
**Pacific Northwest
National Laboratory**

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FRAMES User Defined Atmospheric Concentration and Deposition File Module Documentation

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December 2000



Prepared for the U.S. Department of Energy
under Contract DE-AC06-76RL01830

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1.0 Introduction

The Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) Atmospheric Transport Output (ATO) File provides data for use by exposure pathway modules for airborne releases and atmospheric transport and deposition of pollutants. 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 ATO file is to allow the user to input user-defined airborne releases and the deposition rate of pollutants to generate the appropriate FRAMES data files to be used by exposure pathway modules. Both radionuclides and chemicals can be input into this module. These constituent rates are used to describe the amount of pollutant present in the atmosphere 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: The 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 comprehensive description of how a piece of software will function (i.e., how it will meet its requirements).
- ! Specifications: 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 ATO File. 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 ATO file. Detailed requirements are described in the sections that follow.

The FRAMES ATO file will:

- 1) Allow the user to input different flux types, and time- varying air concentration, external dose and deposition rates, and flux density for each data set.
- 2) Allow unlimited constituents, progeny, and concentrations.
- 3) Operate under Windows 95 and have a user-friendly interface with a standard windows look and feel.
- 4) Produce ATO following the FRAMES data file specifications

2.2 Input Requirements

The user will enter the input data required for the FRAMES User-Defined Atmospheric Concentration and Deposition Module via the Module User Interface (MUI). The MUI will allow the user to define the concentration and deposition.

Following are some general requirements associated with the MUI:

- 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 can be referenced if the user desires.

The MUI for the FRAMES atmospheric 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, hourly or annual average contaminant concentrations, external dose, and deposition rates for air medium.

The data requirements for the **ATO file** category are:

- 1) Flux types (gas 1, particle 1, particle 2, or particle 3)
- 2) Flux type flux density (gas and particles), particle radius (particles only), and reactive fraction (gas only)
- 3) Type of release (acute or chronic)

- 4) Spatial type (point or grid)
- 5) Coordinate grid type (polar or cartesian)
- 6) Reporting points (point)
- 7) Types of output products (air concentration, external dose, and deposition rate) (for “Deposition Rate” would be “total,” “dry,” or “wet”)
- 8) User-defined, time-varying, hourly or annual average contaminant air concentration for each contaminant
- 9) User-defined, time-varying annual average deposition rates (gas or particle).

2.3 Output Requirements

The FRAMES Atmospheric Module is required to output time-varying, pollutant emission rates. These outputs must meet the specifications of FRAMES (Whelan et al. 1997). The pollutant emission rates for atmosphere media in the *.ATO file in FRAMES is output by the atmospheric module.

- 1) Time-varying, instantaneous, annual average contaminant mass fluxes and media release rates for air medium (ATO).

2.4 Scientific Requirements

The FRAMES ATO file 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 ATO file provides data for use by exposure-pathway modules for airborne releases and atmospheric transport and deposition of pollutants. The following outline is a description of the basic information important to the atmospheric transport output file. An example an ATO 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 ATO file. Lines beginning with ';' are descriptive comments only and will not appear in the actual ATO file. The basic data sets are provided as point values at specific locations relative to the release point. Use of keywords is suggested, although other methods of describing data types could be used (e.g. logical or integer flags).

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:

Number of Flux Types - (integer)

Data Set name - (string)

For each 'Flux Type' a line with:

Flux Type Name - (string)

;If Gas, then "Gas 1"

;If particle then "Particle " followed by the particle count

; "Particle 1", "Particle 2", "Particle 3", ...

If Type Name = "Gas #" then

Reactive Gas fraction - (float)

Reactive Gas fraction unit - (string) - "fraction"

Else

Particle Radius - (float)

Particle Radius unit - (string) - "um"

End If

Flux Type Density - (float)

Flux Type Density unit - (string) - "g/cm3"

Next 'Flux Type'

Line with:

Release type - (string) - "acute" / "chronic"

Co-ordinate grid type - (string) - "polar" / "cartesian"

Spatial type - (string) - "grid" / "points"

Number of Constituents (parent) - (integer)

For each 'Constituent' a line with:

Constituent Name - (string)

Constituent ID - (string)

```

Number of Time Periods - (integer)
Number of Progeny - (integer)
For each 'Time Period' line with:
  Time - (float)
  If 'Release type' = "acute" then
    Time unit - (string) - "hr"
  Else 'Release type' = "chronic"
    Time unit - (string) - "yr"
  End if
Number of Output Products - (integer)
For each 'Output Product' line with:
  Output Product Name - (string) - "Air Concentration" / "Deposition Rate" / "External Dose"
  If 'OutPut Product Name' = "Air Concentration" or "Deposition Rate" then
    Output Product Source 'Flux Type' - (string)
  Else
    Blank entry - (string) - ""
  End If
  If 'Output Product Name' = "Deposition Rate" then
    Relative Moisture of Output Product - (string) - "wet" / "dry" / "total"
  Else
    Blank entry - (string) - ""
  End If
  If 'OutPut Product Name' = "Air Concentration"
    If 'Constituent' is a Radionuclide then
      Output Product unit - (string) - "Bq/m3"
    Else
      Output Product unit - (string) - "kg/m3"
    End If
  ElseIf 'OutPut Product Name' = "Deposition Rate"
    If 'Constituent' is a Radionuclide then
      Output Product unit - (string) - "Bq/m2/yr"
    Else
      Output Product unit - (string) - "kg/m2/yr"
    End If
  Else 'OutPut Product Name' = "External Dose" then
    Output Product unit - (string) - "Sv"
  End If
  If 'Co-ordinate grid type' = "polar" and 'Spatial type' = "grid" then
    Number of Radial Distances - (integer)
  ElseIf 'Co-ordinate grid type' = "cartesian" and 'Spatial type' = "grid" then
    Number of x Co-ordinates - (integer)
  Else 'Co-ordinate grid type' = "cartesian" and 'Spatial type' = "points" then
    Number of x,y coordinate points - (integer)
  End If
  Unit of Radial Distances or x Co-ordinates - (string) - "m"
  If 'Co-ordinate grid type' = "polar" and 'Spatial type' = "grid" then
    Number of Directions - (integer)
  ElseIf 'Co-ordinate grid type' = "cartesian" and 'Spatial type' = "grid" then

```

```

    Number of y Co-ordinates - (integer)
Else 'Co-ordinate grid type' = "cartesian" and 'Spatial type' = "points" then
    Number - (integer) - 1
End If
If 'Co-ordinate grid type' = "polar" then
    Unit of Directions - (string) - "deg"
Else 'Co-ordinate grid type' = "cartesian"
    Unit of y Co-ordinate - (string) - "m"
End If
If 'Spatial type' = "grid" then line with:
    All Radial Distances or x Co-ordinates - (set of float)
    If 'Co-ordinate grid type' = "polar" then
        For each 'Direction' line with:
            Direction - (float)
            Output Product Value for the 'Radial Distance' and 'Direction' - (float)
        Next 'Direction'
    Else 'Co-ordinate grid type' = "cartesian" then line with:
        For each 'y Co-ordinate' line with:
            y Co-ordinate - (float)
            Output Product Value for the 'x,y Co-ordinate' pair - (float)
        Next 'Direction'
    End If
Else 'Spatial type' = "points"
    A line with: Name of Reporting Points - (set of strings)
    A line with: Values of x Co-ordinates for each point - (set of float)
    A line with: Values of y Co-ordinates for each point - (set of float)
    A line with:
        Number - (integer) - 99
        Output Product Values for each point - (set of float)
    End If
Next 'Output Product'
Next 'Time Period'
For each 'Progeny' a line with:
    Progeny Name-(string)
    Progeny ID-(string)
    Number of Time Periods - (integer)
    Parent Name-(string)
    Parent ID-(string)
For each 'Time period' a line with:
    Time - (float)
    Time unit - (string) - "hr" / "yr"
    Number of Output Products - (integer)
For each 'Output Product' line with:
    Output Product Name - (string) - "Air Concentration" / "Deposition Rate" / "External
Dose"
    If 'OutPut Product Name' = "Air Concentration" or "Deposition Rate" then
        Output Product Source 'Flux Type' - (string)
    Else

```

```

    Blank entry - (string) - ""
End If
If 'Output Product Name' = "Deposition Rate" then
    Relative Moisture of Output Product - (string) - "wet" / "dry" / "total"
Else
    Blank entry - (string) - ""
End If
If 'OutPut Product Name' = "Air Concentration"
    If 'Constituent' is a Radionuclide then
        Output Product unit - (string) - "Bq/m3"
    Else
        Output Product unit - (string) - "kg/m3"
    End If
Elseif 'OutPut Product Name' = "Deposition Rate"
    If 'Constituent' is a Radionuclide then
        Output Product unit - (string) - "Bq/m2/yr"
    Else
        Output Product unit - (string) - "kg/m2/yr"
    End If
Else 'OutPut Product Name' = "External Dose" then
    Output Product unit - (string) - "Sv"
End If
If 'Co-ordinate grid type' = "polar" and 'Spatial type' = "grid" then
    Number of Radial Distances - (integer)
Elseif 'Co-ordinate grid type' = "cartesian" and 'Spatial type' = "grid" then
    Number of x Co-ordinates - (integer)
Else 'Co-ordinate grid type' = "cartesian" and 'Spatial type' = "points" then
    Number of x,y coordinate points - (integer)
End If
Unit of Radial Distances or x Co-ordinates - (string) - "m"
If 'Co-ordinate grid type' = "polar" and 'Spatial type' = "grid" then
    Number of Directions - (integer)
Elseif 'Co-ordinate grid type' = "cartesian" and 'Spatial type' = "grid" then
    Number of y Co-ordinates - (integer)
Else 'Co-ordinate grid type' = "cartesian" and 'Spatial type' = "points" then
    Number - (integer) - 1
End If
If 'Co-ordinate grid type' = "polar" then
    Unit of Directions - (string) - "deg"
Else 'Co-ordinate grid type' = "cartesian"
    Unit of y Co-ordinate - (string) - "m"
End If
If 'Spatial type' = "grid" then line with:
    All Radial Distances or x Co-ordinates - (set of float)
    If 'Co-ordinate grid type' = "polar" then
        For each 'Direction' line with:
            Direction - (float)
            Output Product Value for the 'Radial Distance' and 'Direction' - (float)
    End If
End If

```

```
    Next 'Direction'
  Else 'Co-ordinate grid type' = "cartesian" then line with:
    For each 'y Co-ordinate' line with:
      y Co-ordinate - (float)
      Output Product Value for the 'x,y Co-ordinate' pair - (float)
    Next 'Direction'
  End If
Else 'Spatial type' = "points"
  Line with: Name of Reporting Points - (set of strings)
  Line with: Values of x Co-ordinates for each point - (set of float)
  Line with: Values of y Co-ordinates for each point - (set of float)
  Line with:
    Number - (integer) - 99
    Output Product Values for each point - (set of float)
  End If
Next 'Output Product'
Next 'Time Period'
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 FRAMES ATO file. The ATO provides data for use by exposure-pathway modules for airborne releases and atmospheric transport and deposition of pollutants. The purpose of the ATO is to allow the user to input user-defined airborne releases and the deposition rate of pollutants to generate the appropriate FRAMES data files to be used by exposure-pathway modules. Both radionuclides and chemicals can be input into this module. These constituent rates are used to describe the amount of pollutant present in the atmosphere 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 ATO is being baseline tested for FRAMES Version 1.1. 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 ATO are described in the paper entitled, *Requirements for the FRAMES Atmospheric Output 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 ATO Module

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, including user-defined, time-varying, annual average contaminant mass fluxes, and media-release rates for air medium.
8	Allow unlimited constituents, progeny, and concentrations.
9	Produce ATO following the FRAMES data file specifications.

Output Requirements for the WCF	
10	Time-varying, instantaneous, annual average contaminant mass fluxes, and media release rates for air medium.

Scientific Requirements	
11	The ATO 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.

There are no test cases for Requirement 8. This is because the ATO cannot currently read or write an unlimited number of flux records, and there are no designated warning conditions that could occur during the simulation.

4.2 Test Cases and Baseline Testing Results

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

4.3 ATO1

4.3.1 Description and Rationale

This is designed to test the user-defined Atmospheric Transport to check if it correctly requests and transfers all necessary data to complete the ATO. The MUI should be checked to see if it allows the following: flux types (gas 1, particle 1, particle 2, or particle 3); flux type flux density (gas and particles), particle radius (particles only) and reactive fraction (gas only); type of release (acute or chronic); spatial type (point or grid); coordinate grid type (polar or cartesian); reporting points (point); types of output products (air concentration, external dose and deposition rate) (for 'Deposition Rate' would be "total", "dry" or "wet"); user-defined, time-varying, hourly or annual average contaminant air concentration for each contaminant; user-defined, time-varying annual average deposition rates (gas or particle). Also, error checking of the user input flux data will be evaluated.

4.3.2 Input Data

Build a case using Appendix A. Save the file as ATOTest1.gid. Select antimony, antimony-125, benzene, beryllium, and strontium-90 from the list of contaminants (see Table 4.2).

Chronic data type

Gas1 with default data, referenced one

Select Turn progeny on.

Table 4.2. Input Data for ATOTest1.gid

Contaminant	Output Type	Time	External	AC Gas	Deposition Gas
Antimony	Air concentration	0 yr		25 kg/m ³	
		10 yr		60	
ANTIMONY-125	Air concentration	2 yr	5 Sv	4 Bq/m ³	
	External dose	4	6	79	
TELLURIUM-125	Air concentration	1 yr		41 Bq/m ³	
		3		5	
Benzene	Total deposition	900 yr			569 kg/m ²
		400 yr			798
Beryllium	Air concentration Wet deposition	0 yr		4 kg/m ³	2 kg/m ²
		1			6
		2			8
		3			10
		4			12
Strontium-90	Air concentration	0 day		6 Bq/m ³	90 Bq/m ²
	Total deposition	10		7	100
		20		8	110
Yttrium-90					

1) After the Benzene out of flux error, deleted 400 yr. After the error message for one, replaced the 400 line with 1900.

4.3.3 Expected Results

1) The expected results for this test case will be that it creates an ATO 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: flux types (gas 1, particle 1, particle 2, or particle 3); flux type flux density (gas and particles), particle radius (particles only) and reactive fraction (gas only); type of release (acute or chronic); spatial type (point or grid); coordinate grid type (polar or cartesian); reporting points (point); types of output products (air concentration, external dose and deposition rate) (for

“Deposition Rate” would be “total,” “dry,” or “wet”); user-defined, time-varying, hourly or annual average contaminant air concentration for each contaminant; user-defined, time-varying annual average deposition rates (gas or particle).

2) It is expected that both Radionuclide and chemicals can be input. It is expected that the transfer of data from the MUI to the ATO 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 (ATOtest1.ato). It is expected that the MUI will not continue until all data have been entered completely and within the correct specifications shown in the scroll bar and the online help. If data entered are incorrect or incomplete, an error message should appear.

4.3.4 Testing Results

Several of the data requirements listed in the Requirements data were not included as part of the User Interface. These should be added in the future, including reactive fraction (gas only), spatial type (point or grid), and coordinate grid type (polar or Cartesian). All other expected results were met.

4.4 ATO2

4.4.1 Description and Rationale

This is designed to test the user-defined Atmospheric Transport to check if it correctly requests and transfers all necessary data to complete the ATO. The MUI should be checked to see if it allows the following: flux types (gas 1, particle 1, particle 2, or particle 3); flux type flux density (gas and particles), particle radius (particles only) and reactive fraction (gas only); type of release (acute or chronic); spatial type (point or grid); coordinate grid type (polar or Cartesian); reporting points (point); types of output products (air concentration, external dose and deposition rate) (for ‘Deposition Rate’ would be “total,” “dry,” or “wet”); user-defined, time-varying, hourly or annual average contaminant air concentration for each contaminant; user-defined, time-varying annual average deposition rates (gas or particle). Also, error checking of the user input flux data will be evaluated.

4.4.2 Input Data

Build a case using Appendix A. Attach two exposure icons to the air module. Save the file as ATOtest2.gid. Select benzene and strontium-90 from the list of contaminants (see Table 4.3).

Acute release type

Default data for start date/time and particles 1,2,3

Table 4.3. Input Data for ATOtest2.gid

Contaminant	Time	Ext.	P1 Total	P2 Wet	AC P1	AC P2	AC P3
Fcm3 Benzene	0 hr		1 kg/m ²		2 kg/m ³		
	3		4		5		

	6		7		8		
Strontium-90	100 hr	101 Sv		102 Bq/m ²		103 Bq/m ³	
	104	105		106		107	
	108	109		110		111	
Fcm4 Benzene	0 hr		569 kg/m ²				
	2		41548				
Strontium-90	0 hr				1 Bq/m ³	4 Bq/m ³	7 Bq/m ³
	10				2	5	8
	20				3	6	9

Contaminant	P3 Total	P1 Dry	P2 Dry	P3 Dry
Fcm4 Benzene	542 kg/m ²			
	4887			
Strontium-90		30 Bq/m ²	60 Bq/m ²	90 Bq/m ²
		40	70	91
		50	80	92

In Fcm3, General Info screen type in the Installation Relative Easting 20 km, Installation Relative Northing 400 km, and Elevation 30 km. In Fcm4, General Info screen type in the Installation Relative Easting 99 km, Installation Relative Northing 450 km, and Elevation 700 km.

4.4.3 Expected Results

The expected results for this test case will be that it creates an ATO in accordance with the FRAMES specifications. It is expected that the MUI will request only the following information: flux types (gas 1, particle 1, particle 2, or particle 3); flux type flux density (gas and particles), particle radius (particles only) and reactive fraction (gas only); type of release (acute or chronic); spatial type (point or grid); coordinate grid type (polar or cartesian); reporting points (point); types of output products (air concentration, external dose and deposition rate) (for 'Deposition Rate' would be "total", "dry" or "wet"); user-defined, time-varying, hourly or annual average contaminant air concentration for each contaminant; user-defined, time-varying annual average deposition rates (gas or particle).

It is expected that the transfer of data from the MUI to the ATO 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 (ATOtest2.ato). It is expected that the MUI will not continue until all data have been entered completely. If data entered are incorrect or incomplete, an error message should appear.

4.4.4 Testing Results

All expected results 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.

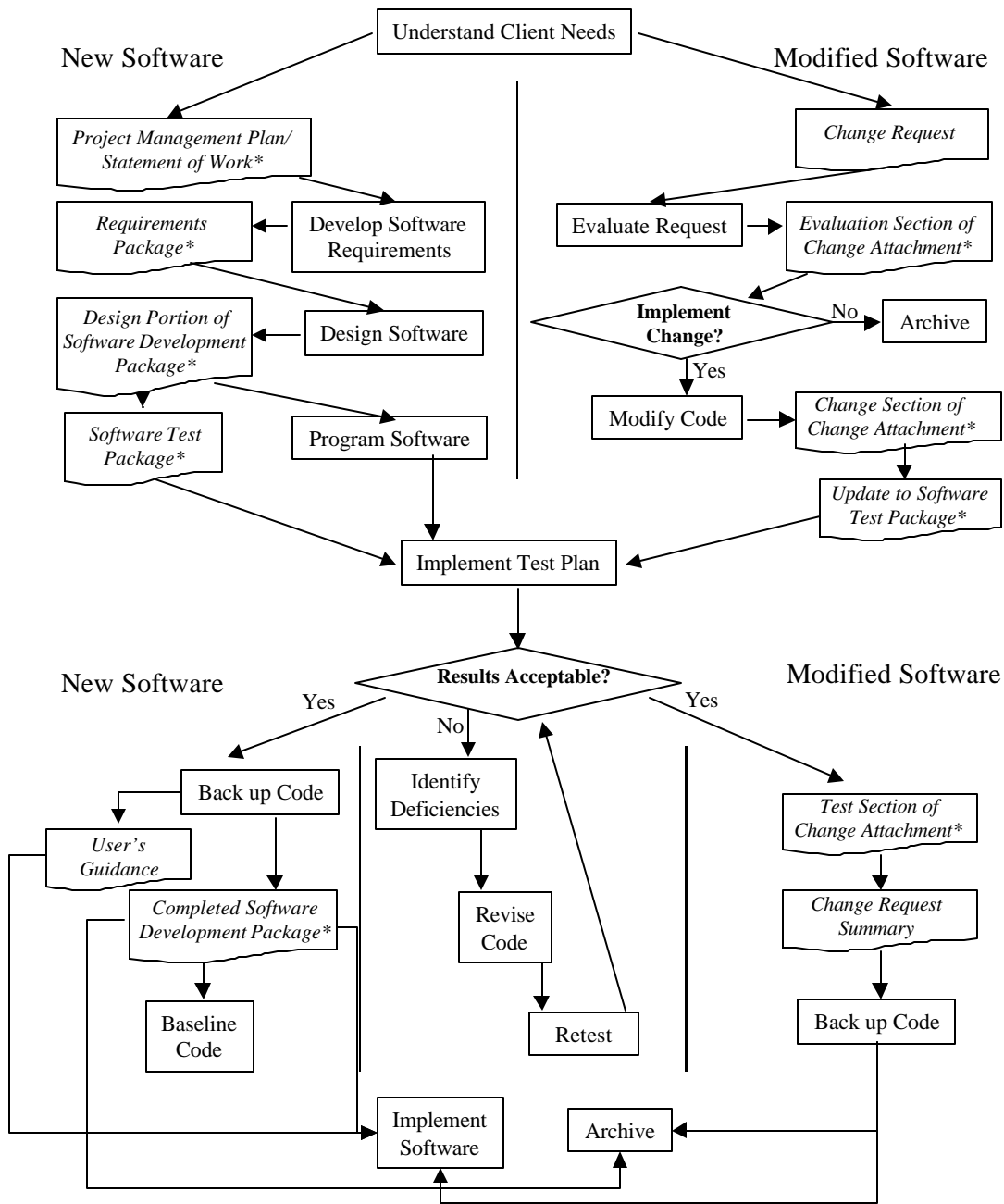


Figure 5.1 Ensuring Quality in the Environmental Software Development Process

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	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
 - ___ hardware and software needed to implement plan
 - ___ test case specifications
 - ___ expected results

Figure 5.2. Quality Assurance Implementation Checklist for the FRAMES Technology Software System

<p>F. User's Guidance</p> <p>--Documented in</p> <p><input type="checkbox"/> hardcopy printout of user's guidance for system</p> <p>--Contains information on (all of the following)</p> <p><input type="checkbox"/> description of software</p> <p><input type="checkbox"/> description of use of user interface</p> <p><input type="checkbox"/> mathematical formulations</p> <p><input type="checkbox"/> example problems</p> <p><input type="checkbox"/> explanation of modules included</p>	
<p>G. General Quality Assurance Documentation</p> <p>--Documented in</p> <p><input type="checkbox"/> Quality Assurance Program Document</p> <p><input type="checkbox"/> Quality Assurance Software-Specific Checklist</p> <p>--Contains information on (all of the following)</p> <p><input type="checkbox"/> purpose of quality assurance program</p> <p><input type="checkbox"/> client-specified activities</p> <p><input type="checkbox"/> activities required to ensure quality in software</p>	
<p>H. Quality Assurance Archive</p> <p>--Documented in</p> <p><input type="checkbox"/> hard-copy files</p> <p><input type="checkbox"/> back up disk files in multiple storage locations</p> <p>--Contains information on (all of the following)</p> <p><input type="checkbox"/> all quality assurance documentation</p> <p><input type="checkbox"/> client correspondence regarding software</p> <p><input type="checkbox"/> modifications made to baselined software</p> <p><input type="checkbox"/> disk copy back ups</p> <p><input type="checkbox"/> reproducibility of code (check code for comments)</p>	
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, the air-module icon, and the exposure icon. Connect both the air and exposure icon to the contaminant icon. Connect the air and exposure icons together (from air to exposure). To do this, hold down the shift key, click on the air icon, and drag the mouse to the exposure icon. Release mouse button and shift key. A line will connect the two icons with an arrow pointing from the air 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. An icon can have more than one connection (i.e., the air module can be connected to two different viewer icons).

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 air module you placed on the main screen and choose General Info. Choose Module: FRAMES Known Atmospheric Concentrations. Click OK. The signal light will turn from black into red.

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

Fill in all the required information on every tab then click save and exit; the light will turn from red into yellow.

Right click on the air 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 viewer/print module output.

Appendix B

ATO Viewer Results

Appendix B- ATO Viewer Results

* File: C:\FRAMES\ATOTEST1.ATO

* Section: air2

* Date: 6/26/00 11:45:48 AM

8

"=====

" FUI Known Air Concentration Module"

" Version 1.00 August 1, 1998"

" Run: C:\FRAMES\ATOTEST1.GID"

" Site: Scenario 1"

" Glyph: air2"

" 06-26-2000"
"=====

1

1,"air2"

"Gas 1",0,"um",1.5,"g/cm^3"

"chronic","cartesian","points",5

"Antimony","7440360",2,0

0,"yr",1

"Air Concentration","Gas",,"kg/m3",1,"m",1,"m"

"fcm3"

0

0

-99,0

10,"yr",1

"Air Concentration","Gas",,"kg/m3",1,"m",1,"m"

"fcm3"

0

0

-99,0

"ANTIMONY-125","SB125",2,1

2,"yr",2

"External Dose",,"","Sv",1,"m",1,"m"

"fcm3"

0

0

-99,5

"Air Concentration","Gas",,"Bq/m3",1,"m",1,"m"

"fcm3"

0

0

-99,0

4,"yr",2

"External Dose",,"","Sv",1,"m",1,"m"

"fcm3"

0

0

-99,6

"Air Concentration","Gas",,"Bq/m3",1,"m",1,"m"

"fcm3"

0

0
-99,0
"TELLURIUM 125M","TE125M",2,"ANTIMONY-125","SB125"
1,"yr",1
"Air Concentration","Gas","", "Bq/m3",1,"m",1,"m"
"fcm3"
0
0
-99,0
3,"yr",1
"Air Concentration","Gas","", "Bq/m3",1,"m",1,"m"
"fcm3"
0
0
-99,0
"Benzene","71432",2,0
900,"yr",1
"Deposition","Gas","", "kg/m2",1,"m",1,"m"
"fcm3"
0
0
-99,0
1900,"yr",1
"Deposition","Gas","", "kg/m2",1,"m",1,"m"
"fcm3"
0
0
-99,0
"Beryllium","7440417",5,0
0,"yr",0
"Deposition","Gas","", "kg/m2",1,"m",1,"m"
"fcm3"
0
0
-99,0
"Air Concentration","Gas","", "kg/m3",1,"m",1,"m"
"fcm3"
0
0
-99,0
1,"yr",0
"Deposition","Gas","", "kg/m2",1,"m",1,"m"
"fcm3"
0
0
-99,0
"Air Concentration","Gas","", "kg/m3",1,"m",1,"m"
"fcm3"
0
0
-99,0
2,"yr",0
"Deposition","Gas","", "kg/m2",1,"m",1,"m"
"fcm3"
0
0

-99,0
"Air Concentration", "Gas", "", "kg/m3", 1, "m", 1, "m"
"fcm3"
0
0
-99,0
3, "yr", 0
"Deposition", "Gas", "", "kg/m2", 1, "m", 1, "m"
"fcm3"
0
0
-99,0
"Air Concentration", "Gas", "", "kg/m3", 1, "m", 1, "m"
"fcm3"
0
0
-99,0
4, "yr", 0
"Deposition", "Gas", "", "kg/m2", 1, "m", 1, "m"
"fcm3"
0
0
-99,0
"Air Concentration", "Gas", "", "kg/m3", 1, "m", 1, "m"
"fcm3"
0
0
-99,0
"STRONTIUM-90", "SR90", 3, 1
0, "yr", 0
"Deposition", "Gas", "", "Bq/m2", 1, "m", 1, "m"
"fcm3"
0
0
-99,0
"Air Concentration", "Gas", "", "Bq/m3", 1, "m", 1, "m"
"fcm3"
0
0
-99,0
10, "yr", 0
"Deposition", "Gas", "", "Bq/m2", 1, "m", 1, "m"
"fcm3"
0
0
-99,0
"Air Concentration", "Gas", "", "Bq/m3", 1, "m", 1, "m"
"fcm3"
0
0
-99,0
20, "yr", 0
"Deposition", "Gas", "", "Bq/m2", 1, "m", 1, "m"
"fcm3"
0
0
-99,0

"Air Concentration", "Gas", "", "Bq/m3", 1, "m", 1, "m"
"fcm3"
0
0
-99,0
"YTTRIUM-90", "Y90", 0, "STRONTIUM-90", "SR90"

* File: C:\FRAMES\ATOTEST2.ATO
* Section: air2
* Date: 6/26/00 12:36:25 PM

8
"=====
" FUJ Known Air Concentration Module"
" Version 1.00 August 1, 1998"
" Run: C:\FRAMES\ATOTEST2.GID"
" Site: Scenario 1"
" Glyph: air2"
" 06-26-2000"
"====="

2
3, "air2"
"Particle 1", 0.03, "um", 1.5, "g/cm^3"
"Particle 2", 3, "um", 1.5, "g/cm^3"
"Particle 3", 10, "um", 1.5, "g/cm^3"
"acute", "cartesian", "points", 2, 2000, 6, 22, 9, 18
"Benzene", "71432", 2, 0
0, "hr", 2
"Deposition", "Particle 1", "total", "kg/m2", 1, "m", 1, "m"
"fcm3"
20
400
-99,1
"Air Concentration", "Particle 1", "", "kg/m3", 1, "m", 1, "m"
"fcm3"
20
400
-99,2
2, "hr", 2
"Deposition", "Particle 1", "total", "kg/m2", 1, "m", 1, "m"
"fcm3"
20
400
-99,4
"Air Concentration", "Particle 1", "", "kg/m3", 1, "m", 1, "m"
"fcm3"
20
400
-99,5
"STRONTIUM-90", "SR90", 3, 1
0, "hr", 3
"External Dose", "", "", "Sv", 1, "m", 1, "m"
"fcm3"
20
400

-99,101
 "Deposition","Particle 2","wet","Bq/m2",1,"m",1,"m"
 "fcm3"
 20
 400

-99,102
 "Air Concentration","Particle 2","", "Bq/m3",1,"m",1,"m"
 "fcm3"
 20
 400

-99,103
 10,"hr",3
 "External Dose","", "Sv",1,"m",1,"m"
 "fcm3"
 20
 400

-99,105
 "Deposition","Particle 2","wet","Bq/m2",1,"m",1,"m"
 "fcm3"
 20
 400

-99,106
 "Air Concentration","Particle 2","", "Bq/m3",1,"m",1,"m"
 "fcm3"
 20
 400

-99,107
 20,"hr",3
 "External Dose","", "Sv",1,"m",1,"m"
 "fcm3"
 20
 400

-99,109
 "Deposition","Particle 2","wet","Bq/m2",1,"m",1,"m"
 "fcm3"
 20
 400

-99,110
 "Air Concentration","Particle 2","", "Bq/m3",1,"m",1,"m"
 "fcm3"
 20
 400

-99,111
 "YTTRIUM-90","Y90",0,"STRONTIUM-90","SR90"
 3,"air2"
 "Particle 1",0.03,"um",1.5,"g/cm^3"
 "Particle 2",3,"um",1.5,"g/cm^3"
 "Particle 3",10,"um",1.5,"g/cm^3"
 "acute","cartesian","points",2,2000,6,22,9,18
 "Benzene","71432",2,0
 0,"hr",2
 "Deposition","Particle 1","total","kg/m2",1,"m",1,"m"
 "fcm4"
 99
 450

-99,569
 "Deposition","Particle 3","total","kg/m2",1,"m",1,"m"

"fcm4"
99
450
-99,542
2,"hr",2
"Deposition","Particle 1","total","kg/m2",1,"m",1,"m"
"fcm4"
99
450
-99,41548
"Deposition","Particle 3","total","kg/m2",1,"m",1,"m"
"fcm4"
99
450
-99,4887
"STRONTIUM-90","SR90",3,1
0,"hr",6
"Deposition","Particle 1","dry","Bq/m2",1,"m",1,"m"
"fcm4"
99
450
-99,30
"Deposition","Particle 2","dry","Bq/m2",1,"m",1,"m"
"fcm4"
99
450
-99,60
"Deposition","Particle 3","dry","Bq/m2",1,"m",1,"m"
"fcm4"
99
450
-99,90
"Air Concentration","Particle 1","", "Bq/m3",1,"m",1,"m"
"fcm4"
99
450
-99,1
"Air Concentration","Particle 2","", "Bq/m3",1,"m",1,"m"
"fcm4"
99
450
-99,4
"Air Concentration","Particle 3","", "Bq/m3",1,"m",1,"m"
"fcm4"
99
450
-99,7
10,"hr",6
"Deposition","Particle 1","dry","Bq/m2",1,"m",1,"m"
"fcm4"
99
450
-99,40
"Deposition","Particle 2","dry","Bq/m2",1,"m",1,"m"
"fcm4"
99
450

-99,70
"Deposition","Particle 3","dry","Bq/m2",1,"m",1,"m"
"fcm4"
99
450
-99,91
"Air Concentration","Particle 1","", "Bq/m3",1,"m",1,"m"
"fcm4"
99
450
-99,2
"Air Concentration","Particle 2","", "Bq/m3",1,"m",1,"m"
"fcm4"
99
450
-99,5
"Air Concentration","Particle 3","", "Bq/m3",1,"m",1,"m"
"fcm4"
99
450
-99,8
20,"hr",6
"Deposition","Particle 1","dry","Bq/m2",1,"m",1,"m"
"fcm4"
99
450
-99,50
"Deposition","Particle 2","dry","Bq/m2",1,"m",1,"m"
"fcm4"
99
450
-99,80
"Deposition","Particle 3","dry","Bq/m2",1,"m",1,"m"
"fcm4"
99
450
-99,92
"Air Concentration","Particle 1","", "Bq/m3",1,"m",1,"m"
"fcm4"
99
450
-99,3
"Air Concentration","Particle 2","", "Bq/m3",1,"m",1,"m"
"fcm4"
99
450
-99,6
"Air Concentration","Particle 3","", "Bq/m3",1,"m",1,"m"
"fcm4"
99
450
-99,9
"YTTRIUM-90","Y90",0,"STRONTIUM-90","SR90"