration above the LC-50 curve, below the Chronic Limit curve, or in between the curves for acute and chronic exposures is determined by summing the duration of exposure that the solid line in Figure 3.2 is above, below, or in between the dotted lines representing the toxicity benchmark curves.

Table 3.4 and Figure 3.3 tabularize and pictorially illustrate, respectively, a summary of the results for acute and chronic exposures, where the 96-hr duration represents the demarcation. The six regions of the curve (Figure 3.3) can be interpreted as follows:

1.   For 1% of the time, the lifeform is exposed to concentrations that are equal to or above the LC-50 curve with durations of exposure less than or equal to 96 hr.

2.   For 58% of the time, the lifeform is exposed to concentrations that are equal to or above the LC-50 curve with durations of exposure greater than 96 hr.

3.   For 3% of the time, the lifeform is exposed to concentrations that are between the LC-50 and Chronic Limit curves with durations of exposure less than or equal to 96 hr.

4.   For 33% of the time, the lifeform is exposed to concentrations that are between the LC-50 and Chronic Limit curves with durations of exposure greater than 96 hr.

5.   For 0% of the time, the lifeform is exposed to concentrations that are below the Chronic Limit curve with durations of exposure less than or equal to 96 hr.

6.   For 5% of the time, the lifeform is exposed to concentrations that are below the Chronic Limit curve with durations of exposure greater than 96 hr.

3.3.2   Ecological Hazard Quotient, Based on Dose or Body Burden, Versus Period of Record

WEAP tabulates the time-varying EHQ, based on dose or body burden in mg/kg, by chemical and lifeform. The time-varying body-burden information is supplied by BPF, and the ecological benchmarks are supplied by the EBF. WEAP calculates the EHQ, as a function of time, based on the time-varying dose or body burden versus time. A pictorial representation of this table is illustrated in Figure 3.4.

Table 3.1 Hypothetical Chemical Water-Column Concentration Versus Time, as Contained in a WCF

Time (d)	Water Concentration (mg/L)
0	0
10	100
12	5
30	90
40	60
45	85
50	30
60	75
70	10
80	15
90	5
95	95
100	20

Table 3.3 Theoretical Water-Column Concentration Versus Duration of Exposure, Equaling or Exceeding a Concentration

Duration of Exposure, Equaling or Exceeding a Concentration (d)	Concentration (mg/L)
100	0
95	10
73	20
66	30
57	40
48	50
37	60
24	70
11	80
2	90
0	100

Table 3.2 Hypothetical Time-Varying Toxicological Data, Represented by Duration of Exposure, LC for 50% Mortality, and Acceptable Chronic Limit Concentration, Obtained from a Hypothetical Ecological Benchmark Database

Duration of Exposure (d)	LC for 50% Mortality (mg/L)	Acceptable Chronic Limit Concentration (mg/L)
0	95	10
4	95	10
20	50	10
60	30	10
100	30	10

Table 3.4 Theoretical Percent of Time Associated with Three Regions (i.e., #Chronic Limit, $LC-50, between the the Chronic Limit and LC-50) for Acute (i.e., #96-hr) and Chronic Limits

Region	Percent of Time Associated with Region (%)	
	Acute (<= 96-hr exposure duration)	Chronic (>96-hr exposure duration)
$LC-50	1	58
<LC-50 & >Chronic Limit	3	31
#Chronic Limit	0	7

3.3.3 Probability of Exceedence versus Concentration, EHQ, or Dose or Body Burden

Probability of exceedence tables, based on the period of record (i.e., assumed to equal the duration of exposure), are developed as a function of water-column concentration, EHQ, or lifeform dose/body burden.

1.   Probability of exceedence tables for water-column concentrations are based on the WCF. A pictorial representation of this table is illustrated in Figure 3.5.

2.   Probability of exceedence tables for EHQs are based on the time-varying body burden information supplied by a BPF and the ecological benchmarks supplied by an EBF. A pictorial representation of this table is illustrated in Figure 3.6.

3.   Probability of exceedence tables for doses/body burdens are based on the time-varying body-burden information supplied by a BPF. A pictorial representation of this table is illustrated in Figure 3.7.

The procedure outlined in Section 3.3.1 is also used to produce the probability of exceedence curves in this section.

3.4 Scientific Design

WEAP is written in C^{++} and operates within a Windows-95 or higher environment.
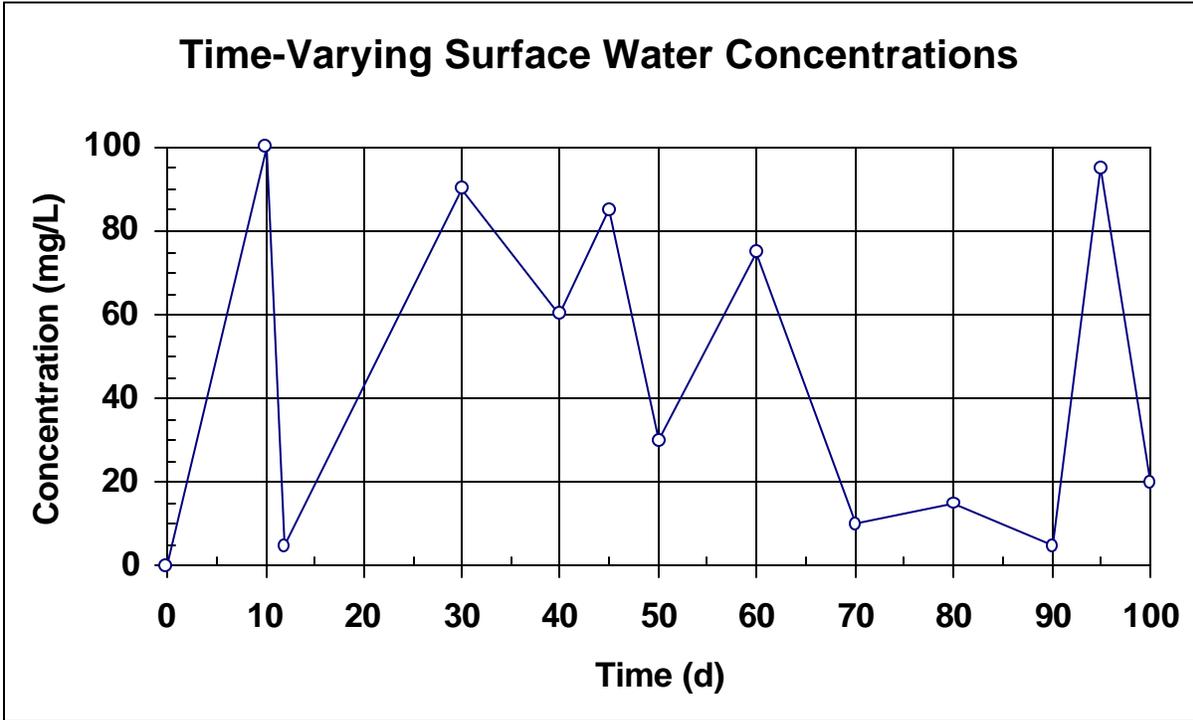
Figure 3.1. Hypothetical Time-Varying Surface Water Concentrations
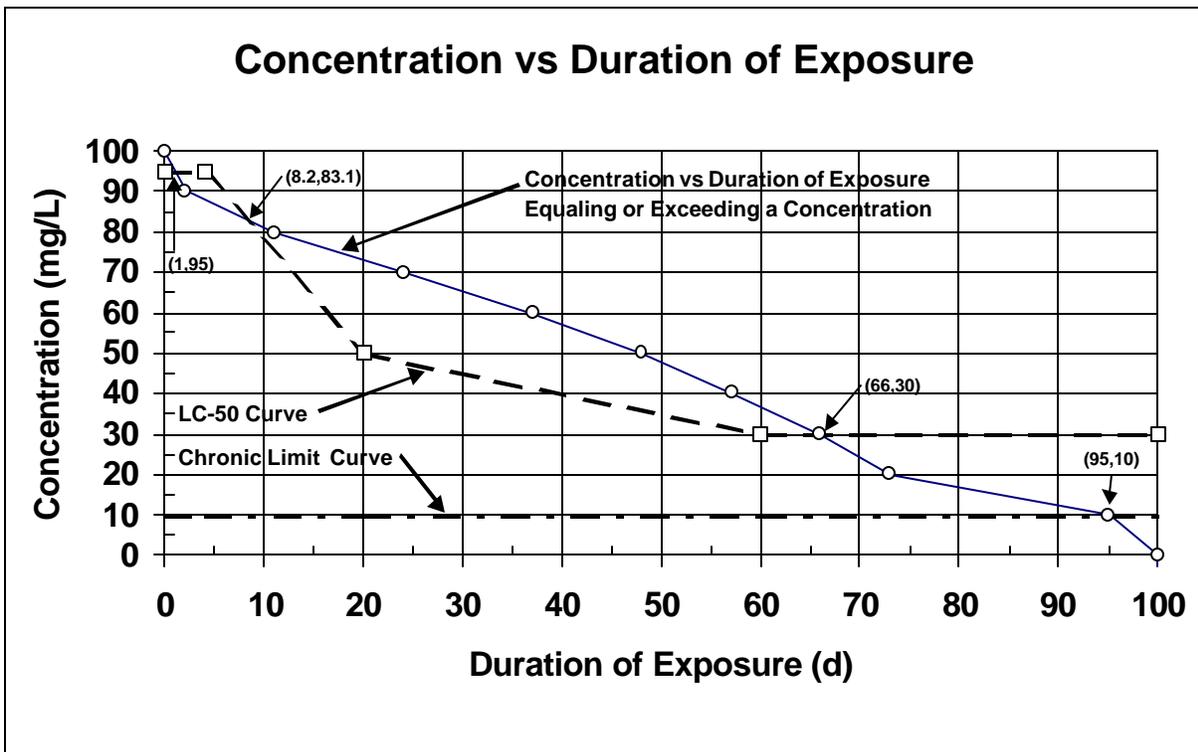
Figure 3.2. Theoretical Concentration Versus Duration of Exposure Curves

3.5
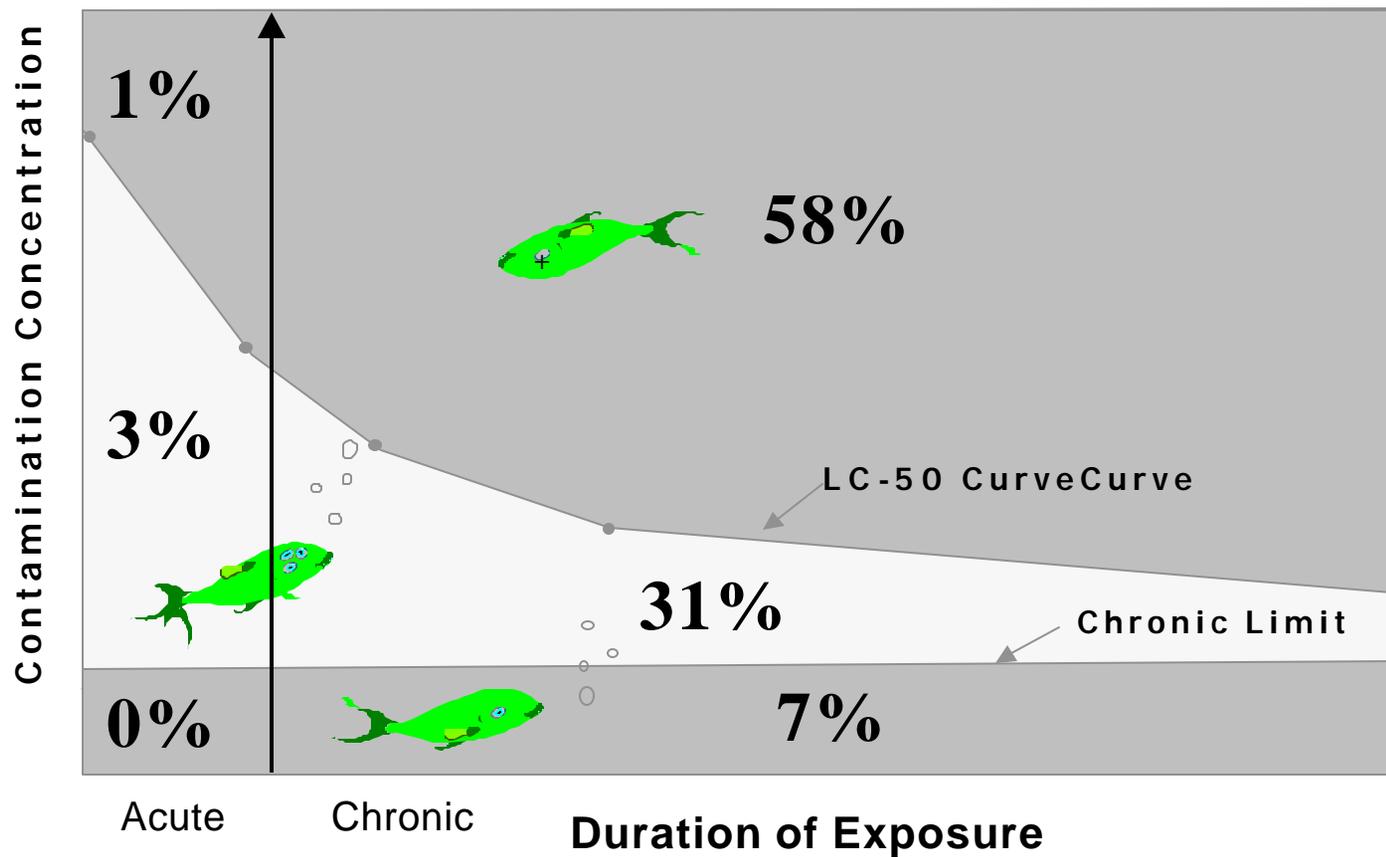
Figure 3.3. Pictorial WEAP Output Depicting the Percentage of Time that Aquatic Life are Exposure to Concentrations Below the Chronic Limit, Above the LC-50 Curve, and In Between Each Curve for Acute and Chronic Durations of Exposure
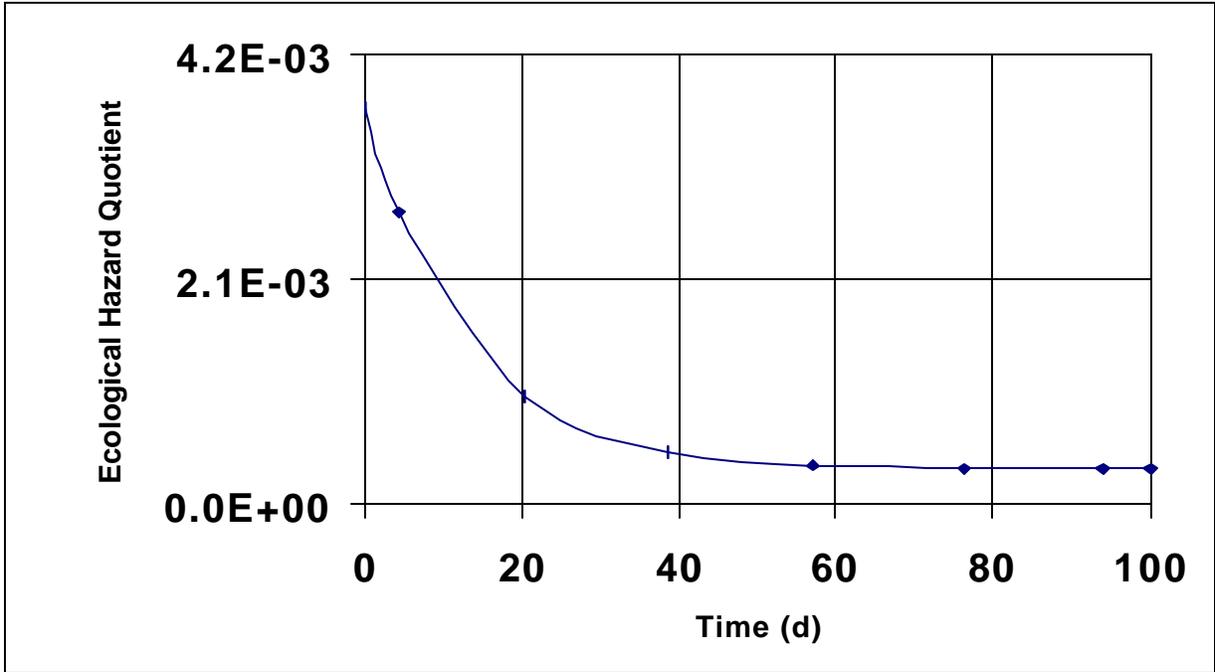
Figure 3.4. Illustrative Example Depicting WEAP Results Plotting EHQ Versus Time, Based on a Specified Toxicity Benchmark at a Given Duration of Exposure
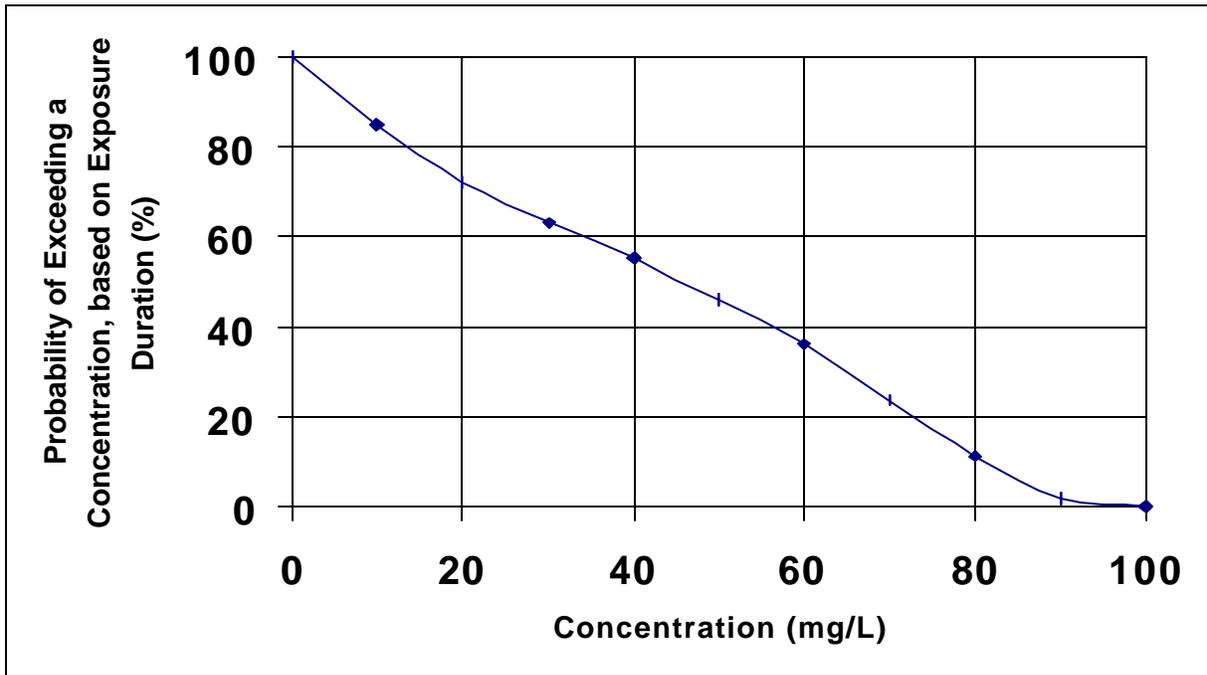
Figure 3.5. Illustrative WEAP Output Depicting the Probability of Equaling or Exceeding a Concentration, Based on Exposure Duration
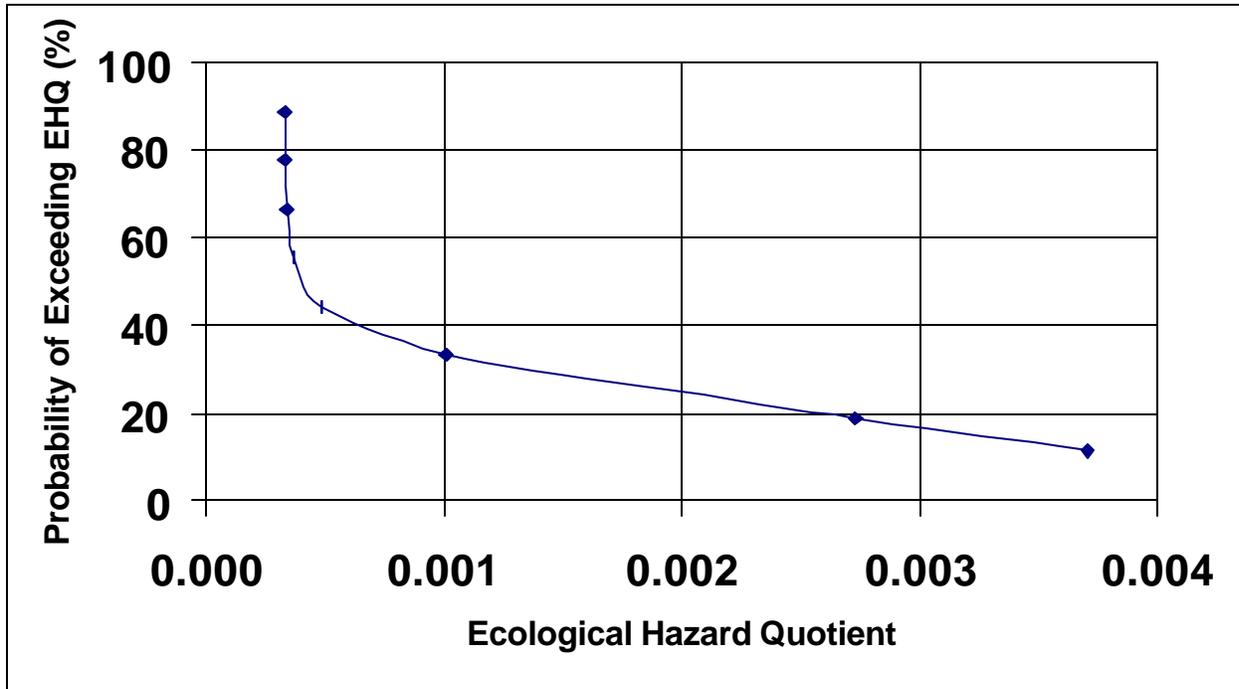
Figure 3.6. Illustrative WEAP Output Depicting the Probability of Equaling or Exceeding an EHQ, Based on Exposure Duration
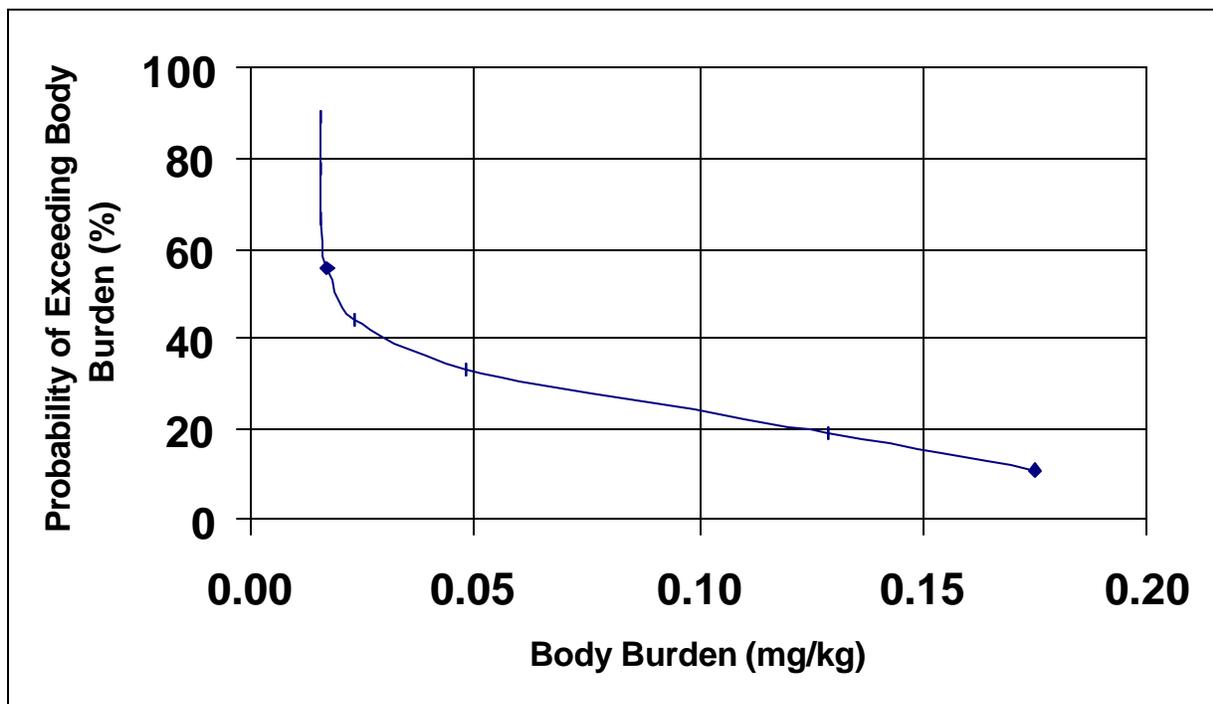
Figure 3.7. Illustrative WEAP Output Depicting the Probability of Equaling or Exceeding a Body Burden, Based on Exposure Duration

4.0 SPECIFICATIONS

4.1 File Input Specifications

There are three types of input files, the Global Input Data (GID) file, BBF, and WCF files. The GID file contains Eco Benchmarks information in a section name EBF#, where # is the identifying number. The format of a GID file and the contents of the EBF section is laid out in Appendix B. The BBF file is describe in Appendix A. The WCF is in http://mepas.pnl.gov:2080/earth/earth.htm and earlier documented in Whelan et al. (1997).

4.2 File Output Specifications

There are two kinds of output for the WEAP model. This output is based on the type of modeled input given: WCF or BBF. Two types of output are described in Sections 4.1.1 and 4.1.2. Both types of output are expected to be placed in the same comma-separated file with an EXF extension. If both types of output are present, then the output described in Section 4.1.2 can be placed first in the file, followed the output described in Section 4.1.1.

4.2.1 EXF Output from a WCF Connection

This section describes the format of the output from a Surface Water (WCF) connection to WEAP. Pseudo code is used to describe the following file format:

```
For each Species a line with
  Species Common Name - (string)
  Species Scientific Name - (string)
  A line with:
    Constituent Name - (string)
    Constituent CASID - (string)
  For each 'Effect Region' a line with
    Percent time at given Effect Region - (float)
    Effect Region description - (string)
  Next 'Effect Region'
  A line with:
    1st Column Label - (string)
      ; "Concentration in g/mL"
    2nd Column Label - (string)
      ; "Probability of Equaling or Exceeding a Concentration, based on Exposure Duration (%)"
    For 'I' = 1 to 11 a line with:
      Concentration - (float)
      Probability of Equaling or Exceeding a Concentration
    Next 'I'
Next 'Species'
```

4.2.2 Example EXF Output from a WCF Connection

"Starfish","Asterias rubens"
"FLUORANTHENE","206440"
3.71,"% time >= effect and < acute duration"
0,"% time >= effect and >= acute duration"
0.304,"% time < effect and > no effect level and < acute duration"
96,"% time < effect and > no effect level and > acute duration"
0,"% time < no effect level and < acute duration"
0,"% time < no effect level and > acute duration"
"Concentration in g/mL","Probability of Equaling or Exceeding a Concentration"
0,100.0
9.5E-06,25.8
1.9E-05,9.2
2.85E-05,8.1
3.8E-05,7.0
4.75E-05,5.8
5.7E-05,4.6
6.65E-05,3.5
7.6E-05,2.3
8.55E-05,1.2
9.5E-05,0.0
"Rotifer","Brachionus calyciflorus"
"FLUORANTHENE","206440"
0.912,"% time >= effect and < acute duration"
57.8,"% time >= effect and >= acute duration"
3.11,"% time < effect and > no effect level and < acute duration"
30.7,"% time < effect and > no effect level and > acute duration"
0,"% time < no effect level and < acute duration"
7.45,"% time < no effect level and > acute duration"
"Concentration in g/mL","Probability of Equaling or Exceeding a Concentration"
0,100.0
1E-05,92.6
2E-05,72.1
3E-05,66.0
4E-05,56.8
5E-05,47.6
6E-05,38.4
7E-05,23.8
8E-05,11.2
9E-05,1.8
0.0001,0.0

4.2.3 EXF Output from a BBF Connection to WEAP

This section describes the format of the output from an Eco Exposure File (BBF) connection to WEAP. Pseudo code is used to describe the following file format:

```
For each Life Form
  For each Constituent
    For each ED Level
      For each Body Part of Concern
        For each Type of Effect
          For each ED Concentration a line with
            Description of output
            A line with:
              1st Column Label - (string)          ; "EHQ"
              1st Column Units - (string)          ; ""
              2ndt Column Label - (string)         ; "Time"
              2nd Column Units - (string)          ; "yr"
            A Line with:
              Number of Time Periods
            For each 'Time Period' a line with:
              EHQ - (float)
              Time - (float)
            Next 'Time Period'
            A line with:
              1st Column Label - (string)          ; "EHQ"
              1st Column Units - (string)          ; ""
              2ndt Column Label - (string)         ;"Probability of Equaling or Exceeding EHQ"
              2nd Column Units - (string)          ; "%"
            A Line with:
              Number of Time Periods
            For each 'Time Period' a line with:
              EHQ - (float)
              Probability of Equaling or Exceeding EHQ - (float)
            Next 'Time Period'
            A line with:
              1st Column Label - (string)          ;"Body Burden"
              1st Column Units - (string)          ;"mg/kg"
              2ndt Column Label - (string)         ;"Probability of Equaling or Exceeding Body burden"
              2nd Column Units - (string)          ;"%"
            A Line with:
              Number of Time Periods
            For each 'Time Period' a line with:
              Body burden - (float)
              Probability of Equaling or Exceeding Body burden - (float)
            Next 'Time Period'
          Next 'ED Concentration'
        Next 'Type of Effect'
      Next 'Body Part of Concern'
```

Next 'ED Level'
  Next 'Constituent'
Next 'Life Form'

4.2.4 Example EXF Output from a BBF Connection to WEAP

"Oncorhynchus mykiss exposed to FLUORANTHENE(206440) using an ED50 level at a concentration of
47.3 mg/kg at duration of 4 days resulting in Mortality for the Whole Body"
"EHQ","","Time","yr"
7
5.48E-05,0
0.000179,5.72
0.000369,24.7
0.00042,44.3
0.000433,63.6
0.000437,82.5
0.000437,100
"EHQ","","Probability of Equaling or Exceeding EHQ","%"
11
0,100
4.37E-05,100
8.75E-05,98.5
0.000131,96.5
0.000175,94.5
0.000219,90.3
0.000262,85.9
0.000306,81.6
0.00035,77.2
0.000394,65.8
0.000437,0
"Body Burden","mg/kg","Probability of Equaling or Exceeding Body burden","%"
11
0,100
0.00207,100
0.00414,98.5
0.00621,96.5
0.00828,94.5
0.0103,90.3
0.0124,85.9
0.0145,81.6
0.0166,77.2
0.0186,65.8
0.0207,0

5.0 TESTING APPROACH AND RESULTS

As noted previously, WEAP is a program that correlates simulated, modeled, or measured ecological contaminant levels (e.g., concentration, body burden, dose) with toxicological levels and provides a statistical analysis of this comparison.

This section describes the type of testing conducted for the WEAP, summarizes the requirements on which testing was based, and describes test cases and the results of their implementation. GID files for each test case and spreadsheet files used in hand calculations are included with the test package. The GID files generated during independent testing should match the GID files included in this test package.

5.1 Summary of Requirements

Requirements for the WEAP are described in Section 2.0. of this document. These requirements were reworded, as necessary, to create a list of fundamental requirements that are suitable for testing. Table 5.1 lists these requirements. To ensure that the WEAP meets the requirements listed in Table 5.1, test cases were developed to check performance. Table 5.2 shows the relationship between these requirements and the test cases described in Section 5.2.

Table 5.1. Fundamental Requirements for Testing the WEAP

Requirement Number	Requirement
1	WEAP shall be capable of connecting to a Surface Water module that produces a WCF.
2	WEAP shall be located under the Eco Effects Icon.
3	WEAP shall be capable of connecting to an Eco Exposure module that produces an ecological BBF.
4	WEAP shall connect to an Ecological Benchmark module that produces an EBF.
5	WEAP shall be able to access and read a WCF, which contains a time series of water concentrations (i.e., concentration versus time), associated with the surface water icon.
6	WEAP shall be able to access and read a BBF, which contains a time series of body burden or doses containing units of mg/Kg (i.e., dose/body burden versus time).
7	WEAP shall be able to access and read an EBF, which contains ecological benchmark information, as described by an EBF Dictionary (EBF.DIC) file. A Dictionary file describes the parameters and the characteristics of the parameters (e.g., name, value, definition, units, etc.).

8	When consuming information from a WCF, WEAP shall produce results computing acute (i.e., #96-hr) and chronic exposures (e.g., >96-hr), for the percentage of time that a time series of concentrations, doses, or body burdens are
	
	    a. below an acceptable limit (e.g., Chronic Limit, CCC, NOEL, NOAEL, etc.),
	    b. above an unacceptable limit (e.g., exposure duration curves associated with LC for 50% mortality [LC-50], LD for 50% mortality [LD-50], ED at 50% [ED-50], etc.), or
	    c. in between acceptable and unacceptable limits.
	
	There will be six result values. These results should be output in a format that can easily be incorporated into a table.

9	When consuming information from a WCF, WEAP shall produce results reporting the Probability of Exceedence, based on the Period of Record (i.e., assumed equal to the Exposure Duration) versus Concentration: probability that concentration will be equal to or greater than a selected value. These results should be output in a format that can easily be incorporated into a table.
10	When consuming a BBF, WEAP shall produce results reporting the EHQ versus time. The EHQ is defined as the ratio of the body burden to the benchmark dose. These results should be output in a format that can easily be incorporated into a table.
11	When consuming a BBF, WEAP shall produce results reporting the Probability of Exceedence, based on the Period of Record (i.e., assumed equal to the Exposure Duration) versus EHQ: probability that an EHQ will be equal to or greater than a selected value. These results should be output in a format that can easily be incorporated into a table.
12	When consuming a BBF, WEAP shall produce results reporting the Probability of Exceedence, based on the Period of Record (i.e., assumed equal to the Exposure Duration) versus Dose or Body Burden: probability that dose/body burden will be equal to or greater than a selected value. These results should be output in a format that can easily be incorporated into a table.
13	WEAP shall operate within FRAMES using Windows-95 or a more current version of Windows.

Table 5.2. Relationship Between Test Cases and Fundamental Requirements

		Test Case Name (WEAP_xx)		
		01	**02**	**03**
R e q u i r e m e n t s	1	X		X
	2	X		
	3		X	X
	4	X		X
	5	X		
	6		X	
	7	X		
	8	X		
	9	X		
	10		X	
	11		X	
	12		X	
	13	X		

5.2 TEST CASES

5.2.1 WEAP_01

5.2.1.1 Description and Rationale

This test case addresses the capability of WEAP to compute acute and chronic exposures for the percentage of time that a time series of concentrations, doses, or burdens are below acceptable limits, above unacceptable limits, and in between acceptable and unacceptable limits. The case specifically will involve the assessment of the effect of the contaminant Fluorenthene on rotifers in a surface water body.

This test case also addresses the basic functionality of the WEAP; therefore, several of the other requirements are addressed in this case. The requirements addressed are listed below. These requirement numbers are referenced in the expected results and results sections (Note: the requirement numbers used below do not correspond to the requirement numbers listed in Table 5.1.).

5.3

1. WEAP shall operate within FRAMES using Windows-95 or a more current version of Windows.
2. WEAP shall be located under the Ecological Icon.
3. WEAP shall be capable of connecting to a Surface Water Icon which produces a WCF.
4. WEAP shall connect to an Ecological Benchmark Icon that produces an EBF.
5. WEAP shall be capable of accessing and reading a WCF, which contains a time series of water concentrations (i.e., concentration versus time), associated with the surface water icon.
6. WEAP shall be capable of accessing and reading an EBF, which contains ecological benchmark information, as described by an EBF Dictionary (EBF.DIC) file. A Dictionary file describes the parameters and the characteristics of the parameters (e.g., name, value, definition, units, etc.).
7. When consuming information from a WCF, WEAP shall produce results computing acute (i.e., #96 hr) and chronic exposures (e.g., >96 hr), for the percentage of time that a time series of concentrations, doses, or body burdens are
   a. below an acceptable limit (e.g., Chronic Limit, CCC, NOEL, NOAEL, etc.)
   b. above an unacceptable limit (e.g., exposure duration curves associated with LC for 50% mortality [LC-50], LD for 50% mortality [LD-50] , ED at 50% [ED-50], etc.), or
   c. in between acceptable and unacceptable limits.
   There will be a maximum of six result values. These results should be output in a format that can easily be incorporated into a table.
8. When consuming information from a WCF, WEAP shall produce results reporting the Probability of Exceedence, based on the Period of Record (i.e., assumed equal to the Exposure Duration) versus Concentration: probability that concentration will be equal to or greater than a selected value. These results should be output in a format that can easily be incorporated into a table.

5.2.1.2 Input Data

Contaminant Database Model (FRAMES Default Chemical Selection)

The constituent "Fluorenthene" should be selected through the contaminant-selection model.

Surface Water Model (FRAMES Known Surface Water Concentration/Flux)

The Concentration/Time sample data for Surface Water module are listed in Table 5.3.

Table 5.3. Hypothetical Time-Varying Water Concentrations

Time	Concentration
(d)	(mg/L)
0	0
10	100
12	5
30	90
40	60
45	85
50	30
60	75
70	10
80	15
90	5
95	95
100	20

Ecological Benchmark Model (ERED) (see Table 5.4)

Table 5.4. Chemical and Lifeform Aliases

Parameter	Selection	Alias in ERED
Constituent	206440	100-02-7
Lifeform Species	Brachionus calyciflorus (rotifer)	Brachionus calyciflorus

Ecological Effects Model (WEAP) (see Table 5.5)

Table 5.5. Rotifer Input Data

Time of Acute Exposure and Chronic Limit Information	
Time of Acute Exposure (d)	4
Chronic Limit Concentration (mg/L)	10
Duration of Exposure at a Specified Location	
Time (d)	**Location**
0	Location (Riv3)
100	Location (Riv3)
Toxicity Benchmark LC-50 Curve Information	
Duration of Exposure (d)	**Water-Column Concentration (mg/L)**
0	95
4	95
20	50
60	30
100	30

5.2.1.3 Expected Results

1. WEAP shall operate within FRAMES using Windows-95 or a more current version of Windows.
2. WEAP shall be located under the Ecological Icon.
3. WEAP shall be capable of connecting to a Surface Water Icon.
4. WEAP shall connect to an Ecological Benchmark Icon.
5. WEAP shall be capable of accessing and reading a WCF associated with the surface water icon.
6. WEAP shall be capable of accessing and reading an Ecological Benchmark File (EBF), which contains ecological benchmark information, as described by an EBF Dictionary (EBF.DIC) file.
7. When consuming information from a WCF, WEAP shall produce results computing acute (i.e., #96 hr) and chronic exposures (e.g., >96 hr), for the percentage of time that a time series of concentrations, doses, or body burdens are
   a. below an acceptable limit (e.g., Chronic Limit, Criterion Continuous Concentration [CCC], No Observable Effects Level [NOEL], No Observable Adverse Effects Level [NOAEL], etc.)
   b. above an unacceptable limit (e.g., exposure duration curves associated with LC for 50% mortality [LC-50], LD for 50% mortality [LD-50], ED at 50% [ED-50], etc.), or
   c. in between acceptable and unacceptable limits.

There will be a maximum of six result values. These results should be output in a format that can easily be incorporated into a table. It is expected that WEAP will compute results that match hand calculations performed. The expected results are listed in Table 5.6.

Table 5.6. Percentage of Time Associated with Regions Above, Below, and Between the LC-50 and Chronic Limit Curves, as Estimated by Hand-Calculations

Percent of Time Associated with Region (%)		
Region	**Acute (<= 96-hr Exposure Duration)**	**Chronic (> 96-hr Exposure Duration)**
>= LC-50	1	58
< LC-50 & > Chronic Limit	3	33
<= Chronic Limit	0	5

8. When consuming information from a WCF, WEAP shall produce results reporting the Probability of Exceedence, based on the Period of Record (i.e., assumed equal to the Exposure Duration) versus Concentration: probability that concentration will be equal to or greater than a selected value. These results should be output in a format that can easily be incorporated into a table. It is expected that WEAP will compute results that match hand calculations performed. The expected results are listed in Table 5.7:

Table 5.7. Predicted Probability of Equaling or Exceeding
Concentrations, Based on Exposure Durations

Concentration (g/mL)	Probability of Equaling or Exceeding a Concentration, Based on Exposure Duration (%)
0.0	100
1.0E-5	95
2.0E-5	73
3.0E-5	66
4.0E-5	57
5.0E-5	48
6.0E-5	37
7.0E-5	24
8.0E-5	11
9.0E-5	2
1.0E-4	0

5.2.1.4 Procedure

Open the Multimedia Framework (FUI.exe).[a] Select New from the File menu. Enter a file name and select Open. Enter a site name at the prompt and select Ok.

Double click on the **Contaminant** icon and it will appear on the upper left corner of the main screen. Then drag the icon to the desired location on the screen. Repeat this process to place the **Eco Benchmark** icon, **Surface Water** icon, and the **Ecological Effects** icon onto and positioned in the main screen.

Connect the Contaminant icon and Surface Water icons together. Next, connect the Surface Water icon to the Ecological Effects icon.   Also connect the Contaminants icon to the Eco benchmark icon, the Eco Benchmark icon to the Ecological Effects icon, and the Contaminants icon to the Ecological Effects icon. (Note: To connect icons, hold down the shift key, click on the first icon, and drag the mouse to the second icon. Release mouse button and shift key. A line will connect the two icons with an arrow pointing from the first icon to the second icon. To remove this line, repeat the steps used to connect it. To remove an icon from the screen, right click and a menu will appear with the different options—one option is delete; highlight that, and the icon will be taken out.

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[a] FUI = Framework User Interface

Contaminant Database Module

Right click the Contaminant icon and choose General Info. When the General Info screen opens, enter "Contaminants" in the Label text box and select "FRAMES Default Chemical Database Selection" in the "Select from applicable models" text box. Click OK at the bottom of the screen to return to the work area. The signal light attached to the contaminant icon will change from black into red. Right click on the contaminant icon in the main screen and choose User Input on the menu that appears. The Contaminant Selection screen will open. Select "All Contaminants" from the "Possible Contaminants" drop-down box. The contaminant used in this case is Flouranthene. Scroll to select Flouranthene from the contaminants list or use the Find option to search for it. Click "OK" to return to the work screen. The Contaminant icon's status light will change from red to green.

Surface Water Concentration Module

Right click on the Surface Water icon and choose General Info. In the "Select from Applicable Models" box, choose "FRAMES Know Surface Water Concentration/Flux." Click OK. The signal light will turn from black to red. Right click on the Surface Water icon and choose User Input. The "FRAMES Know Surface Water Concentration/Flux Module" screen will open. Begin to input your data. For this case, use the data shown in Section 5.2.1.2 under the Surface Water module heading. Click on File -> Save and Exit when you have completed entering your data. The main screen returns, and the light on the icon will turn yellow. Now you can right click the icon and select "Run Model."

To view results, drag a viewer icon onto the main screen. Connect the Surface Water module to the viewer icon. Right click on the viewer icon and select General Info. In this screen, name the viewer and select WCF Chart. Then click Ok. The light will turn from black into red. Right click on the chart icon again and select Run Model. The results of the model will be displayed as a Microsoft Excel Chart.

Eco Benchmark Module (ERED Database)

Right click the Eco Benchmark icon and select General Info. Choose the ERED database and click OK. The light will change to red. Right Click and choose Run Model. This model does not request user input, so the light will change from red to green. When run, the Database interface will appear. The ERED Editor module functions using an outline menu. If a + sign appears to the left of a category, it indicates that there is additional information under that category. Double click the + sign to expand a list and Double click a - sign to contract a list.

Choose an alias for the chemical in the first screen. Both chemical name and CAS Id can be used. Select the alias for the contaminant as indicated in Section 5.2.1.2 in the Ecological Benchmark Model section.

Next choose the Life Form Alias. Both scientific name and common name can be used. Click on the box to the left of the species name to select that species. Select the alias for the contaminant as indicated in Section 5.2.1.2 in the Ecological Benchmark Model section.

Click on the Data option. Click the Retrieve Data button to collect the data from the ERED database. Expand the Data option to reveal the data type options. Select ED Effect Concentration Values. Select the

combination of interest. ED Percentages: ED50, Body Part: Whole Body and Description of Effect: Mortality. 5 values will appear in the table at the bottom of the screen.

Go to the File menu, save and close the ERED editor.

WEAP Module

The Surface Water model and the Eco Dose Data model must be run before running the WEAP (the Ecological icon). In this case, both models have been run, so proceed to the Eco Dose Data model.

Right click the Ecological icon and choose General Info. The icon may be labeled using the Label text box. Select "Wildlife Ecological Assessment Program" from the "Select from Applicable Models" field and then click "Ok." A red light will now appear on the Ecological icon.

Right click the Ecological icon and choose User Input. The "Wildlife Ecological Assessment Program" window will appear.

The WEAP module functions using an outline menu. If a + sign appears to the left of a category, it indicates that there is additional information under that category. Double-click the + sign to expand a list and Double-click a - sign to contract a list. Relevant data for this case can all be entered as follows:

Click on "Rotifer." Enter the time and location data listed in Section 5.2.1.2. The location for each time should be selected from the available choices in the corresponding list box.

Double-click "Rotifer." One item (Flouranthene) will appear in the data tree. Click on Fluoranthene and fill in the data for Rotifer listed in Section 5.2.1.2 under the heading Ecological Effects Model.

Double click "Rotifer" again to close its segment of the data tree.

Once all tables are filled out, click File -> Save and Exit to close the window.

Then right click on the Ecological icon and click Run Model. This will run the model and output the results to a file. This file will have an EDF extension.

5.2.1.5 Results

1. WEAP operated within FRAMES using Windows-95.
2. WEAP model was located under the Ecological Icon within FRAMES.
3. WEAP was capable of connecting to a Surface Water Icon.
4. WEAP was capable of connecting to an Ecological Benchmark Icon.
5. WEAP was capable of accessing and reading a WCF associated with the surface water icon.
6. WEAP was capable of accessing and reading an Ecological Benchmark File (EBF), which contains ecological benchmark information, as described by an EBF Dictionary (EBF.DIC) file.
7. WEAP computed results that compared well with hand calculations. The hand calculations are estimates and are not exact, where as the WEAP calculations are exact. The WEAP results for the rotifer are listed below alongside the expected results in Table 5.8.

8. WEAP computed results that compared well with hand calculations performed. The hand calculations are estimates and are not exact, where as the WEAP calculations are exact. The WEAP results for the rotifer are listed below along side the expected results in Table 5.9.

Table 5.8. Comparison of Expected and Actual Results Between Estimated Hand Calculations and WEAP Output, for the Percentage of Time Associated with the Regions Below, Above, and Between the LC-50 and Chronic Limit Curves for Acute and Chronic Exposures

Percent of Time Associated with Region (%)				
Region	Acute (<= 96-hr Exposure Duration)		Chronic (> 96-hr Exposure Duration)	
	Estimated from Hand Calculations	WEAP	Estimated from Hand Calculations	WEAP
>= LC-50	1	0.9	58	57.8
< LC-50 & > Chronic Limit	3	3.1	33	30.7
<= Chronic Limit	0	0.0	5	7.5

Table 5.9. Comparison of Expected and Actual Results Between Estimated Hand Calculations and WEAP Output for Probability of Equaling or Exceeding a Concentration, Based on Exposure Duration

Concentration (mg/L)	Probability of Equaling or Exceeding a Concentration, Based on Exposure Duration (%)	
	Estimated from Hand Calculations	WEAP
0.0	100	100.0
1.0E-5	95	92.6
2.0E-5	73	72.1
3.0E-5	66	66.0
4.0E-5	57	56.8
5.0E-5	48	47.6
6.0E-5	37	38.4
7.0E-5	24	23.8
8.0E-5	11	11.2
9.0E-5	2	1.8
1.0E-4	0	0.0

5.2.2 WEAP_02

5.2.2.1 Description and Rationale

This test case addresses the capability of WEAP to produce results computing the Probability of Exceedence versus Concentration, Dose, or Body Burden (i.e., probability that concentration/dose/body burden will be equal to or greater than a selected value). WEAP should output these results in a format that can easily be incorporated into a table.

The case starts with contaminated water column and sediments as predicted by Recovery and transports contaminants though the surface water with Recovery to produce time-varying water-column concentration levels. These concentrations are used by the Theoretical Bioaccumulation Potential (TBP) model to produce time-varying body burdens. WEAP uses the time-varying body burdens, couples these with Toxicity Reference Value (TRV) end points (e.g., NOAEL, NOEL) to compute EHQs. Probability of Exceedence (i.e, equal to or greater than) will be calculated as it relates to body-burden levels and EHQs. This example uses Recovery, TBP, and WEAP models, with linkages to the ERED database and demonstrates the

Recovery, TBP, and WEAP models integration into FRAMES and the new Ecological icon feature. The contaminant that will be evaluated is fluoranthene, and Diporeia will be the species.

This test case also addresses several of the other basic functionality requirements of the WEAP. The requirements addressed are listed below. These requirement numbers are referenced in the expected results and results sections. (Note: the requirement numbers used below do not correspond to the requirement numbers listed in Table 5.1.)

1. WEAP shall be capable of connecting to an Eco Exposure Icon that produces an ecological Body Burden File (BBF).
2. WEAP shall be capable of accessing and reading a BBF, which contains a time series of body burden or doses containing units of mg/Kg (i.e., dose/body burden versus time).
3. When consuming a BBF, WEAP shall produce results reporting the EHQ versus time. The EHQ is defined as the ratio of the body burden to the benchmark dose. These results should be output in a format that can easily be incorporated into a table.
4. When consuming a BBF, WEAP shall produce results reporting the Probability of Exceedence, based on the Period of Record (i.e., assumed equal to the Exposure Duration) versus EHQ: probability that an EHQ will be equal to or greater than a selected value. These results should be output in a format that can easily be incorporated into a table.
5. When consuming a BBF, WEAP shall produce results reporting the Probability of Exceedence, based on the Period of Record (i.e., assumed equal to the Exposure Duration) versus Dose or Body Burden: probability that dose/body burden will be equal to or greater than a selected value. These results should be output in a format that can easily be incorporated into a table.

5.2.2.2 Input Data

Contaminant Database Model (FRAMES Default Chemical Selection)

The constituent "Fluorenthene" should be selected through the contaminant selection model.

Source Term Model (Recovery 3.0 Source - Known Contaminant) (see Table 5.10)

Table 5.10. Recovery 3.0 Source Data

Description	Units / Comments	Value
Contaminant Initial Concentration	micrograms/m^3	1.0E-06
Contaminant Inflow Concentration	micrograms/m^3	0.005
Atmospheric Contaminant External Loading	not applicable to scenario	-
Time Series Contaminant External Loading	Not Currently Supported	-
Constant Contaminant External Loading	kg/yr	50.0
X Distance to Lake	km- not applicable to scenario	-
Y Distance to Lake	km- not applicable to scenario	-

Surface Water Model (RECOVERY 3.0 Surface Water Module) (see Tables 5.11 through 5.16)

Table 5.11. RECOVERY 2.0 HK-Editor' Screen Data

Description	Units	Value
Simulation Period:	yr	100
Number of Time Steps Between Printing:		
for water Column (20 to 100)	-	50
for Sediment Profile (20 to 100)	-	50
Maximum Sediment Profile Depth for	cm	100
Enhanced Biodiffusion	cm^2/sec	2.5E-05
Enhanced Biodiffusion Depth Below the	cm	0

Table 5.12. "MORPHOMETRY AND HYDROLOGY" Screen "Water" Data

Description	Units	Value
Water Surface Area	m^2	1E+05
Water Depth	m	3
Flow Through	m^3/yr	0
Residence Time	years	.3

Table 5.13. "MORPHOMETRY AND HYDROLOGY" Screen "Deep Contaminated Sediments" Data

Description	Units	Value
L = Contaminated Sediment Depth	m	0.3
Z = Depth of Mixed Layer	cm	10
Mixed Layer Surface Area	m^2	1E+05
Initial Concentrations ($\mu g/m^3$)		
Mixed Layer	$\mu g/m^3$	1000
Deep Contaminated Sediments	$\mu g/m^3$	1000

When prompted for a Fixed or Variable concentration, choose Fixed.

Table 5.14. "SYSTEM PROPERTIES" Screen Data

Description	Units	Value
Suspended Solids Concentration in Water	g/m^3	30
Mixed Sediment Porosity	-	0.9
Deep Sediment Porosity	-	0.4
Mixed Sediment Particle Density	g/m^3	2.65E+06
Deep Sediment Particle Density	g/m^3	2.65E+06
Wind Speed	m/sec	2
Weight fraction carbon in solid - water	-	0.02
Weight fraction carbon in solid - mixed layer	-	0.05
Weight fraction carbon in solid - sediments	-	0.05
Resuspension Velocity	m/yr	0
Burial Velocity	m/yr	0.001
Settling Velocity	m/yr	0

Table 5.15. "FLUORANTHENE Properties" Screen Data (Part I)

Description	Units	Value
Molecular Diffusivity	cm2/sec	5.0E-06
Decay Coefficients for Dissolved and Particulate Contaminant Phases (1/yr)		
Dissolved Contaminant Phase:		
In Water	-	0
In Mixed Layer	-	0
In Deep Sediments	-	0
Particulate Contaminant Phase:		
In Water	-	0
In Mixed Sediments	-	0
In Deep Sediments	-	0

Table 5.16. "FLUORANTHENE Properties" Screen Data (art II)

Description	Units	Value
Henry's Constant	atm-m^3/gmole	9.31E-06
Molecular Weight	-	202.3
Octanol-Water Partition Coefficient	-	1.445E+05

In the screen that appears, select "1" to save and exit.

Eco Benchmark (ERED Database) (see Table 5.17)

Table 5.17. Chemical and Lifeform Selections and Aliases

Description	Selection	Alias in ERED
Constituent	206440	100-02-7
Species 1	Asterias rubens (starfish)	Balanus crenatus
Species 2	Oncorhynchus mykiss(trout)	Oncorhynchus mykiss

Eco Effects (Theoretical Bioaccumulation Potential) (see Table 5.18)

Table 5.18. TBP Input

Organism Selected in ERED	Comparable Organism in BSAF Database
Asterias rubens	Diporeia sp
Oncorhynchus mykiss	Hyalella azteca

Ecological (WEAP)

Ecological Dose Selections: Check the box next to "Effective Dose" (see Table 5.19).

Table 5.19. Ecological Benchmark Selections

Description	Selection
ED	ED50
Body part of Concern	Whole Body
Type of Effect	Mortality

5.2.2.3 Expected Results

1. WEAP shall be capable of connecting to an Eco Exposure Icon.
2. WEAP shall be capable of accessing and reading a BBF, which contains a time series of body burden or doses containing units of mg/Kg (i.e., dose/body burden versus time).
3. When consuming a BBF, WEAP shall produce results reporting the EHQ versus time. The EHQ is defined as the ratio of the body burden to the benchmark dose. These results should be output in a format that can easily be incorporated into a table. Hand calculations were performed for the first ED50 value (47.3 mg/kg) and are listed in Table 5.20. (Note: The spreadsheet containing the hand calculations for this test case is called "WEAP02_bbf_expResults.xls" and is included in the test bed.)

Table 5.20. Predicted EHQ Versus Time by WEAP

EHQ	Time (years)
0.0037	0.00
0.0121	5.72
0.0249	24.65
0.0284	44.32
0.0292	63.61
0.0295	82.50
0.0295	100.0

4. When consuming a BBF, WEAP shall produce results reporting the Probability of Exceedence, based on the Period of Record (i.e., assumed equal to the Exposure Duration) versus EHQ: probability that an EHQ will be equal to or greater than a selected value. These results should be output in a format that can easily be incorporated into a table. Hand calculations were performed for the first ED50 value (47.3 mg/kg) and are listed in Table 5.21.

Table 5.21. Probability of Equaling or Exceeding EHQ, as Predicted by WEAP

EHQ	Probability
0	100
0.00295	100
0.0059	98
0.00885	97
0.0118	95
0.01475	90
0.0177	86
0.02065	82
0.0236	77
0.02655	66
0.0295	0

5. When consuming a BBF, WEAP shall produce results reporting the Probability of Exceedence, based on the Period of Record (i.e., assumed equal to the Exposure Duration) versus Dose or Body Burden: probability that dose/body burden will be equal to or greater than a selected value. These results should be output in a format that can easily be incorporated into a table. Hand calculations were performed for the first ED50 value (47.3 mg/kg) and are listed in Table 5.22.

5.2.2.4 Procedure

Open the Multimedia Framework (fui.exe). Select New from the File menu. Enter a file name and select Open. Enter a site name at the prompt and select Ok.

Double click on the **Contaminant** icon and the icon will appear in the upper left corner of the main screen. Drag the icon to the desired location on the screen.   Do the same to add the following:

An **Eco Benchmarks** icon

A **Source** icon

A **Surface Water** icon

An **Eco Exposure** icon

An **Eco Effects** icon

Four **Viewer** icons

Table 5.22. Probability of Equaling or Exceeding Body Burden, as Predicted by WEAP

Body Burden (mg/kg)	Probability
0	100
0.140	100
0.279	98
0.419	97
0.559	95
0.698	90
0.838	86
0.977	82
1.117	77
1.257	66
1.396	0

Next connect the icons. To connect icons, hold down the shift key, click on the first icon, and drag the mouse to the second icon. Release mouse button and shift key. A line will connect the two icons with an arrow pointing from the first icon to the second icon. To remove this line, repeat the steps used to connect it. To remove an icon from the screen, right click and a menu will appear with the different options—one option is delete; highlight that, and the icon will be taken out.

Create the following connections:
Contaminants
–> Eco Benchmarks
Contaminants
–> Source
Contaminants
–> Surface Water
Contaminans
–> Eco Exposure
Contaminans
–> Eco Effects
Source
–> Surface Water

Source
–> Viewer #1
SurfaceWater
–> Eco Exposure
SurfaceWater
–> Viewer #2
Eco Exposure
–> Eco Effects
Eco Exposure
–> Viewer #3

Eco Effects
–> Viewer #4
Eco Benchmarks
–> Eco Exposure
Eco Benchmarks
–> Eco Effects

Each icon must be given *General Info* and *User Input* before the *Run Model* command is run. The *General Info, User Input,* and *Run Model* commands are accessed by right clicking the icon and clicking the desired command from the pop up menu. The following is a list of the data that should be entered and the procedure for this example.

Contaminants
General Info
A window titled "Object General Information" will appear.

! Under "Label," type "Chemicals."
! In the "Select from Applicable Models" box, select "FRAMES Default Chemical Database Selection." Click "OK."
! A red traffic light should appear next to the Contaminants icon.

User Input
A window titled "FRAMES Contaminant Selection" will appear.

! For this case, select "Flouranthene" as the contaminant. This can be done by searching by contaminant name or contaminant CAS ID.

! To search by name, simply type "Flouranthene" in the "Search for:" box and click "Find Next."   Keep clicking "Find Next" until "Flouranthene" appears in the selection box. Click the "Add >>>" button to add Flouranthene to the list of contaminants for use in the model.

! Searching by CAS ID is a similar process. Check "Show CAS ID" and then enter Flouranthene's CAS ID (206440) into the "Search for:" box. Click "Add >>>" to add Flouranthene to the list of contaminants for use in the model.

! Click "OK."

!   The traffic light by the Contaminants icon should turn green.

Source Term

General Info

A window titled "Object General Information" will appear.

!   Under "Label," type "Recovery."
!   In the "Select from Applicable Models" box, select "RECOVERY 3.0 Source - Known Contaminant."
!   Click "OK."
!   A red traffic light should appear next to the Source icon.

User Input

A window titled "RECOVERY 2.0 Source Term" will appear.

!   Enter the source term model data listed in Section 5.2.2.2.
!   Click "Save and Exit."
!   The traffic light by the Source icon should turn yellow.

Run Model
!   Click "Run Model." The model will run automatically in the background.
!   The traffic light by the Source icon should turn green.

Viewer #1

General Info

A window titled "Object General Information" will appear.

!   Under "Label," type "Viewer1."
!   In the "Select from Applicable Models" box, select "WCF Viewer."
!   Click "OK."
!   A red traffic light should appear next to the Viewer icon.

Run Model
A text window containing the contents of the WCF file will appear. Close the window when done viewing the results.

Surface Water

General Info

A window titled "Object General Information" will appear.

!   Under "Label," type "Surface Water"

!   In the "Select from Applicable Models" box, select "RECOVERY 3.0 Surface Water Module."

! Click "OK."

! A red traffic light should appear next to the Surface Water icon.

User Input

A window titled "RECOVERY 2.0 HK-Editor" will appear.

! Enter the data listed in Section 5.2.2.2 for the *"RECOVERY 2.0 HK-Editor"* screen.

! Click "OK." to save and exit.

! The first screen, "A Decision Support Model for Screening the Fate of In-Place Contaminated Sediments in Aquatic Environments," will now run in a disk operating system (DOS) window.

! Push any key at the title screen.

! At the second screen (titled "RECOVERY"), press Enter.

! On the "MORPHOMETRY AND HYDROLOGY" screen, type in the "Water" data listed in Section 5.2.2.2. Then Press F10 to move to the next screen.

! Enter the "Deep Contaminated Sediments" data listed in Section 5.2.2.2.

! When prompted for a Fixed or Variable concentration, choose Fixed.

! On the "SYSTEM PROPERTIES" screen, enter the data listed in Section 5.2.2.2 for this screen. Then Press F10 to move to the next screen.

! On the "FLUORANTHENE Properties" screen, enter the data listed in Section 5.2.2.2 for this screen. Then Press F10 to move to the next screen.

! A second "FLUORANTHENE Properties" screen will appear. Enter the data listed in Section 5.2.2.2 for this screen. Then Press F10 to move to the next screen.

! On the "RECOVERY" screen, select "1. Save into FRAMES.REC then exit" and press Enter. When prompted whether or not to quit, select "EXIT" and press enter.

! The traffic light by the Surface Water icon should turn yellow.

Run Model

! Click "Run Model." The model will run automatically in the background.

! The traffic light by the Surface Water icon should turn green.

Viewer #2

General Info

A window titled "Object General Information" will appear.

5.24

! Under "Label," type "Viewer2."

! In the "Select from Applicable Models" box, select "WCF Viewer."

! Click "OK."

! A red traffic light should appear next to the Viewer icon.

Run Model
A text window containing the contents of the WCF file will appear. Close the window when done viewing the results.

Eco Benchmarks

General Info
A window titled "Object General Information" will appear.

! Under "Label," type "Eco Benchmarks."

! In the "Select from Applicable Models" box, select "ERED Database."

! Click "OK."

! A red traffic light should appear next to the Eco Dose Data icon.

Run Model

! At the "Login" window, you will be prompted for a valid User Name and Password for access to the ERED database. Enter both and click "OK."

! In the tree view diagram on the left, click "Chemical Aliases." Click on the number "206440" in the lower window. Select "100-02-7" from the dropdown list under the title "Aliased CAS ID for selected chemical."

! In the tree view diagram at left, click "LifeForm Selection." A list of lifeforms in the database will appear to the right. Check "Asterias rubens" (a.k.a. Starfish,) and "Oncorhynchus mykiss" (a.k.a. Trout - Rainbow) by clicking the small box to the left of the corresponding names. It may be easier to select by common name; check "Use Common Names" at the bottom of the screen. Now all lifeforms are sorted in alphabetical order according to their common name.

! In the tree view diagram at left, click "LifeForm Aliases." A list of lifeforms selected in the previous window will appear. Click on "Asterias rubens" (a.k.a. Starfish). In the list box above entitled "Aliased Scientific name for selected liferorm," select "Balanus crenatus." Next click on "Oncorhynchus mykiss" (a.k.a. Trout - Rainbow). In the list box above entitled "Aliased Scientific name for selected liferorm" select "Oncorhynchus mykiss."

! In the tree view, click "Viewing and Editing Data." A button titled "Retrieve Data" will appear. Click it to begin retrieval of necessary information from the database.

! When all data have been retrieved, they can be viewed and edited. From the tree-view diagram, select "ED effect concentration values."

! Set the drop-down boxes to the following values:

Chemical common name:	"Flouranthene"
Lifeform scientific name...:	"Oncorhynchus mykiss"
Short description for ED percentages:	"ED50"
Body part description:	"Whole Body"
Description of effect:	"Mortality"
Number of ED values:	"5"

! The following data should appear (see Table 5.23):

Table 5.23. Effective Dose (ED) Values in ERED

Value	Units
47.3	mg/kg
47.0	mg/kg
61.2	mg/kg
190.0	mg/kg
75.0	mg/kg

! In the tree view, click "ED effect duration."
! Set the drop-down boxes to the following values:

Chemical common name:	"Flouranthene"
Lifeform scientific name...:	"Oncorhynchus mykiss"
Short description for ED percentages:	"ED50"
Body part description:	"Whole Body"
Description of effect:	"Mortality"
Number of ED values:	"5"

! The following data should appear (see Table 5.24):

Table 5.24. Duration of Exposure Corresponding to the Effective Dose (ED) Values in ERED

Value	Units
4	day
4	day
4	day
4	day
4	day

! Click File -> Save Changes and Exit.

Eco Exposure

General Info

A window titled "Object General Information" will appear.

! Under "Label," type "TBP."

! In the "Select from Applicable Models" box, select "#1 Theoretical Bioaccumulation Potential."

! Click "OK."

! A red traffic light should appear next to the Ecological #1 icon.

User Input
A window titled "Match organism" will appear.

! Select the comparable organisms as listed in Section 5.2.2.2. Then click on the "Save Settings" button to exit.

! The traffic light next to the Ecological icon should turn yellow.

Run Model

! After clicking "Run Model," the model will run automatically in the background.

! The traffic light by the Ecologica icon should turn green.

Viewer #3

General Info

5.27

A window titled "Object General Information" will appear.

! Under "Label," type "Viewer3."
! In the "Select from Applicable Models" box, select "Body Burden Viewer."
! Click "OK."
! A red traffic light should appear next to the Viewer icon.

Run Model

A text window containing the contents of the BBF file will appear. Close the window when done viewing the results.

Eco Effects

General Info

A window titled "Object General Information" will appear.

! Under "Label," type "WEAP."

! In the "Select from Applicable Models" box, select "Wildlife Ecological Assessment Program."

! Click "OK."

! A red traffic light should appear next to the Ecological #2 icon.

User Input

A window titled "Wildlife Ecological Assessment Program" will appear.

! Click File -> Save and Exit

! The traffic light next to the Ecological #2 icon should turn yellow.

Run Model

! After clicking "Run Model," the model will run automatically in the background.

! The traffic light by the Ecological #2 icon should turn green.

Viewer #4

General Info

A window titled "Object General Information" will appear.
! Under "Label," type "Viewer4."
! In the "Select from Applicable Models" box, select "Ecological Dose Viewer."
! Click "OK."
! A red traffic light should appear next to the Viewer icon.

Run Model

A text window containing the contents of the EXF file will appear. Close the window when done viewing the results.

5.2.2.5 Results

1. WEAP connected to an Eco Exposure Icon.

2. WEAP was able to access and read a BBF, which contains a time series of body burden or doses containing units of mg/Kg (i.e., dose/body burden versus time).

3. When consuming a BBF, WEAP shall produce results reporting the EHQ versus time. The EHQ is defined as the ratio of the body burden to the benchmark dose. These results should be output in a format that can easily be incorporated into a table. The results are listed in Table 5.25 along with the expected results.

Table 5.25. EHQ vs. Time Results

Hand Calculations		WEAP	
EHQ	Time (yrs)	EHQ	Time (yrs)
0.0037	0.00	0.0037	0.00
0.0121	5.72	0.0121	5.72
0.0249	24.65	0.0249	24.7
0.0284	44.32	0.0284	44.3
0.0292	63.61	0.0292	63.6
0.0295	82.50	0.0295	82.5
0.0295	100.0	0.0295	100

4. When consuming a BBF, WEAP shall produce results reporting the Probability of Exceedence, based on the Period of Record (i.e., assumed equal to the Exposure Duration) versus EHQ: probability that an EHQ will be equal to or greater than a selected value. These results should be output in a format that can easily be incorporated into a table. The results are listed in Table 5.26 along with the expected results.

Table 5.26. Probability of Equaling or Exceeding EHQ Results

Hand Calculations		WEAP	
EHQ	**Probability**	**EHQ**	**Probability**
0	100	0	100
0.00295	100	0.00295	100
0.0059	98	0.0059	98.5
0.00885	97	0.00886	96.5
0.0118	95	0.0118	94.5
0.01475	90	0.0148	90.3
0.0177	86	0.0177	85.9
0.02065	82	0.0207	81.6
0.0236	77	0.0236	77.2
0.02655	66	0.0266	65.8
0.0295	0	0.0295	0

5. When consuming a BBF, WEAP shall produce results reporting the Probability of Exceedence, based on the Period of Record (i.e., assumed equal to the Exposure Duration) versus Dose or Body Burden: probability that dose/body burden will be equal to or greater than a selected value. These results should be output in a format that can easily be incorporated into a table. The results are listed in Table 5.27 along with the expected results.

Table 5.27. Probability of Equaling or Exceeding Body Burden Results

Hand Calculations		WEAP	
EHQ	Probability	EHQ	Probability
0	100	0	100
0.140	100	0.14	100
0.279	98	0.279	98.5
0.419	97	0.419	96.5
0.559	95	0.559	94.5
0.698	90	0.698	90.3
0.838	86	0.838	85.9
0.977	82	0.977	81.6
1.117	77	1.12	77.2
1.257	66	1.26	65.8
1.396	0	1.4	0

5.2.3 WEAP_03

5.2.3.1 Description and Rationale

This test case addresses the capability of WEAP to determine if a valid conceptual site model has been developed for a modeling scenario. The FRAMES User Interface (FUI) follows a logic defined in each modules Description (DES) file to determine which module connections to allow. The WEAP module DES file should specify that it can connect with the Contaminant Database, Eco Benchmark, Surface Water, and Eco Exposure modules. This case will check that those are the only valid connections that WEAP will accept. Error message should appear when attempts to make different connections are made.

5.2.3.2 Input Data

Contaminant Database Model (FRAMES Default Chemical Selection)

The constituent "Fluorenthene" should be selected through the contaminant selection model.

Source Term Module (MEPAS Computed Source Term Module) (see Table 5.28)

Table 5.28. Input Data for MEPAS Computed Source Term Module

Parameter	Value	Units
medium type for waste zone	Soil/Vadose	none
leaching loss route	Known infiltration rate	none
overland runoff loss route	Turn off pathway	none
suspension loss route	Turn off pathway	none
volatilization loss route	Turn off pathway	none
known source/sink	Turn off pathway	none
time interval for simulation	1	years
time period for simulation	200	years
residual mass for simulation	0.01	fraction
thickness of clean overburden	0	cm
thickness	10	m
length	10	m
width	10	m
bulk density	1.5	g/cm^3
total porosity	0.25	fraction
moisture content	0.1	fraction
volumetric air content	autofilled	fraction
average air temperature	25	C
height above ground of local wind measure	10	m
equilibrium coefficient Kd	0	mL/g
Inventory	1000	g
darcy infiltration rate	2	cm/yr

Ecological Benchmark Model (ERED) (see Table 5.29)

Table 5.29. Input Data for ERED

	Selection	**Alias in ERED**
Constituent	206440	100-02-7
Species	Brachionus calyciflorus (rotifer)	Brachionus calyciflorus

Aquifer (FRAMES Known Aquifer Concentration/Flux) (see Table 5.30)

Table 5.30. Input for FRAMES Known Aquifer Concentration/Flux Module

Time	**Concentration**
yr	g/mL
0	1
1	1

5.2.3.3 Expected Results

Note that FRAMES allows the user to connect Source icon and Aquifer icon to WEAP. This is because both of these modules are capable of creating a WCF file, which is a file that WEAP can use as input. The WEAP model should be able to determine however that these models are not producing surface water results and should reject the connection and provide a message to the user specifying that valid connections have not been made (see Table 5.31).

Table 5.31. Expected Connections for WEAP

Module Type	Icon Connection Allowed by FRAMES	WEAP Connection Allowed
Contaminant	*Yes*	*Yes*
Eco Benchmarks	*Yes*	*Yes*
Air	No	No
Aquifer	Yes	No
Eco Effects	No	No
Eco Exposure	*Yes*	*Yes*
Exposure Pathways	No	No
Health Impacts	No	No
Overland Flow	No	No
Receptor Intake	No	No
Source	Yes	No
Surface Water	*Yes*	*Yes*
Vadose Zone	No	No

5.2.3.4 Procedure

Open the Multimedia Framework (fui.exe). Select New from the File menu. Enter the file name "WEAP03.GID" and select Open. Enter a site name and select Ok.

Double click on the **Contaminant** icon and the icon will appear in the upper left corner of the main screen. Drag the icon to the desired location on the screen. Do the same to add the following:

An **Eco Benchmarks** icon

An **Air** icon

An **Aquifer** icon

An **Eco Effects** icon

A **Eco Exposure** icon

A **Exposure Pathways** icon

A **Health Impacts** icon

An **Overland Flow** icon

A **Receptor** icon

A **Source** icon

A **Surface Water** icon

A **Vadose Zone** icon.

Next connect the Contaminants icon to the Eco Benchmarks icon and the Eco Effects icon (The WEAP module is an eco effects model and will be located under this icon). To connect icons, hold down the shift key, click on the first icon and drag the mouse to the second icon. Release mouse button and shift key. A line will connect the two icons with an arrow pointing from the first icon to the second icon. To remove this line, repeat the steps used to connect it. To remove an icon from the screen, right click, and a menu will appear with the different options—one option is delete; highlight that, and the icon will be taken out.

Next attempt to make the following connections:

Air	–>	Eco Effects
EcoEffects	–>	Eco Effects
Exposure Pathways	–>	Eco Effects
Health Impacts	–>	Eco Effects
Overland Flow	–>	Eco Effects
Receptor Intake	–>	Eco Effects
Vadose Zone	–>	Eco Effects

After each attempt, an error message stating that the connection is not allowed should appear on the screen.

Next attempt to make the connections listed below. After each successful attempt, use the method described previously to disconnect the module icons.

Contaminant	–>	Eco Effects
EcoBenchmarks	–>	Eco Effects
Surface Water	–>	Eco Effects
Eco Exposure	–>	Eco Effects

5.35

Source   –>   Eco Effects

Aquifer   –>   Eco Effects

The FUI should allow these connections because they could all potentially produce results that could be consumed by WEAP. The exceptions are the Source and Aquifer modules. They both produce water concentration results; however, they do not produce surface water results, which are a criterion for WEAP input. For this reason, the WEAP module will not accept them as valid connections. WEAP cannot determine this, however, until the input data have been entered for the unacceptable scenarios.

To check the Source module connection, connect the Contaminants icon to the Source icon and the Source icon to the Eco Effects icon. Enter the data from Section 5.2.3.2 for the Contaminants, Eco Benchmarks, and Source modules. Then run each module. You will need a user name and a password to fill out the ERED data. This information can be provided upon request. The signal light for each module should turn green. Then right click on the Eco Effects icon and select "User Input" to attempt to bring up the WEAP user interface. An error message should appear stating that acceptable connections have not been made.

Next check the Aquifer module connection. Disconnect the Source icon and replace it with the Aquifer icon using the same procedure used to connect the Source icon. Enter the Aquifer module data listed in Section 5.2.3.2 for the Aquifer module. Then run the Contaminants, Eco Benchmarks, and Aquifer modules. The signal light for each module should turn green. Then right click on the Eco Effects icon and select "User Input" to attempt to bring up the WEAP user interface. An error message should appear stating that acceptable connections have not been made.

Save and exit the FUI.

5.2.3.5 Results

The testing results matched the expected results listed in Section 5.2.1.3. WEAP was capable of connecting to only the specified model types, which are the contaminant database, eco benchmark, surface water, and eco exposure. Frames allowed the WEAP icon to connect to several other model icons (source and aquifer), but the WEAP model would not work with those models. Appropriate error messages were written to the screen.

6.0 QUALITY ASSURANCE PROGRAM

Updates to the FRAMES technology software system will be developed under a quality assurance program documented in Gelston et al. (1998). Quality is defined as the capability of the software to meet client needs. Meeting client needs starts with a shared understanding of how the software must perform and continues throughout the software life cycle of design, development, testing, and implementation through attention to details.

Figure 6.1 outlines the software-development process that will be used for the FRAMES technology software system highlighting the quality check points. The FRAMES technology software system activities flow down the left side of Figure 6.1 because it is software developed for the first time as opposed to a modification to existing software. The process shown is designed for compatibility with similar processes used by other government agencies. For example, this quality process compares favorably with that in U.S. Environmental Protection Agency (EPA) Directive 2182*, System Design and Development Guidance* (EPA 1997). It also compares favorably with the Office of Civilian Radioactive Waste Management's *Quality Assurance Requirements and Description, Supplement I, Software* (OCRWM 1995).   Activities roughly equivalent across these processes are shown in Table 6.1.

Development of the FRAMES technology software system includes the implementation of a quality assurance checklist (see Figure 6.2). All team members understand the component requirements and design necessary to ensure quality. Completion of this checklist verifies that all documentation will be complete for transfer of the software to client use.
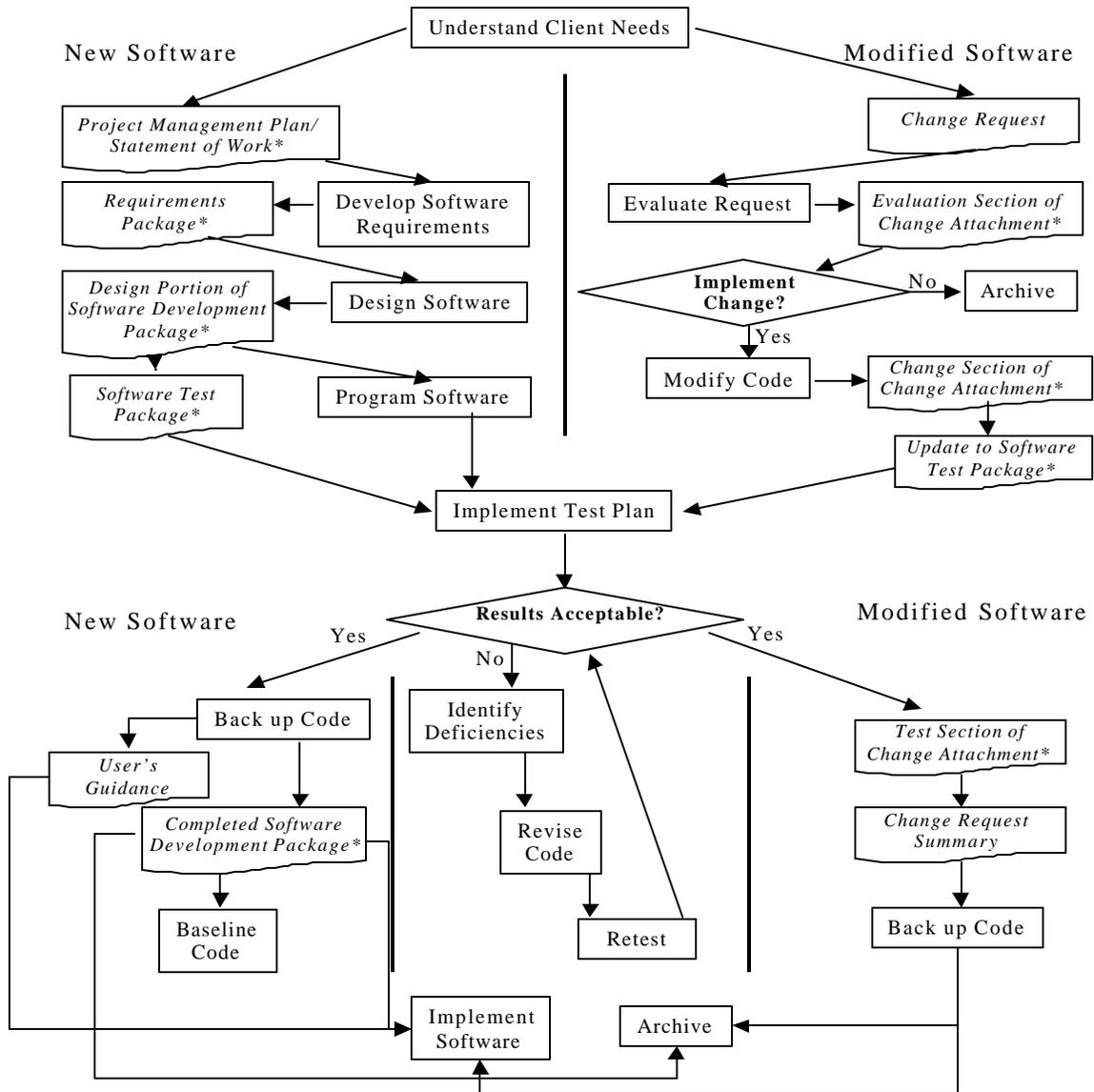
Figure 6.1. Ensuring Quality in the Environmental Software Development Process (* indicates quality review stage; box with wavy bottom line and italics font indicates a document rather than an activity)

6.2

Table 6.1. Relationship of Pacific Northwest National Laboratory (PNNL) Environmental Software Development Process to Quality Assurance Requirements (OCRWM 1995; EPA 1997)

OCRWM Quality Assurance Requirement[a]	EPA Essential Element of Information[b]	Environmental Software Process Equivalent (Section)
	4—System Implementation Plan	Project Management Plan or Statement of Work
I.2.5A Functional Requirements Information Documentation; I.2.5C Requirements and Design Documentation	5—System Detailed Requirements Document	Requirements Package
I.2.1 Software Life Cycles, Baselines (see their Appendix C), and Controls	6—Software Management Plan	Project Management Plan or Statement of Work and Gelston et al. (1998)
I.2.2 Software Verification[c] and Software Validation; I.2.4 Software Validation[d]	7—Software Test and Acceptance Plan	Software Test Package
I.2.3 Software Verification; I.2.5C Requirements and Design Information Documentation	8—Software Design Document	Design Portion of Software Development Package
I.2.6A Configuration Identification		Completed Software
I.2.6B Configuration Control; I.2.6C Configuration Status; I.2.7 Defect Reporting and Resolution[e]	9—Software Maintenance Document	Modification Documentation
	10—Software Operations Document	User's Guidance and Training
I.2.5B User Information Documentation	11—Software User's Reference Guide	User's Guidance and Training
	12—System Integration Test Reports	Software Test Package

(a) Note that OCRWM requirement I.2.8, Control of the Use of Software, is the responsibility of the OCRWM-related client.

(b) Elements 1 through 3 are generally completed by clients in the U.S. Environmental Protection Agency before contract initiation with the project team.

(c) Verification includes informal code testing by software engineers to ensure that code functions as required.

(d) Validation includes testing by those other than the software engineers who developed the code to provide an independent confirmation that software functions as required.

(e) Note that some changes requested by clients may not be made in the software unless funding has been allocated for such modifications.

```
A.  General Requirements Analysis
          --Documented in
          _____Statement of Work
          --Contains information on (all of the following)
          _____problem description
          _____deliverables
          _____project team
          _____capabilities to be used
          _____restrictions
          _____difficulties envisioned
          _____compatibilities with existing software/hardware
          _____scope of the project
B.  Specific Requirements Analysis
          --Documented in
          _____requirements section of documentation.
          --Contains information on (all of the following)
          _____purpose of the software
          _____structure of the software
          _____hardware and software requirements
          _____input and output requirements
          _____scientific basis
          _____assumptions
          _____limitations
C.  Design Documentation
          --Documented in
          _____design portion of documentation.
          _____team task plans/Project Management Plan
          --Contains information on (all of the following)
          _____code type and description
          _____development team members
          _____specifications
          _____logic diagrams
          _____"help" descriptions
          _____methods to ensure consistency in components
          _____mathematical formulations
          _____need for pre/post-processors
D.  Development Documentation
          --Documented in
          _____Specifications Document
          _____Quality Assurance Archive
          --Contains information on (all of the following)
          _____baseline hard copy of the source code
          _____diskette copy
          _____name of computer language(s) used
E.  Testing Documentation
          --Documented in
          _____test plan that meets quality assurance requirements
          --Contains information on (all of the following)
          _____description of software
          _____testing scope
```

Figure 6.2. Quality Assurance Implementation Checklist for the FRAMES Technology Software System

F. User's Guidance
      --Documented in
      _____hardcopy printout of user's guidance for system
      --Contains information on (all of the following)
      _____description of software
      _____description of use of user interface
      _____mathematical formulations
      _____example problems
      _____explanation of modules included

G. General Quality Assurance Documentation
      --Documented in
      _____Quality Assurance Program Document
      _____Quality Assurance Software-Specific Checklist
      --Contains information on (all of the following)
      _____purpose of quality assurance program
      _____client-specified activities
      _____activities required to ensure quality in software

H. Quality Assurance Archive
      --Documented in
      _____hard-copy files
      _____back up disk files in multiple storage locations
      --Contains information on (all of the following)
      _____all quality assurance documentation
      _____client correspondence regarding software
      _____modifications made to baselined software
      _____disk copy back ups
      _____reproducibility of code (check code for comments)

Completed by _____   Date _____

Approved by
System/Module Manager _____   Date _____

Figure 6.2. Quality Assurance Implementation Checklist for FRAMES Technology Software System
(contd)

7.0 REFERENCES

Gelston, G. M., R. E. Lundgren, J. P. McDonald, and B. L. Hoopes. 1998. *An Approach to Ensuring Quality in Environmental Software*, PNNL-11880, Pacific Northwest National Laboratory, Richland, Washington.

Office of Civilian Radioactive Waste Management (OCRWM). 1995. *Quality Assurance Requirements and Description, Supplement I, Software*, U.S. Department of Energy, Washington, D.C.

U.S. Environmental Protection Agency (EPA). 1997. *System Design and Development Guidance*, EPA Directive Number 2182, Washington, D.C.

Whelan, G., K.J. Castleton, J.W. Buck, G.M. Gelston, B.L. Hoopes, M.A. Pelton, D.L. Strenge, and R.N. Kickert. 1997. *Concepts of a Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES),* PNNL-11748, Pacific Northwest National Laboratory, Richland, Washington.

Appendix A

Body Burden File (BBF)

Appendix A: Body Burden File (BBF)

This file format is given in psuedo code format. The file contains body burden information for different life-form over time. All body burdens are given in mg/kg for chemicals, pCi/kg for radionuclides. The file is not considered to be a FRAMES system files.

For each 'Module' a line with:

  Module Name -(string)

  Number of Lines that follow for this module's section

  A line with:

    Number of Header Lines -(integer)

  For each 'Header Line' a line with:

    Header line information -(string)

  Next 'Header Line'

  A line with:

    Number of Data Sets -(integer)

  For each 'Data Set' a line with:

    Data Set name -(string)

      ; "All" / "eco#"

      ; where 'eco' is the module type and '#' is the id number

    Usage Location Type -(string)

     ; "All" / "Eco Concentrations" / "Exposure Pathways" / any glyph type...

    Number of Species -(integer)

    For each 'Specie' a line with:

      Species Name -(string)

      Number of Constituents -(integer)

      For each 'Constituent' a line with:

        Constituent Name -(string)

        Constituent ID -(string)

        Time units -(string) - "yr"

Concentration units -(string) - "mg/kg"

Number of Time concentrations pairs -(integer)

Number of progeny -(integer)

For each 'Time Concentration Pair' a line with:

  Time -(float)

  Concentration -(float)

Next 'Time-Concentration Pair'

For each 'Progeny' a line with:

  Progeny Name -(string)

  Progeny ID -(string)

  Time units -(string) - "yr"

  Concentration units -(string) - "mg/kg"

  Number of Time Concentrations Pairs -(integer)

  Parent Name -(string)

  Parent ID -(string)

  For each 'Time Concentration Pair' a line with:

    Time -(float)

    Concentration -(float)

  Next 'Time-Concentration Pair'

Next 'Progeny'

Next 'Constituent'

Next 'Species'

Next 'Data Set'

Next 'Module'

A.2

Appendix B

Ecological Benchmark File (EBF)

Appendix B: Ecological Benchmark File (EBF)

B.1 Ecological Benchmark Dictionary File (EBF.DIC)

51,EcoBenchMarks

Code,Dimensions,DataType,Min,Max,Units,Description,Key1,Key2,Key3,Key4,Key5,Key6

NumLifeForm,0,INTEGER,0,0,,"Number of life-forms"

LifeFormSci,1,STRING,0,80,,"Life-form scientific name (Genus species)",NumLifeForm

LifeformName,1,STRING,0,80,,"Life-form common name",NumLifeForm

akaLifeFormSci,1,STRING,0,80,,"Life-form scientific name (Genus species)",NumLifeForm

akaLifeFormName,1,STRING,0,80,,"Life-form common name",NumLifeForm

NumChems,0,INTEGER,0,,,"Number of chemicals",,

ChemID,1,STRING,0,20,,"Chemical CAS ID",NumChems

ChemName,1,STRING,0,80,,"Chemical common name",NumChems

NumLCDescript,0,INTEGER,0,,,"Number of LC descriptions"

LCDescript,1,STRING,0,80,,"Short description for LC percentages",NumLCDescript

NumLDDescript,0,INTEGER,0,,,"Number of LD descriptions"

LDDescript,1,STRING,0,80,,"Short description for LD percentages",NumLDDescript

NumECDescript,0,INTEGER,0,,,"Number of EC descriptions"

ECDescript,1,STRING,0,80,,"Short description for EC percentages",NumECDescript

NumEDDescript,0,INTEGER,0,,,"Number of ED descriptions"

EDDescript,1,STRING,0,80,,"Short description for ED percentages",NumEDDescript

NumBodypart,0,INTEGER,0,,,"Number of body part descriptions"

Bodypart,1,STRING,0,80,,"Body part description",NumBodyPart

NumEffect,0,INTEGER,0,,,"Number of effect types descriptions"

Effect,1,STRING,0,80,,"Description of effect",NumEffect

NumLCChem,3,INTEGER,0,,,"Number of LC values",ChemID,LifeFormSci,LCDescript

LCChemCom,4,STRING,0,100,,"Comment on conditions of measurement for LC values",ChemID,LifeFormSci,LCDescript,NumLCChem

LCChem,4,FLOAT,0,,"mg/kg","LC effect concentration values",ChemID,LifeFormSci,LCDescript,NumLCChem

LCChemDur,4,FLOAT,0,,"day","LC effect duration",ChemID,LifeFormSci,LCDescript,NumLCChem

NumLDChem,3,INTEGER,0,,,"Number of LD values",ChemID,LifeFormSci,LDDescript

LDChemCom,4,STRING,0,100,,"Comment on conditions of measuement for LD values",ChemID,LifeFormSci,LDDescript,NumLDChem

LDChem,4,FLOAT,0,,"mg/kg","LD effect concentration value",ChemID,LifeFormSci,LDDescript,NumLDChem

LDChemDur,4,FLOAT,0,,"day","LD effect duration",ChemID,LifeFormSci,LDDescript,NumLDChem

NumECChem,5,INTEGER,0,,,"Number of EC values",ChemID,LifeFormSci,ECDescript,Bodypart,Effect

ECChemCom,6,STRING,0,100,,"Comment on conditions of measuement for EC values",ChemID,LifeFormSci,ECDescript,Bodypart,Effect,NumECChem

ECChem,6,FLOAT,0,,"mg/kg","EC effect concentration values",ChemID,LifeFormSci,ECDescript,Bodypart,Effect,NumECChem

ECChemDur,6,FLOAT,0,,"day","EC effect duration",ChemID,LifeFormSci,ECDescript,Bodypart,Effect,NumECChem

NumEDChem,5,INTEGER,0,,,"Number of ED values",ChemID,LifeFormSci,EDDescript,Bodypart,Effect

EDChemCom,6,STRING,0,100,,"Comment on conditions of measuement for ED values",ChemID,LifeFormSci,EDDescript,Bodypart,Effect,NumEDChem

EDChem,6,FLOAT,0,,"mg/kg","ED effect concentration values",ChemID,LifeFormSci,EDDescript,Bodypart,Effect,NumEDChem

EDChemDur,6,FLOAT,0,,"day","ED effect duration",ChemID,LifeFormSci,EDDescript,Bodypart,Effect,NumEDChem

LOELChemCom,4,STRING,0,100,,"Comment on conditions of measuement for LOEL values",ChemID,LifeFormSci,Bodypart,Effect

LOELChem,4,FLOAT,0,,"mg/kg","Lowest concentration to cause an effect",ChemID,LifeFormSci,Bodypart,Effect

LOELChemDur,4,FLOAT,0,,"mg/kg","Duration for lowest concentration to cause an effect",ChemID,LifeFormSci,Bodypart,Effect

NOELChemCom,2,STRING,0,100,,"Comment on conditions of measuement for NOEL values",ChemID,LifeFormSci

NOELChem,2,FLOAT,0,,"mg/kg","Highest concentration not to cause an effect",ChemID,LifeFormSci

NOELChemDur,2,FLOAT,0,,"mg/kg","Duration for highest concentration not to cause an effect",ChemID,LifeFormSci

~Table,2,LifeFormSci,LifeFormName

~Table,2,ChemID,ChemName

~Table,3,LCChem,LCChemDur,LCChemCom

~Table,3,LDChem,LDChemDur,LDChemCom

~Table,3,ECChem,ECChemDur,ECChemCom

~Table,3,EDChem,EDChemDur,EDChemCom

~Table,3,NOELChem,NOELChemDur,NOELChemCom

~Table,3,LOELChem,NOELChemDur,LOELChemCom

B.2 Ecological Benchmarks File (EBF)

This file is stored as a section in the FRAMES GID file. The section name is EBF# where # is the identifying number. The specification for the EBF section is:

For each Parameter

Line with:

  Parameter Name (string)

  Index 1 (integer)

  Index 2 (integer)

  Index 3 (integer)

  Index 4 (integer)

  Index 5 (integer)

  Index 6 (integer)

  Reference (integer)

  User Units (string)

  Units (string)

  Value (string),(integer), or (float)

Example Lines

NumLifeform,0,0,0,0,0,0,0,,,1

LifeFormSci,1,0,0,0,0,0,0,,,"Brachionus calyciflorus"

LifeFormName,1,0,0,0,0,0,0,,,"Rotifer"

akaLifeFormSci,1,0,0,0,0,0,0,,,"Brachionus calyciflorus"

akaLifeFormName,1,0,0,0,0,0,0,,,"Rotifer"

NumChems,0,0,0,0,0,0,0,,,1

ChemID,1,0,0,0,0,0,0,,,"71432"

ChemName,1,0,0,0,0,0,0,,,"Benzene"

NumLCDescript,0,0,0,0,0,0,0,,,2

LCDescript,1,0,0,0,0,0,0,,,"LC50"

LCDescript,2,0,0,0,0,0,0,,,"LC80"

All values are stored as text; this allows each module to use its own storage format (Big-Endian, Little-Endian, 32 bit real, 64 bit real ...). The number of digits of precision should be set by the model developer when floating point numbers are being written.