

FRAMES User Defined Water Concentration File Module

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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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1.0 Introduction

The Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) Water Concentration File (WCF) contains time-varying, instantaneous, aqueous phase, constituent concentrations for water media (i.e., vadose zone, aquifer, and surface water). 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 WCF is to allow the user to input user-defined contaminant concentration in water to generate the appropriate FRAMES data files to be used by fate and transport and exposure modules. Both radionuclides and chemicals can be input into this module. These constituent concentrations are used to describe the amount of contaminant present in the aqueous media and passed into the exposure pathways. 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, which would make proper use of 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 phenomenon 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 WCF. Detailed requirements are described in the sections that follow.

2.1 Summary of Requirements

This section provides an overall summary of the requirements for the FRAMES WCF. Detailed requirements are described in the sections that follow.

The FRAMES WCF will:

- 1) Allow user to input time varying, instantaneous, aqueous phase, and constituent concentrations for water media (i.e., vadose zone, aquifer, and surface water).
- 2) Allow unlimited constituents, progeny, concentrations, or media.
- 3) Operate under Windows 95 and have a user-friendly interface with a standard windows look and feel.
- 4) For all input parameters having dimensions associated with them, the MUI will provide users with a choice of units.
- 5) Produce WCF following the FRAMES data-file specifications

2.2 Input Requirements

The user will enter the input data required for the FRAMES User-Defined Source Release Module via the Module User Interface (MUI). The MUI will allow the user to define the source problem and associated data. The three main inputs to the FRAMES User-Defined Source Release Module MUI are 1) the medium type of source being modeled, 2) time-varying, contaminant concentrations, and 3) time-varying, media release rates. The media-release-rate types depend on which modules are connected to this source module. If a vadose or aquifer module is connected, water fluxes will be required; if an overland or surface water module is connected, sediment fluxes will be required. The appropriate tabs should appear in the MUI based on the modules connected.

The following general requirements are associated with the MUI:

- 1) User-defined, time-varying, instantaneous contaminant mass fluxes and media release rates for overland medium

The data requirements for the **Water Concentration** category are:

- 1) Usage location
- 2) User-defined, time-varying, instantaneous contaminant mass concentrations for each contaminant
- 3) User-defined, time-varying, instantaneous medium release rates.

2.3 Output Requirements

The FRAMES User-Defined Source Release Module is required to output time-varying, contaminant mass fluxes for water. These outputs must meet the specifications of the FRAMES (Whelan et al. 1997). The constituent concentration for aqueous media in the *.WCF file in FRAMES is output by the aqueous modules selected (i.e., vadose zone, aquifer, and surface water).

Time-varying, instantaneous, aqueous phase, constituent concentration for water media (WCF)

2.4 Scientific Requirements

The FRAMES WCF 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 include a reference feature in which the source of the specified value for each input item can be referenced if the user desires.
- 3) 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 concentrations are in pCi/mL or g/mL, depending whether the constituent is a radionuclide or chemical. These concentration values are the instantaneous values at that time, not an average at the location specified. There are NO limits on the number of constituents, progeny, concentrations, or receptors. The x is the easterly distance of the receptor from the source, y is the northerly, and z is the relative altitude from the source. The following outline is a description of the basic information important to the WCF. An example WCF 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 WCF. Lines beginning with ';' are descriptive comments only and will not appear in the actual WCF.

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)

Usage Location Type -(string) - "Vadose" / "Aquifer" / "Surface water"

Number of Constituents -(integer)

For each 'Constituent' a line with:

Constituent name -(string)

Constituent ID -(string)

Time unit -(string) - "yr"

Concentration unit -(string) - "pCi/ml" / "g/ml"

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 unit -(string) - "yr"

Concentration unit -(string) - "pCi/ml" / "g/ml"

Number of Time Concentration 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 '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 Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) WCF. The purpose of the WCF is to allow the user to input user-defined contaminant concentration in water to generate the appropriate FRAMES data files to be used by fate and transport and exposure modules. Both radionuclides and chemicals can be input into this module. These constituent concentrations are used to describe the amount of contaminant present in the aqueous media and passed into the exposure pathways. The constituent concentrations are time varying, and the user must define the time steps required. FRAMES is a platform that allows for the linking of various multimedia modules into complete transport/exposure assessment systems (Whelan et al. 1997).

The WCF is being baseline tested for FRAMES Version 1.3. 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 Requirements

Requirements for the WCF are described in the paper entitled, *Requirements for the FRAMES Water Concentration File*. 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 Water Concentration 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	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.
3	Each module will contain an About tab to inform the user of the module title, version number and brief description.
4	For all input parameters having dimensions associated with them, the MUI will provide users with a choice of units.
5	The MUI will include a reference feature in which the source of the specified value for each input item can be referenced if the user desires.
6	The MUI will show the range of values allowed for each input data item, when the cursor is positioned on the 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 background.

7	The MUI must allow the user to input all the required data to execute the module.
8	Allow unlimited constituents, progeny, concentration, or media.
9	Produce WCF following the FRAMES data file specifications.

Output Requirements for the WCF	
10	Time-varying, instantaneous, aqueous phase, constituent concentration for water media

Scientific Requirements	
11	The WCF 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.

Recommendations	
12	Allow the user to enter known ground water or surface water concentrations (WCF format)
13	Although the MUI will convert the dimensions of user input data values into the units needed by the model, the MUI will always display the approximate value and units in which the user originally entered each input data item.

Table 4.2 shows the relationship between these requirements and the test cases described in Section 3. Although some requirements are applicable to all test cases (e.g., function within Windows 95), this table mainly shows which requirements are intended to be tested by each case. There are no test cases for Requirement 8. This is because the WCF cannot currently read or write an unlimited number of flux records, and there are no designated warning conditions that could occur during the simulation. Number 12 is a recommendation that is not tested for either.

Table 4.2. Relationship Between Test Cases and Requirements for the Water Concentration File

		Test Case Number					
		01	02	03	04	05	06
Requirement	1	X					
	2	X				X	
	3	X	X	X	X	X	X
	4	X	X	X	X	X	X
	5	X				X	
	6	X					
	7	X	X	X	X	X	X
	8						
	9	X	X	X	X	X	X
	10	X				X	
	11	X	X	X	X	X	X
	12						
	13	X	X	X	X	X	X

4.2 Test Cases and Baseline Testing Results

This section describes the specific test cases used for baseline testing of the FRAMES WCF. Appendix A describes the general procedure for conducting the tests.

4.3 WCF01

4.3.1 Description and Rationale

The data requirements for the Vadose zone flux are the following: medium type, width of flux plane, length of flux plane, distance below water table, natural recharge rate, user-defined, time-varying, instantaneous contaminant mass fluxes for each contaminant, and user-defined, time-varying, instantaneous medium release rates.

4.3.2 Input Data

Build a case using Appendix A. The water module for this case is a Vadose module. Attach this to an Aquifer, and connect the Aquifer to an Exposure icon. Save the file as test01.gid. Select benzene and strontium-90 from the list of contaminants. In the Vadose Object Information screen, type in Label: Vadose and select the Applicable Model: FRAMES Known Vadose Zone Flux.

In the User Input screen, enter this data, and then returned to the main screen.

Width	5	Yd
Length	10	M
Distance	20	Cm
Recharge rate	3	M/yr

Return to User Input and entered one time flux under the parent water. Time: 1 yr. Flux rate: 2 m³/yr. After returning to the main screen again enter information under water.

Time	Flux rate
0 yr	2 m ³ /yr
1 yr	3 m ³ /yr

Return to the main screen to see if the module ran correctly, and then input the following fluxes under benzene.

Time	Flux rate
0 day	6 g/day
1 day	7 g/day
2 day	8 g/day
3 day	9 g/day
4 day	10 g/day
5 day	11 g/day

Enter this information under strontium-90.

Time	Flux Rate
0 yr	59 pCi/yr
10	63
4	50

Enter this information under the progeny yttrium-90.

Time	Flux Rate
0 yr	53 pCi/yr
900	95

Go back and remove the strontium-90 out-of-sequence flux. Put an empty line between 0/59 and 10/63.

4.3.3 Expected Results

The expected results for this test case will be that it creates a WCF in accordance with the FRAMES specifications. It is expected that the MUI will be easy to use, have a functionality consistent with standard Windows software and that the online help will be clear and consistent. It is expected that the MUI will request only the following information: medium type, width of flux plane, length of flux plane, distance below water table, natural recharge rate, user-defined, time-varying, instantaneous contaminant mass fluxes for each contaminant, user-defined, time-varying, instantaneous medium release rates.

It is expected that both radionuclides and chemicals can be input. It is expected that the transfer of data from the MUI to the WCF 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 (test01.wff). It is expected that the MUI will not continue until all data have been entered completely and within the correct specifications shown in the scrollbar and the online help. If data entered are incorrect or incomplete, an error message should appear.

4.3.4 Testing Results

The MUI performed as expected by only requesting necessary information and allowing all required data to be input. It was easy to use with Windows interface, allowed both Radionuclide and chemicals to be input, the transfer of data from the MUI to the WFF occurred properly with the necessary unit conversions. The About tab showed information, and a choice of units was available for all parameters. The water concentration was in the output. The results were in the right format.

4.4 WCF02

4.4.1 Description and Rationale

This is designed to test the user-defined Overland flux to check if it correctly requests and transfers all necessary data to complete the WCF. The MUI should be checked to see if it allows the following: medium type; width of flux plane; height of flux plane; distance below water table; natural recharge rate; user-defined,

time-varying, instantaneous contaminant mass fluxes for each contaminant; user-defined, time-varying, instantaneous medium release rates. Also, error checking of the user input flux data will be evaluated.

4.4.2 Input Data

Build a case using Appendix A. The water module for this case is an Overland module. Attach this to a Surface Water, and connect the Surface Water to an Exposure icon. Save the file as test02.gid. Select antimony-125, benzene, beryllium, and strontium-90 from the list of contaminants. In the Overland Object Information screen, type in Label: Vadose and select the Applicable Model: FRAMES Known Overland Flow Flux.

In the User Input screen, enter this data, and then returned to the main screen.

Width	2	In
Length	25	M
Distance	10	Ft
Recharge rate	100	M/s

	Time	Flux rate	Dissolved
Water	0 yr	25 cm ³ /yr	2

I went back and entered the rest of the information.

	Time	Flux rate	Dissolved
Water	0 yr	25 cm ³ /yr	
	10	30	
	20	60	
Antimony-125	0 yr	5 pCi/yr	
	14	6	
Tellurium-125			
Benzene	5 yr	63 g/yr	
	12	45	
Beryllium	45 yr	78 g/yr	
	65	41	
Strontium-90	0 yr	1 pCi/yr	50
	66	23	80
Yttrium-90	0	29	
	51	76	
	69	83	
	100	50	
	5	49	

After deleting out-of-sequence flux, attach a WFF viewer to see results.

4.4.3 Expected Results

The expected results for this test case will be that it creates a WCF file in accordance with the FRAMES specifications. It is expected that the MUI will request only the necessary information for generating a WCF file and allow all the required data to be input with the user's choice of units. It is expected that the transfer of data from the MUI to the WCF file 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 (test02.wff). It is expected that the MUI will not continue until all data have been entered completely, and if data entered are incorrect or incomplete, an error message should appear. The About tab should show module information.

4.4.4 Testing Results

When saving and exiting after typing only one water flux, the right error message appeared. The time and flux stayed the same. When saving and exiting after entering the rest of the input. The error message detected a flux out of sequence correctly; deleting the out-of-sequence flux, returns the module to running correctly. All other expected results were met.

4.5 WCF03

4.5.1 Description and Rationale

This is designed to test the user-defined Aquifer flux to check if it correctly requests and transfers all necessary data to complete the WCF. The MUI should be checked to see if it allows the following: medium type; width of flux plane; height of flux plane; distance below water table; natural recharge rate; user-defined, time-varying, instantaneous contaminant mass fluxes for each contaminant; user-defined, time-varying, instantaneous medium release rates. Also, error checking of the user input flux data will be evaluated.

4.5.2 Input Data

Build a case using Appendix A. The water module for this case is an Aquifer module. Attach this to an Aquifer, and connect the Aquifer to an Exposure icon. Save the file as test03.gid. Select benzene and strontium-90 from the list of contaminants. In the Aquifer Object Information screen, type in Label: Aquifer and select the Applicable Model: FRAMES Known Aquifer Concentration/ Flux Module.

In the User Input screen, enter this data, and then returned to the main screen.

Width	6	Km
Length	7	Cm
Distance	8	Cm
Recharge rate	9	M/yr

	Time	Flux Rate
Water	0 yr	52 yd ³ /s
	4	69
Benzene	0yr	4 g/yr
	1	5
	2	6
	3	9
Strontium-90	10 day	56 pCi/yr
	20	98
	30	58

Yttrium-90	0 yr	12 pCi/yr
	4	57
	23	46
	9	45

After the error message for Yttrium flux out of sequence, delete the out-of-sequence flux. Run the model and then select a viewer for WCF file and WFF file.

4.5.3 Expected Results

The expected results for this test case will be that it creates a WCF file in accordance with the FRAMES specifications. It is expected that the MUI will request only the necessary information for generating a WCF file and allow all the required data to be input with the user's choice of units. It is expected that the transfer of data from the MUI to the WCF file 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 (test03.wff). It is expected that the MUI will not continue until all data have been entered completely, and if data entered are incorrect or incomplete, an error message should appear. The About tab should show module information.

4.5.4 Testing Results

All parameters had a choice of units, the necessary information was requested, and everything transferred correctly. The correct error messages appeared. The approximate value was shown for user input that the user originally entered. The WFF was in accordance with FRAMES specs.

4.6 WCF04

4.6.1 Description and Rationale

This is designed to test the user-defined Surface Water flux to check if it correctly requests and transfers all necessary data to complete the WCF. The MUI should be checked to see if it allows the following: medium type; width of flux plane; height of flux plane; distance below water table; natural recharge rate; user-defined, time-varying, instantaneous contaminant mass fluxes for each contaminant; user-defined, time-varying, instantaneous medium release rates. Also, error checking of the user input flux data will be evaluated.

4.6.2 Input Data

Build a case using Appendix A. The water module for this case is a Surface Water module. Attach this to another Surface Water, and connect the Surface Water to an Exposure icon. Save the file as test04.gid. Select benzene and strontium-90 from the list of contaminants. In the Object Information screen, type in Label: Surface and select the Applicable Model: FRAMES Known Surface Water Concentration/ Flux Module.

In the User Input screen, enter this data, and then returned to the main screen.

Width	9	M
Length	8	Yd

Distance	7	Cm
Recharge rate	6	M/yr

	Time	Flux Rate	Dissolved
Water	0 yr	4 m ³ /yr	2
	10	5	3
	20	6	4
	30	7	5
Benzene	10 yr	50 g/yr	0 g/yr
	25	55	2
	30	60	3
	35	65	4
Strontium-90	900 hr	54 Bq/s	3 Bq/s
	4800	64	4
	2700	74	5
Yttrium-90	0 yr	3 pCi/yr	6 pCi/yr
	2	5	9

4.6.3 Expected Results

The expected results for this test case will be that it creates a WCF file in accordance with the FRAMES specifications. It is expected that the MUI will request only the necessary information for generating a WCF file and allow all the required data to be input with the user's choice of units. It is expected that the transfer of data from the MUI to the WCF file 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 (test04.wff). It is expected that the MUI will not continue until all data have been entered completely, and if data entered are incorrect or incomplete, an error message should appear. The About tab should show module information.

4.6.4 Testing Results

All results were as expected.

4.7 WCF05

4.7.1 Description and Rationale

This is designed to test the user-defined Aquifer concentration to check if it correctly requests and transfers all necessary data to complete the WCF. The MUI should be checked to see if it allows the following: usage location; user-defined, time-varying, instantaneous contaminant mass concentrations for each contaminant; user-defined, time-varying, instantaneous medium release rates. Also, error checking of the user input flux data will be evaluated.

4.7.2 Input Data

Usage Location (Fcm4)

	Time	Concentration
Antimony	0 yr	23 g/mL
	100	25
Benzene	0 yr	52 g/mL
	45	56
Strontium-90	0 yr	6 pCi/mL
	10	8
Yttrium-90	0 yr	74 pCi/mL
	5	29

Usage Location (Fcm5)

	Time	Concentration
Antimony	0 yr	23 g/mL
	100	25
Benzene	0 yr	52 g/mL
	45	56
Strontium-90	0 yr	6 pCi/mL
	10	8
Yttrium-90	0 yr	74 pCi/mL
	5	29

4.7.3 Expected Results

The expected results for this test case will be that it creates a WCF file in accordance with the FRAMES specifications. It is expected that the MUI will request only the necessary information for generating a WCF file and allow all necessary information to be entered. It is expected that the transfer of data from the MUI to the WCF file 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 (test05.WCF). It is expected that the MUI will not continue until all data have been entered completely and within the correct specifications shown in the scrollbar and the online help. If data entered are incorrect or incomplete, an error message should appear. The About tab will contain the appropriate information. There will be a choice of units for all user-input parameters. The reference feature will work correctly.

4.7.4 Testing Results

All of the requirements were met.

4.8 WCF06

4.8.1 Description and Rationale

This is designed to test the user-defined Surface Water concentration to check if it correctly requests and transfers all necessary data to complete the WCF. The MUI should be checked to see if it allows the following: usage location; user-defined, time-varying, instantaneous contaminant mass concentrations for each

contaminant; user-defined, time-varying, instantaneous medium release rates. Also, error checking of the user input flux data will be evaluated.

4.8.2 Input Data

Select the following Contaminants: Antimony, Benzene, Beryllium, Strontium-90. Type in Label: SW and choose FRAMES Known Surface Water Concentration/ Flux Module. Attach a surface water to two different exposure icons. Pull down a second Surface Water, attach the first one to it then to an exposure icon.

On the Flux tab enter this data:

Width	10	Km
Length	9	Cm
Distance	8	Ft
Recharge rate	7	M/yr

	Time	Flux Rate	Dissolve d
Water	10 yr	23 m ³ /yr	3
	20	32	4
	30	45	5
Antimony	0 day	5 g/day	23 g/day
	1	4	60
Benzene	97 yr	86 g/yr	56 g/yr
	456	98	45321
Beryllium	0 yr	10 g/yr	
	95	15	
Strontium-90	0 yr	1 pCi/yr	2 pCi/yr
	3	4	5
	6	7	8
Yttrium-90	9	10	11
	12	13	14
	15	16	17

4.8.3 Expected Results

The expected results for this test case will be that it creates a WCF file in accordance with the FRAMES specifications. It is expected that the MUI will request only the necessary information for generating a WCF file and will allow all necessary data to be entered. It is expected that the transfer of data from the MUI to the WCF file 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 (WCF). It is expected that the MUI will not continue until all data have been entered. If data entered are incorrect or incomplete, an error message should appear.

4.8.4 Testing Results

All results are as expected.

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 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 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 that are necessary to ensure quality. Completion of this checklist verifies that all documentation will be complete for transfer of the software to client use.

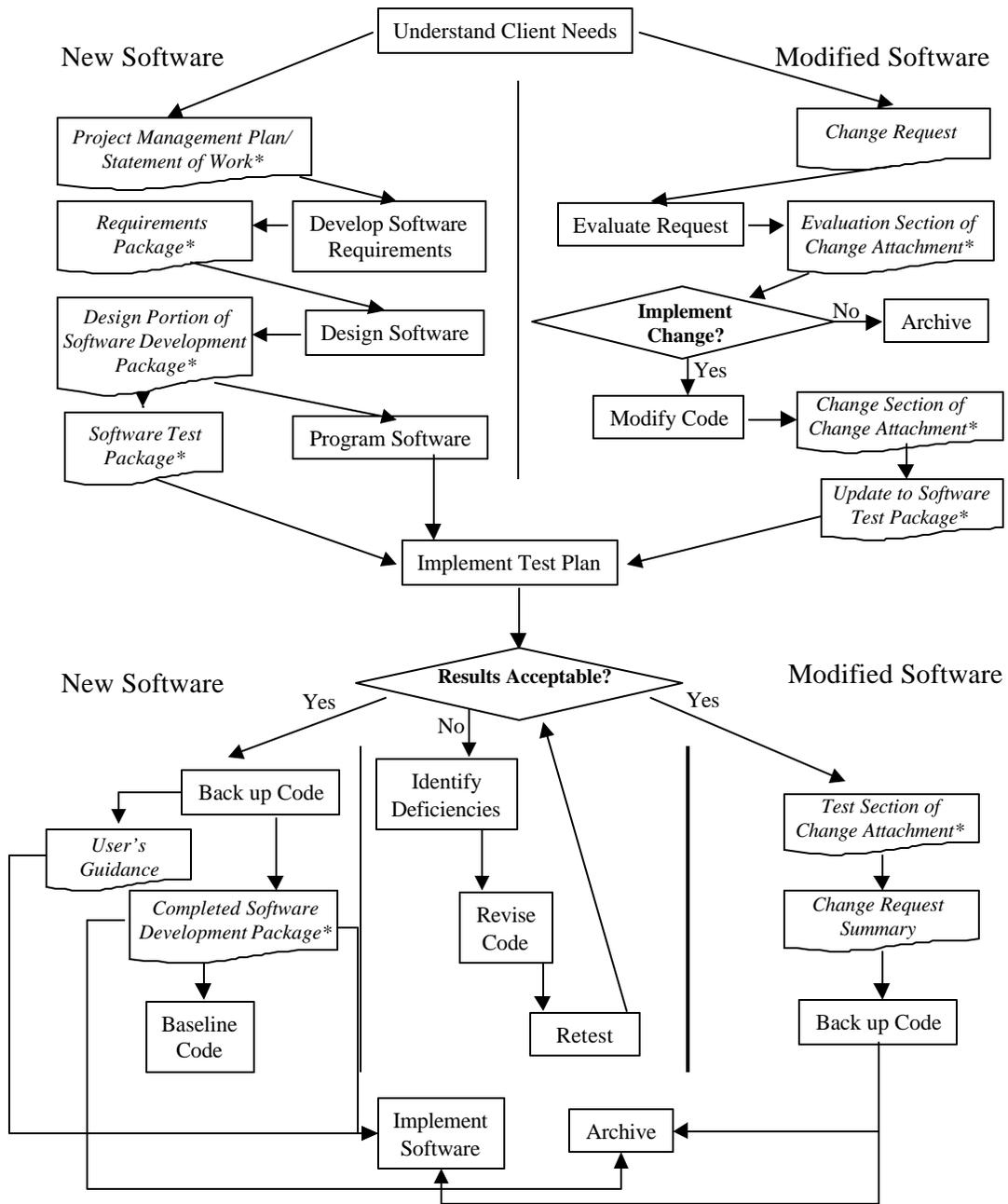


Figure 5.1. Ensuring Quality in the Environmental Software Development Process

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	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

Figure 5.2. 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 _____ Date _____

System/Module Manager _____ Date _____

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

6.0 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

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 desired water module icon. The icons will appear on the main screen. When all icons are in place, connect the icons together. To do this hold down the shift key, click on an icon, and drag the mouse to the next icon. Release mouse button and shift key. A line will connect the two icons with an arrow pointing from the first icon clicked on to the second icon. To remove this line, repeat the steps used to connect it. Continue linking all icons together, moving from left to right across the screen so that the arrows are pointing in the flow of contamination. The contaminant icon needs to be linked to all other icons. To remove an icon from the screen, Right-click and select delete. An icon can have more than one connection (i.e., the aquifer module can be connected to two different exposure modules).

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 to green.

Right click on the water module you placed on the main screen and choose General Info. Choose Label: Source and Module: FRAMES Known Contaminant Flux or Concentration. Click OK. The signal light will turn from black to red.

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

On all the tabs, fill in the red boxes. These boxes will turn to green when the correct information is entered. For guidance on what to enter in the red boxes, click on one of the boxes and look at the scrolling bar at the bottom of the screen. This bar will give you the boundaries for the box. If more guidance is needed, choose the desired box by clicking on it, and press F1. This will open up the online help that will take you directly to the correct section.

Click save and exit; the light will turn from red to yellow.

For each test case, follow the above steps. After these first steps have been followed, continue to build the case using user input information and the same steps used to fill in the

information on the source-term icon. When the test case has been built and you are ready for the results, follow these instructions.

Right click on the water module and choose Run Model. The model will run, and the light will change from yellow to green. Right click on the next icon and choose Run Model. The model will run, and the light will change from yellow to green. Instead of running each model individually, click on the GO button in the toolbar at the top of the screen. This button works if all the lights are yellow. If one is black or red and you wish to leave it this way, then you will have to run each model separately.

To view results, Right click on the icon and select “View/Print module output” and select the desired viewer off the menu.

Appendix B

WCF and WFF Viewer Results

Appendix B: WCF and WFF Viewer Results

```
*****  
* File: C:\FRAMES\test01.WFF  
* Section: vad2  
* Date: 6/13/00 5:24:21 PM  
*****
```

```
1  
"vad2 has known Vadose Zone flux values."  
1  
"aqu6","Vadose Zone",4.572,"m",10,"m",0.2,"m",3,"m/yr",2  
"yr","m^3/yr",2  
0.0,2.0  
1.0,3.0  
"Benzene","71432","yr","g/yr",6,1,0  
0.0,2191.4998  
0.0027,2556.7498  
0.0055,2921.9998  
0.0082,3287.2497  
0.011,3652.4997  
0.0137,4017.7497  
"STRONTIUM-90","SR90","yr","pCi/yr",2,1,1  
0.0,59.0  
10.0,63.0  
"YTTRIUM-90","Y90","yr","pCi/yr",2,"STRONTIUM-90","SR90",1  
0.0,53.0  
900.0,95.0
```

```
*****  
* File: C:\FRAMES\test02.WFF  
* Section: ovl2  
* Date: 6/16/00 2:56:52 PM  
*****
```

```
1  
"ovl2 has known Overland flux values."  
1  
"riv6","Overland",0.0508,"m",25,"m",3.048,"m",3155000000,"m/yr",4  
"yr","m^3/yr",3  
0.0,2.3E-05  
10.0,3.0E-05  
20.0,6.0E-05  
"ANTIMONY-125","SB125","yr","pCi/yr",2,2,1  
0.0,5.0,0.0  
14.0,6.0,0.0  
"TELLURIUM 125M","TE125M","yr","pCi/yr",0,"ANTIMONY-125","SB125",2  
"Benzene","71432","yr","g/yr",2,2,0  
5.0,63.0,0.0  
12.0,45.0,0.0  
"Beryllium","7440417","yr","g/yr",2,2,0  
45.0,78.0,0.0  
65.0,41.0,0.0
```

"STRONTIUM-90","SR90","yr","pCi/yr",2,2,1
0.0,1.0,50.0
66.0,23.0,80.0
"YTTRIUM-90","Y90","yr","pCi/yr",4,"STRONTIUM-90","SR90",2
0.0,29.0,0.0
51.0,76.0,0.0
69.0,83.0,0.0
100.0,50.0,0.0

* File: C:\FRAMES\test03.WFF
* Section: aqu2
* Date: 6/19/00 9:59:22 AM

1
"aqu2 has known Aquifer flux values."
1
"aqu3", "Aquifer",6000,"m",0.07,"m",0.08,"m",9,"m/yr",2
"yr","m^3/yr",2
0.0,1.256E+09
4.0,1.667E+09
"Benzene", "71432", "yr", "g/yr",4,1,0
0.0,4.0
1.0,5.0
2.0,6.0
3.0,9.0
"STRONTIUM-90","SR90","yr","pCi/yr",3,1,1
0.0274,56.0
0.0548,98.0
0.0821,58.0
"YTTRIUM-90","Y90","yr","pCi/yr",3,"STRONTIUM-90","SR90",1
0.0,12.0
4.0,57.0
23.0,46.0

* File: C:\FRAMES\test04.WFF
* Section: riv2
* Date: 6/19/00 11:20:20 AM

1
"riv2 has known Surface water flux values."
1
"riv3", "Surface water",9,"m",7.3152,"m",0.07,"m",6,"m/yr",2
"yr","m^3/yr",4
0.0,4.0
10.0,5.0
20.0,6.0
30.0,7.0
"Benzene", "71432", "yr", "g/yr",4,2,0

10.0,50.0,0
25.0,55.0,0
30.0,60.0,0
35.0,65.0,0
"STRONTIUM-90","SR90","yr","pCi/yr",3,2,1
0.1027,4.615E+10,0
0.2053,5.47E+10,0
0.308,6.325E+10,0
"YTTRIUM-90","Y90","yr","pCi/yr",2,"STRONTIUM-90","SR90",2
0.0,3.0,0
2.0,5.0,0

* File: C:\FRAMES\test05.WCF
* Section: aqu3
* Date: 6/19/00 12:58:04 PM

1
"aqu3 has known Aquifer concentration values."
2
"fcm4","Aquifer",3
"Antimony","7440360","yr","g/ml",2,0
0.0,23.0
100.0,25.0
"Benzene","71432","yr","g/ml",2,0
0.0,52.0
45.0,56.0
"STRONTIUM-90","SR90","yr","pCi/ml",2,1
0.0,6.0
10.0,8.0
"YTTRIUM-90","Y90","yr","pCi/ml",2,"STRONTIUM-90","SR90"
0.0,74.0
5.0,29.0
"fcm5","Aquifer",3
"Antimony","7440360","yr","g/ml",2,0
0.0,23.0
100.0,25.0
"Benzene","71432","yr","g/ml",2,0
0.0,52.0
45.0,56.0
"STRONTIUM-90","SR90","yr","pCi/ml",2,1
0.0,6.0
10.0,8.0
"YTTRIUM-90","Y90","yr","pCi/ml",2,"STRONTIUM-90","SR90"
0.0,74.0
5.0,29.0

* File: C:\FRAMES\test06.WFF
* Section: riv2
* Date: 6/19/00 4:21:03 PM

1
 "riv2 has known Surface water flux values."
 1
 "riv5", "Surface water", 10000, "m", 0.09, "m", 2.4384, "m", 7, "m/yr", 4
 "yr", "m^3/yr", 3
 10.0, 23.0
 20.0, 32.0
 30.0, 45.0
 "Antimony", "7440360", "yr", "g/yr", 2, 2, 0
 0.0, 1826.2499, 0
 0.0027, 1460.9999, 0
 "Benzene", "71432", "yr", "g/yr", 2, 2, 0
 97.0, 86.0, 0
 456.0, 98.0, 0
 "Beryllium", "7440417", "yr", "g/yr", 2, 2, 0
 0.0, 10.0, 0
 95.0, 15.0, 0
 "STRONTIUM-90", "SR90", "yr", "pCi/yr", 3, 2, 1
 0.0, 1.0, 0
 3.0, 4.0, 0
 6.0, 7.0, 0
 "YTTRIUM-90", "Y90", "yr", "pCi/yr", 3, "STRONTIUM-90", "SR90", 2
 9.0, 10.0, 0
 12.0, 13.0, 0
 15.0, 16.0, 0

 * File: C:\FRAMES\test06.WCF
 * Section: riv2
 * Date: 6/19/00 4:22:59 PM

1
 "riv2 has known Surface water concentration values."
 2
 "fcm3", "Surface water", 4
 "Antimony", "7440360", "yr", "g/ml", 0, 0
 "Benzene", "71432", "yr", "g/ml", 0, 0
 "Beryllium", "7440417", "yr", "g/ml", 0, 0
 "STRONTIUM-90", "SR90", "yr", "pCi/ml", 0, 1
 "YTTRIUM-90", "Y90", "yr", "pCi/ml", 0, "STRONTIUM-90", "SR90"
 "fcm4", "Surface water", 4
 "Antimony", "7440360", "yr", "g/ml", 0, 0
 "Benzene", "71432", "yr", "g/ml", 0, 0
 "Beryllium", "7440417", "yr", "g/ml", 0, 0
 "STRONTIUM-90", "SR90", "yr", "pCi/ml", 0, 1
 "YTTRIUM-90", "Y90", "yr", "pCi/ml", 0, "STRONTIUM-90", "SR90"