PNNL-13409

FRAMES User Define Exposure Pathway File Module Documentation

M. A. Pelton
G. M. Gelston
M.A. Eslinger

December 2000

Prepared for the
U.S. Army Research and Development Center
Waterways Experiment Station
U.S. Army Corps of Engineers
3909 Halls Ferry Road
Vicksburg, Mississippi 39180
under Contract DE-AC06-76RL01830

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Richland, Washington 99352

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1.0 Introduction

The Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) User Defined Exposure Pathway File (EPF) module provides concentrations of each pollutant in each exposure medium defined for specific exposure pathways and intake routes. This report contains the requirements for this file and will be used by software engineers and testers to ensure that the file inputs properly. A test plan will be developed from this document. Test cases will be developed from the test plan to ensure that the product meets the needs of the client(s) and to establish a baseline version of the file.

1.1 Objective

The purpose of the FRAMES user-defined EPF module is to allow the user to input user-defined concentration of each pollutant in each exposure medium for specific exposure pathways and intake routes to generate the appropriate FRAMES data files to be used by receptor intake modules. The EPF file contains sets of data for each exposure module included in the current case. The constituent concentrations are time varying, and the user must define the time steps required.

1.2 Definitions

- Requirement: Characteristics and behaviors that a piece of software must possess to function adequately for its intended purpose. A good requirement is also testable. Sometimes a function is called a requirement, although it is not related to a regulatory definition.
- 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 that would make proper use to the subroutines.
- Model/Code: Loosely defined here 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. This section provides an overall summary of the requirements for the FRAMES EPF. Detailed requirements are described in the sections that follow.

2.1 Summary of Requirements for the FRAMES User Defined EPF Module

The FRAMES User Defined EPF Module will:

1) Allow user to input different exposure pathways.
2) Allow user to input different intake routes.
3) Allow unlimited constituents, progeny, and concentrations.
4) Operate under Windows 95 and have a user-friendly interface with a standard windows look and feel.
5) Produce EPF following the FRAMES data file specifications.

2.2 Input Requirements for the FRAMES

The user will enter the input data required for the FRAMES User-Defined Exposure Pathway Module via the Module User Interface (MUI). The MUI will allow the user to define the exposure pathways and associated data. The three main inputs to the FRAMES User-Defined Exposure Pathway Module MUI are 1) different exposure locations in exposure time periods in each exposure medium, 2) average contaminant concentrations, and 3) average contaminant concentrations for each time period, location, and exposure pathway and route.

There are some general requirements associated with the MUI, which are:

1) The MUI will operate in Windows 95 and will have a standard Windows look and feel.
2) For all input parameters having dimensions associated with them, the MUI will provide users with a choice of units.
3) The MUI will include a reference feature in which the source of the specified value for each input item or set of items can be referenced if the user desires.

The MUI for the FRAMES exposure pathway module must allow the user to input all the required data to execute the module. This includes allowing the user to enter data for:

1) User-defined, time-varying, average contaminant concentrations for different exposure pathways and routes at different locations from different transport media.

Based on the media connected, the exposure module has it own data requirements as follows:

The data requirements for the **EPF** category are:

1) Location (x,y)

2) Data set type (acute or chronic)
3) Number of Time Periods
4) Exposure Start Time
5) Exposure Duration
6) Types of Exposure Pathway (air, ground, leafy vegetable, fruit, etc.)
7) Exposure Intake Route (Ingestion, Inhalation, Dermal, External)
8) Exposure Concentration

2.3 Output Requirements

The FRAMES Exposure Pathway Module is required to output user-defined, time-varying, average contaminant concentrations for different exposure pathways and routes at different locations from different transport media. These outputs must meet the specifications of FRAMES (Whelan et al. 1997).

2.4 Scientific Requirements

The FRAMES EPF does not conduct computations that change the values input by the user except to convert units to internal FRAMES units. This is done by the MUI. No other scientific requirements exist for this Module.

2.5 Recommendations

1) The MUI will have online help in an HTML format that provides users with an easy-to-understand description of all input parameters required by the MUI, as well as an About tab to inform the user of the module title, version number, and brief description.

2) The MUI will show the range of values allowed for each input data item, when the cursor is positioned on that item, as a message at the bottom of the screen will appear. When an out-of-range value is entered in a field, the MUI will indicate this by a red background in the input field and an error message in addition to the allowed range message. Data input values within range are shown with a green field background.

3.0 Specifications

The EPF is the input to the Intake Component, which produces estimates of pollutant intakes. The output from the Exposure Pathways component is the concentration of each pollutant for a given route and pathway. The input to the Intake Component is provided in the Primary Data Communication File, "runname".EPF.

The following outline is a description of the basic information important to the EPF. An example EPF file is included after the outline. Comparing the line-by-line description in the outline to the example should clarify and help locate data contained in the EPF file. Lines beginning with ';' are descriptive comments only and will not appear in the actual EPF file.

```
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 type -(string)
      ;"acute" / "chronic"
    Data Set name -(string)
    Exposure Medium Type -(string)
      ;Input Models Qualified type
      ;"Air" / "Aquifer" / "Surface water" / ...
    Number of Exposure Media Points -(integer)
    Number of Constituents -(integer)
    For each 'Exposure Media Point' a line with:
      X coordinate -(float)
      X coordinate unit -(string) - "km"
      Y coordinate -(float)
      Y coordinate unit -(string) - "km"
    Next 'Exposure Media Point'
    For each 'Constituent' a line with:
      Constituent Name -(string)
      Constituent ID -(string)
      Number of Progeny -(integer)
      Number of Exposure Start Times -(integer)
      For each 'Exposure Start Time' a line with:
        Exposure Start Time -(float)
        Exposure Start Time unit -(string) - "yr"
        Exposure Duration -(float)
        Exposure Duration unit -(string) - "yr"
```

```
      Number of Exposure Pathways -(integer)
      For each 'Exposure Pathway' line with:
        Exposure Pathway Name -(string)
          ;"Air" / "Indoor air" / "Ground" / "Leafy vegetables" /
          ;"Root vegetables" / "Fruit" / "Grain" / "Beef" /
          ;"Poultry" / "Milk" / "Eggs" / "Soil" / "Swimming" /
          ;"Boating" / "Shoreline" / "Water" / "Fish" / "Mollusks" /
          ;"Crustacea" / "Aquatic plants" / "Showering" / ...
        Exposure Route -(string)
          ;"Ingestion" / "Inhalation" / "Dermal" / "External"
        Exposure Concentration unit -(string)
          ;"Bq/kg" / "Bq/l" / "Bq/m3"   for radionuclides
          ;"mg/kg" / "mg/l" / "mg/m3"   for non-radionuclides
          ;"Sv"                        for external routes
        A line with:
          Exposure Concentration -(set of float)
            ;a concentration for each 'Exposure Media Point'
      Next 'Exposure Pathway'
      For each 'Progeny' a line with:
        Progeny Name -(string)
        Progeny ID -(string)
        Number of Exposure Pathways -(integer)
        For each 'Exposure Pathway' line with:
          Exposure Pathway Name -(string)
            ;"Air" / "Indoor air" / "Ground" / "Leafy vegetables" /
            ;"Root vegetables" / "Fruit" / "Grain" / "Beef" /
            ;"Poultry" / "Milk" / "Eggs" / "Soil" / "Swimming" /
            ;"Boating" / "Shoreline" / "Water" / "Fish" / "Mollusks" /
            ;"Crustacea" / "Aquatic plants" / "Showering" / ...
          Exposure Route -(string)
            ;"Ingestion" / "Inhalation" / "Dermal" / "External"
          Exposure Concentration unit -(string)
            ;"Bq/kg" / "Bq/l" / "Bq/m3"   for radionuclides
            ;"mg/kg" / "mg/l" / "mg/m3"   for non-radionuclides
            ;"Sv"                        for external routes
          A line with:
            Exposure Concentration -(set of float)
              ;a concentration for each 'Exposure Media Point'
        Next 'Exposure Pathway'
      Next 'Progeny'
    Next 'Exposure Start Time'
  Next 'Constituent'
Next 'Data Set'
Next 'Module'
```

4.0 Test Plan Approach and Internal Testing Results

This paper presents a test plan and the baseline testing results for the FRAMES EPF. FRAMES is a platform that allows for the linking of various multimedia modules into complete transport/exposure assessment systems (Whelan et al., 1997). The purpose of the FRAMES EPF is to allow the user to input user-defined concentrations of each pollutant from an exposure medium for specific exposure pathways and intake routes to generate the appropriate FRAMES data files to be used by receptor intake modules. The EPF contains sets of data for each exposure module included in the current case. The constituent concentrations are time varying, and the user must define the time steps required. Both radionuclides and chemicals can be input into this module. FRAMES is a platform that allows for the linking of various multimedia modules into complete transport/exposure assessment systems (Whelan et al., 1997).

The EPF module is being baseline tested for FRAMES version 1.2. The suite of test cases developed for this testing, and presented in this paper, will also be used for assessing the effects of future code modifications. Each time a modification is made to the program code, these test cases are rerun, and their results are compared to the previous run (regression testing). Changes in the results are evaluated to determine if they were expected due to the modification and are an acceptable change, or if they are an unintended side effect. In the latter case, the program code can be changed and the testing performed again.

4.1 Testable Requirements

Requirements for the EPF are described in the paper entitled, Section 1.0, of this document. These requirements have been reworded into the following list (Table 4.1) of concise, fundamental requirements suitable for testing.

Table 4.1. Testing Requirements for the Exposure Pathway File

Requirement Number	General MUI Requirements
1	The MUI will operate in Windows 95 and have a user-friendly interface with a standard Windows look and feel.
2	Each module will contain an About tab to inform the user of the module title, version number, and brief description.
3	For all input parameters having dimensions associated with them, the MUI will provide users with a choice of units.
4	The MUI will include a reference feature in which the source of the specified value for each input item or set of items can be referenced if the user desires.
5	The MUI must allow the user to input all the required data to execute the module, including user-defined, time-varying, contaminant concentration by location from different transport media by different exposure pathways and routes.

6	Allow unlimited constituents, progeny, and concentrations.
7	Produce EPF following the FRAMES data-file specifications.
8	Allow user to input different exposure pathways.
9	Allow user to input different intake routes.
10	The appropriate tabs and media release rate type should appear in the MUI based on the modules connected.

	Scientific Requirements
11	**The EPF does not conduct computations that change the values input by the user except to convert units to internal FRAMES units. This is done by the MUI.**

4.2 Test Cases and Baseline Testing Results

This section describes the specific test cases used for baseline testing of the FRAMES User-Defined EPF Module. Table 4.2 shows which requirements were the focus of each test case. There are no test cases for Requirement 6. This is because the EPF allows unlimited constituents, progeny, and concentrations and is only limited by the memory of the user's machine. None of the test cases are designed to test the recommendations. Appendix A describes the general procedure for conducting the tests.

Table 4.2. Relationship Between Test Cases and Requirements for the Exposure Pathway File Module

Requirement\Test Case	**EPF01**	**EPF02**
1	X	
2	X	
3	X	
4	X	
5	X	
6		
7	X	
8	X	
9		X
10	X	
11		X

4.2.1 EPF01

4.2.1.1 Description and Rationale

The purpose of this section is to test the user-defined EPF module to ensure that it correctly requests and transfers all necessary data to complete the EPF. This test case is intended to check if the MUI allows

the following: location of each media point (x,y), data-set type (acute or chronic), number of time periods, start time, duration of time period, types of exposure pathway (air, ground, leafy vegetable, fruit, etc.), exposure concentration, and exposure intake route (ingestion, inhalation, dermal, external). Also, error checking of the user input concentration data will be evaluated.

4.2.1.2 Input Data

Build a case using Appendix A. Save the file as EPFtest1.gid. Select chromium III, and strontium-90 from the list of contaminants.

Soil as the Exposure Pathways.

Soil/chronic

0 mi	234
7	894

Chromium III

Time	**Duration**
0 yr	2 yr
5	2
10	2

Ingestion (Meet) mg/kg

yr	mg/kg
0	4.398E-1
5	2.9E-3
10	1.99E-5

*Dermal (Soil)*mg/kg

0	127.4
5	8.586E-1
10	5.785 E-3

Strontium-90

Time	**Duration**
5 yr	1 yr
25	1
50	1

Dermal (soil)

yr	Sv
5	0.02
25	1.23E-4
50	21

Ingestion (soil)

yr	Bq/kg
5	0.02
25	1.23E-4
50	7.3E-7

4.2.1.3 Expected Results

The expected results for this test case will be that it creates an EPF in accordance with the FRAMES specifications. It is expected that the MUI will be easy to use and have a functionality consistent with standard Windows software. It is expected that the MUI will request only the required information.

It is expected that the transfer of data from the MUI to the EPF will occur properly and that any necessary unit conversions will be done correctly. The transfer of data between files can be confirmed by visual inspection of these files (EPFtest1.epf). It is expected that the MUI will not continue until all data have been entered completely and within the correct specifications. If data entered are incorrect or incomplete, an error message should appear.

4.2.1.4 Testing Results

All requirements were met.

4.2.2 EPF02

4.2.2.1 Description and Rationale

The purpose of this section is to test the user-defined EPF module to ensure that it correctly requests and transfers all necessary data to complete the EPF. This test case is intended to check if the MUI allows the following: location of each media point (x,y), data-set type (acute or chronic), number of time periods, start time, duration of time period, types of exposure pathway (air, ground, leafy vegetable, fruit, etc.,), exposure concentration, and exposure intake route (ingestion, inhalation, dermal, external). Also, error checking of the user-input concentration data will be evaluated.

4.2.2.2 Input Data

Build a case using Appendix A. Save the file as EPFtest2.gid. Select antimony, antimony-125, benzene, and strontium-90 from the list of contaminants.

Choose Air and Soil as the Exposure Pathways.

For Air/ Chronic

X	**Y**
0 m	10
10	40
100	90

Antimony

Time	**Duration**
0 yr	20 day
50	40

100	60

Inhalation (indoor air) mg/l

1	2	3
5	6	7
9	10	111

Dermal (showering) Sv

5	10	20
40	50	60

External (soil)

2
4
6

Choose inhalation (showering), dermal (swimming) and ingestion (beef) with no data entered.

Antimony-125

Time	**Duration**
0 yr	50 yr
80	10
90	120

Ingestion (aquatic plants) Bq/kg

5	10
6	7
8	9

Ingestion (beef) Bq/kg

1	2	3
4	5	6
7	8	9

Tellurium-125
Inhalation (indoor air) Bq/L

60	78	51

Soil/Acute

0 mi	234
7	894

Benzene

Time	**Duration**
0 yr	50 yr

80	10
90	120

Ingestion (beef)

1	2
3	4
5	6

Antimony

Time	**Duration**
0 hr	1 hr
10	

Ingestion (beef)

2	5
4	6

Strontium-90

time	duration
5 yr	3 day
25	2
41	8

Dermal (soil)

6	8
4	10
465	21

Yttrium-90
Ingestion (Crustacean)

4	5
87	47
1	2

4.2.2.3 Expected Results

The expected results for this test case will be that it creates an EPF in accordance with the FRAMES specifications. It is expected that the MUI will be easy to use and have a functionality consistent with standard Windows software. It is expected that the MUI will request only the required information.

It is expected that the transfer of data from the MUI to the EPF will occur properly and that any necessary unit conversions will be done correctly. The transfer of data between files can be confirmed by visual inspection of these files (EPFtest1.epf). It is expected that the MUI will not continue until all

data have been entered completely and within the correct specifications. If data entered are incorrect or incomplete, an error message should appear.

4.2.2.4 Testing Results

All requirements were met.

5.0 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 5.1 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 5.1 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 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 5.1.

Development of the FRAMES technology software system includes the implementation of a quality assurance checklist (see Figure 5.2). 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.

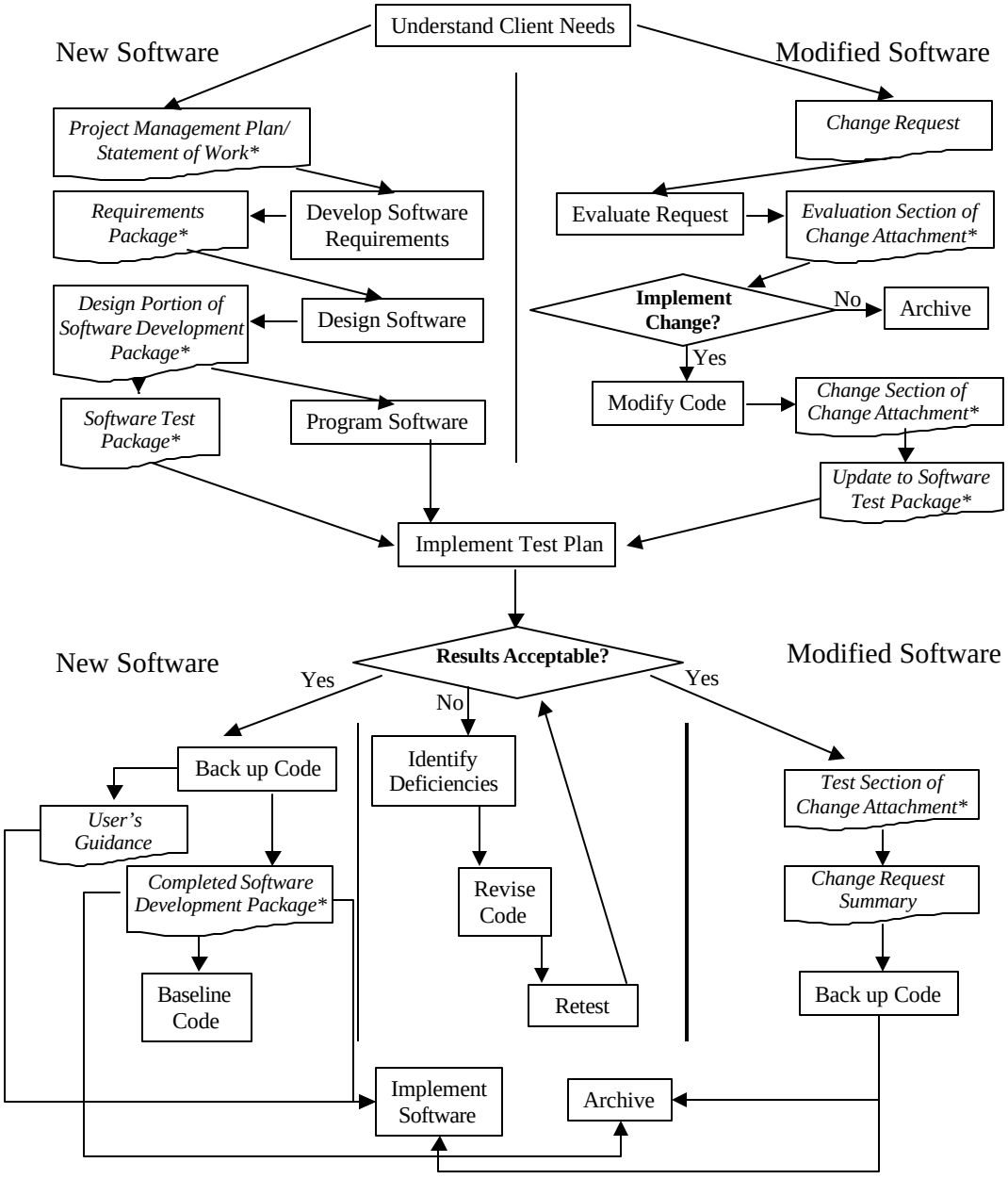

Figure 5.1. Ensuring Quality in the Environmental Software Development Process

Table 5.1. Relationship of 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

_____relationship between test cases and requirements

_____test activity description

Figure 5.2. Quality Assurance Implementation Checklist for 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

Figure 5.2. Quality Assurance Implementation Checklist for FRAMES Technology Software System (contd)

6.0 References

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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

General Procedure for Test Case Implementation

Appendix A: General Procedure for Test Case Implementation

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 exposure module icon. The icons will appear on the main screen. Left click and drag to the desired locations. Connect the contaminant icon to the exposure module. To do this, hold down the shift key, click on the exposure icon, and drag the mouse to the viewer icon. Release mouse button and shift key. A line will connect the two icons with an arrow pointing from the contaminant icon to the exposure icon. To remove this line, repeat the steps used to connect it. To remove an icon from the screen, right click and choose delete from the menu. An icon can have more than one connection.

Right click on the contaminant icon and choose General Info. When the General Info screen opens, select Label: Contaminants and Module: FRAMES Default Chemical Database Selection. Click on OK at the bottom of the screen; this returns you to the work area, and the signal light attached to the contaminant icon changes from black into red. Right click on the contaminant icon in the main screen and choose User Input on the menu that appears and the Contaminant Selection screen will open. Select from Possible Contaminants: All Contaminants. Scroll to select the contaminants or use the Find option on this screen. Click OK to return to the work screen. The light will change from red into green.

Right click on the exposure module you placed on the main screen and choose General Info. Select the applicable model and click OK. The signal light will turn from black into red.

Right click on the exposure module and choose User Input, and the FRAMES Known User Input screen will open.

Fill in all the required information in the menu by following instructions and clicking on each box that looks like this (☒) to expand the menu and then click save and exit; the light will turn from red into yellow.

Right click on the exposure module and choose Run Model. The model will run, and the light will change from Yellow into Green. To view results, Right-click and choose the "view/print module results" menu. Select the desired viewer from the menu.