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**Pacific Northwest  
National Laboratory**

Operated by Battelle for the  
U.S. Department of Energy

**FRAMES 1.x Software System:  
Sensitivity/Uncertainty Multimedia  
Modeling Module (SUMMM)  
Application Manager**

K. J. Castleton  
G. Whelan  
B. L. Hoopes

October 2006



Prepared for  
Engineer Research and Development Center  
U.S. Army Corps of Engineers  
Vicksburg, MS  
under Contract DE-AC05-76RL01830

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## Summary

The Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) is a Windows-based software platform that provides an interactive user interface and, more importantly, specifications to allow a variety of disk operation system (DOS) and Windows-based environmental codes to be integrated within a single framework. The major components of the FRAMES software include modules (module user interface, environmental code and potentially pre- and/or post-processors), the Framework User Interface (FUI), sensitivity/uncertainty module, databases, and data viewers. Although FRAMES is domain independent, it is being used herein to support environmental assessment. Modules represent a particular step in the risk assessment process, such as type of contaminant selection, source release, fate and transport (groundwater, vadose zone, surface water, air, overland), exposure pathway (farm foodchain, ingestion, inhalation, dermal, external), and risk (dose, cancer incidence or fatalities, and hazard quotient). Modules can accept data from the user or other modules and can calculate some portion of the risk assessment. The FUI allows the user to interact with the system. The sensitivity/uncertainty module allows the user to conduct a Monte Carlo (MC) analysis, and the viewers allow results to be reviewed from a particular stage in the process. To achieve realistic scenarios, users often need to combine multiple modules and databases together, where data seamlessly flows from one component to the next.

FRAMES currently has a mechanism to perform MC uncertainty analyses, including Latin Hypercube sampling. Because the user has the ability to link an unlimited number of components together to describe transport, exposure, and risk scenarios, there is the distinct possibility that the execution time for an MC assessment could occur for an extended period of time. Ideally, the execution would be most beneficial if the execution occurs when the computer is not in use, so its central processing unit (CPU) can be focused on completing the MC analysis. To avoid tying up a user's computer while engaging in other activities, the software provides the ability to execute MC runs at a time most convenient for the user. This effort provides the option of executing an MC-based run at a later time (e.g., at night during off hours, when the CPU is not allocated to other activities). As part of the MC user interface, a start time, within the next 24 hours, has been added to the user interface. Working similar to a programmed VCR, the MC assessment begins at the user-specified start time, correlated to the PC's clock, and the program stops when FRAMES has completed its run.

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



## Acronyms

ADDAMS	Automated Dredging Decision, Analysis, and Modeling System
ARAMS	Adaptive Risk Assessment Modeling System
BSAF	Bio-Sediment Accumulation Factor (database)
COC	Compound of concern
CPU	Central processing unit
CSM	Conceptual Site Model, simplified description of the environmental problem to be modeled
DoD	U.S. Department of Defense
DOE	U.S. Department of Energy
DOS	Disk Operation System, basic operation system on the computer
EHQ	Ecological hazard quotient
EPA	U.S. Environmental Protection Agency
ERD	Ecosystems Research Division
ERDC	Engineer Research and Development Center
FRAMES	Framework for Risk Analysis in Multimedia Environmental Systems
FUI	Framework User Interface
GMS	Groundwater Modeling System
MC	Monte-Carlo
MEPAS	Multimedia Environmental Pollutant Assessment System
NERL	National Exposure Research Laboratory
NRC	U.S. Nuclear Regulatory Commission
OCRWM	Office of Civilian Radioactive Waste Management
ORD	Office of Research and Development
ORIA	Office of Radiation and Indoor Air
OSW	Office of Solid Waste
PCB	Polychlorinated biphenyl
PNNL	Pacific Northwest National Laboratory
QA/QC	Quality Assurance and Quality Control, processes that confirm the quality of the product
RAIS	Risk Assessment Information System
SUMMM	Sensitivity/Uncertainty Multimedia Modeling Module
TTD	Terrestrial Toxicity Database



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# 1.0 Introduction

The Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) is a Windows-based software platform that provides an interactive user interface and, more importantly, specifications to allow a variety of disk operations system (DOS) and Windows-based environmental codes to be integrated within a single framework. The major components of the FRAMES software include modules (module user interface, environmental code, and potentially pre- and/or post-processors), the Framework User Interface (FUI), sensitivity/uncertainty module, and data viewers. Modules can accept data from the user or other modules and can calculate some portion of the risk assessment. The FUI allows the user to interact with the system. The sensitivity/uncertainty module allows the user to conduct a Monte Carlo (MC) analysis, and the viewers allow results to be reviewed from a particular stage in the process.

FRAMES is a software platform that allows users the ability to select and implement environmental software models for risk assessment and management problems. This program is a flexible and holistic approach to understanding how activities affect humans and the environment. It links models that integrate across scientific disciplines, allowing for tailored solutions to specific activities, and it provides meaningful information to business and technical managers. FRAMES is the key to identifying, analyzing, and managing potential environmental, safety, and health risks. The purpose of FRAMES is to assist users in developing environmental scenarios and to provide options for selecting the most appropriate computer codes to conduct human and environmental risk-management analyses.

## 1.1 Background

The U.S. Environmental Protection Agency (EPA) is charged with developing, implementing, and enforcing regulations concerning protecting human and ecological health from the myriad of chemical and non-chemical stressors imposed on the environment as a result of human activities. The U.S. Department of Energy (DOE), U.S. Department of Defense (DoD) Army Corps of Engineers, Engineer Research and Development Center (ERDC), and U.S. Nuclear Regulatory Commission (NRC), in response to existing and emerging regulatory requirements for environmental protection, have developed significant programs to assess exposure and risk at their facilities. In pursuing these activities, ERDC, NRC, DOE, and EPA share a common need to understand the environmental processes (physical, biological, and chemical) that collectively release, transform, and transport contaminants and result in exposure and finally a probability of deleterious health effects. At ERDC, NRC, EPA, and DOE, computer models are key tools to organize the knowledge of environmental science and apply it to the decision-making process.

Through the past 13 years, EPA and DOE have jointly pursued common interests related to environmental modeling. For example, in 1995, DOE's Pacific Northwest National Laboratory (PNNL) and the EPA Office of Air and Radiation in the Office of Radiation and Indoor Air (ORIA) joined efforts to design and develop a prototype multimedia modeling system. The unique aspect of this effort was the incorporation of software modules representing individual steps of a risk assessment (e.g., source release of contaminants, fate and transport in surface water, exposure) within a software framework. A module represents the computer model (i.e., code), pre- and post-processors, and user interface. The software framework was designed using "object-oriented" design and, as such, allowed for the decoupling of individual models. This design greatly improved the ability of model developers (e.g., a modeler developing a new surface-water model) to "plug" the new model into a full multimedia modeling system

without the need to develop a complete modeling system. The product of this effort was FRAMES. FRAMES Version 1 allows a user to conduct multimedia simulations of contaminant-based exposure and risk at a single facility.

Concurrent to the development of FRAMES Version 1, DOE and the EPA Office of Research and Development (ORD), Ecosystems Research Division (ERD,) in Athens, Georgia, also initiated a joint effort in 1995 to study existing technology and future needs of EPA and DOE related to multimedia/multi pathway exposure and risk assessment. The latest stage of joint efforts between DOE and EPA (1998 to 2001) was to extend and refine FRAMES to build a modeling system capable of conducting a national assessment of exposure and risk as a result of contaminant releases from hazardous waste sites. This national assessment modeling approach is called FRAMES-3MRA and was developed and implemented for the EPA Office of Solid Waste (OSW). In the past several years, the EPA National Exposure Research Laboratory (NERL) has responded to these needs by establishing specific research and development tasks to “integrate” all multimedia modeling-based activities, including the FRAMES-based efforts. The goal of this initiative is to design and implement, over the next decade, a multimedia integrated modeling system that will facilitate future environmental assessments and related research. EPA-ORD-ERD is currently supporting the merger of the FRAMES Version 1, which is designed for site-specific assessments, with FRAMES-3MRA, which is designed to perform regional and national assessments. The intent is to capture the best attributes of both into one system for use by others to form FRAMES Version 2.

Concurrent to and in parallel with EPA and DOE, ERDC and NRC have programs that support various aspects associated with the FRAMES approach. ERDC initiated the development of the Adaptive Risk Assessment Modeling System (ARAMS) because the military needed a system that was compatible and consistent with similar systems at other agencies. NRC initiated the linkage of various models contained in the Groundwater Modeling System (GMS) with FRAMES, so users would have direct access to more science-supported groundwater models for their assessment exercises. In each case, FRAMES represents middle where that seamlessly connects these disparate components, and FRAMES is used as the execution manager.

ARAMS is a computer-based, information delivery, modeling, and analysis system that integrates multimedia fate/transport, exposure, uptake, and effects of constituents (i.e., compounds of concern [COCs], including chemicals and radionuclides) to assess human and ecological health impacts and risks (<http://www.wes.army.mil/el/arams/arams.html>). ARAMS uses an object-oriented, system framework to construct a computational conceptual site model composed of the environmental pathways and exposure routes linked to various models and databases for exposure and effects assessments.

The Multimedia Environmental Pollutant Assessment System (MEPAS) is one of the modeling systems in ARAMS that helps form the basis for many of the preliminary- or screening-level models/calculations, including releases from contaminant sources; fate/transport in air, streams, vadose zone, and groundwater; multimedia exposure pathways for humans, such as food via uptake through crops and farm animals; human intake; and human health impact/risk calculations. The MEPAS fate/transport models are typically semi-analytical solutions to simplified transport equations for each medium. Other ERDC and related models (e.g., RECOVERY, TPB, TWEM, WEAP, and HELPQ) have been added, and others can be added later as needed. RECOVERY and HELPQ are part of the U.S. Army Corps of Engineers Automated Dredging Decision, Analysis, and Modeling System (ADDAMS).

ARAMS provides additional ecological features that many of the current systems do not. Several web-based ecological databases have been linked to the system, including the Terrestrial Toxicity Database

(TTD), which contains ecological soil screening levels and ecological-effects toxicity reference values for wildlife that can be used to screen soil concentrations and compute ecological hazard quotients (EHQ), respectively. There is also a Bio-Sediment Accumulation Factors (BSAF) database that contains BSAF and percent lipid values for various aquatic organisms. BSAF is used to compute tissue residues (mg/kg) of constituents of concern in aquatic organisms. The system is also linked to the web-based Risk Assessment Information System (RAIS). This allows for the direct download of chemical-specific factors (physicochemical properties, exposure factors, and bioaccumulation factors) and human health toxicity reference values.

The NRC required seamless linkages between numerical groundwater models and models addressing other aspects of the hydrosphere, biosphere, atmosphere, and geosphere. Specifically, when licensed nuclear facilities want to terminate their nuclear operating license, they need to demonstrate that the facility, when vacated, does not create an unacceptable health impact. NRC provides approaches for the license terminations, but those approaches are very conservative and may not show that the site has *de minimus* impacts. As such, NRC wants to provide the license terminations with access to some of the most sophisticated groundwater models in the world, contained in the GMS (<http://www.emrl.byu.edu/gms.htm>). FRAMES provides the ability to link models to GMS, so more sophisticated and science-based models can be used in the license termination process with other non-groundwater modeling systems.

While the various federal agencies (i.e., DoD, EPA, NRC, and DOE) are sponsoring their own individual projects, they are also working together to confirm that their investments in FRAMES are leveraged to the products that are useful to others. The efforts described herein represent a product of the leveraged investment.

## 1.2 Component Description

The FRAMES 2.0/ARAMS 2.0 MC module provides great flexibility in performing probabilistic assessments. As with any MC approach, the number of realizations and run times of the models dictate the length of time the PC may be engaged in calculations. To avoid tying up a computer while the user is engaged in other activities, the software developed under this task will provide the capability to execute MC runs so as to maximize the user's ability perform other tasks while the probabilistic analysis is executing. One method that does not currently appear feasible is the option of running the assessment in the background while the user is simultaneously executing other tasks. FRAMES is structured in a way that does not allow for a mechanism that would not interrupt the user on the computer during simulations. This is because FRAMES uses models that are executables, and, therefore, FRAMES is at the will of the operating system with respect to pop-ups in the Windows environment (e.g., when windows pop up, and which window is the current window). Although it would be worthwhile to run the MC simulation in the background where it does not tie up the desktop too much, Microsoft Windows does not allow for easy control of pop-up windows. Because pop-up windows cannot be easily eliminated, execution in background would not be recommended at this time.

To potentially allow for the efficient execution of MC assessments within the FRAMES-ARAMS paradigm, a query screen will provide with the option of executing an MC-based run at a later time (e.g., at night during off hours when the central processing unit (CPU) is not allocated to other activities). As part of the MC user interface, a start time would be added to the interface. This requires the baseline problem to be pre-established, pre-run, and ready to execute. Working similarly to a programmed VCR,

the MC assessment would begin at the user-specified start time, designated by the user in military time (e.g., 1300 hrs as 1 pm), and the program would run to completion.

The current Sensitivity/Uncertainty Multimedia Modeling Module (SUMMM) executes immediately when the user presses the run button. This modification will add two choices to the user interface, using radio buttons, of which the user must choose one or the other, but not both:

- Delay Execution—Making this choice would prepare the module to execute at a time in the next 24 hours, as specified by the user. This variable will be the time of the day to begin execution. The SUMMM module will read this value and wait until that time within the next 24 hours to begin the actual effort of simulating the MC realizations. Time would be represented as Military Time, using an integer for hours from 1 to 23 (e.g., 1300 hrs for 1 pm). For example, if the current time is 4 pm (i.e., 1600 military time), and the user designated a start time of 2 am, the user would specify 0200 hours or 2.
- Execute Immediately—If the “Delay Execution” option is NOT chosen, then when the user exited the user interface, the module would be ready to execute immediately.

After making the choice (i.e., Run Now or Delay Run), the user would Save and Exit under the File Menu. To execute the choice, the user chooses “Run Model” as part of its Stop Light choices.

## 2.0 Requirements

Requirements are characteristics and behaviors that a piece of software must possess to function adequately for its intended purpose. The main requirements for the modification to SUMMM is presented as follows:

- 1 Confirm that the modified SUMMM should function as before and meet all previous requirements.
- 2 Allow the user to not delay the MC simulations.
- 3 Allow the user to delay the starting time of the MC simulations up to 23 hours by allowing for a user-defined starting time.
- 4 Start the simulations at the user-defined time.

### 3.0 Design

Design elements are strategies for meeting requirements. The SUMMM is designed to meet the requirements identified in Section 2.0. Key to meeting those requirements is adding the capability for the user to delay the MC simulation until a user-specified start time occurs. If the choice is not made to delay the execution, then when the user runs the module, the MC application will begin immediately. One important feature of the design is that the loop that waits for the appropriate time to start needs to consume almost no CPU time. That is to say, the SUMMM module should consume almost no computational resources while it is waiting. This will be accomplished by using MS-Windows operating system “calls,” which allow for the application to be put to sleep from a number of hours to minutes.

Figure 1 presents a modified user interface. If the user does NOT check the “Delay Execution” box, the MC application will execute when the user runs the module. If the user checks the “Delay Execution” box, the start time, which begins as a grayed-out number, becomes active, and the user can specify a start time in military time within in the next 23 hours. So, if the current time is 9 am (i.e., 0900 military time), and a start time of 3 pm is defined, then the user would specify to delay the run until 1500 hours military time, or type in “15.”

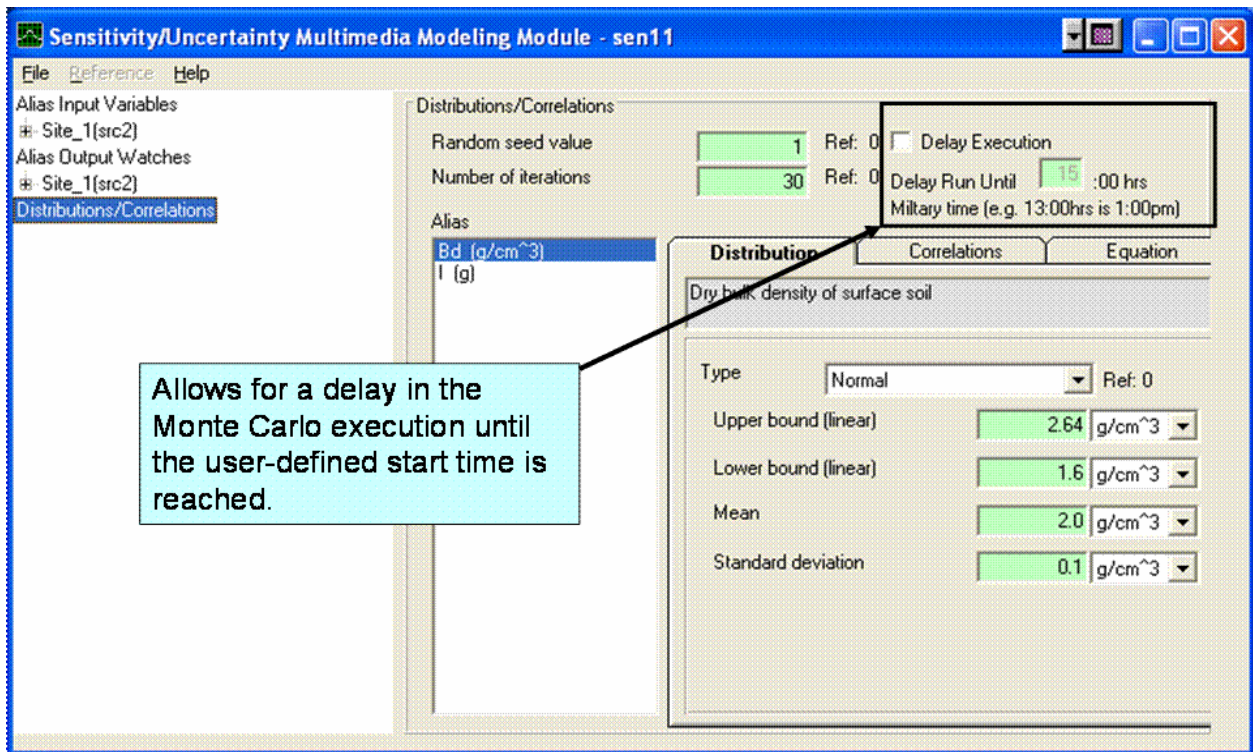
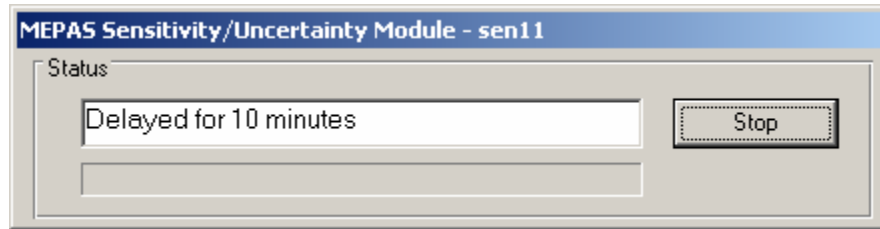


Figure 3.1. The Modified SUMMM User Interface

If the current time is after the requested time, then the delay occurs at the next available time the user-defined military time occurs. This has the effect of having times before the current time delayed until the

next day. So, if it is 10 am (1000 military time), and the requested start time is 5 am (0500 military time), then the SUMMM will begin execution on the morning of the next day. The number of minutes delayed is shown to the user. Figure 2 shows an example of where the start time was 10 minutes into the future. The “Stop” button can be used to terminate the SUMMM if the delay was accidental.



**Figure 3.2.** An Example of the SUMMM that is Delayed



## 4.0 Specifications

Specifications are the descriptions of input and output files that are used during execution of a component. Alongside these input and output descriptions, how the component is invoked and how the component was compiled are also discussed.

This modification to the SUMMM simply adds two new values to the user interface. The integer parameter `StartTime` will be added to the user interface. The default will be 0. The range in acceptable values for this parameter is 0 to 23. `StartTime` represents the military time hour to start the simulations. The second variable is the `NoDelay` flag that defines whether the simulation should or should not be delayed. A value of T will delay the simulation until the user-designated input `StartTime`.

**Table 4.1.** The New Parameters for the SUMMM User Interface

Variable	Units	Minimum	Maximum	Description
<code>StartTime</code>	N/A	0	23	The hour start time the SUMMM simulation
<code>NoDelay</code>	N/A	F	T	A flag indicating whether a delay should occur. T indicates a delay should occur. F indicates it should not.

### 4.1 Command Line

The command line for the SUMMM is the standard FRAMES 1.x module command line. The module when invoked is passed the FRAMES path, the Simulation Name, and the Module Name. These three pieces of information are required to connect to interface to the FRAMES 1.x system.

### 4.2 Compiler Version

The SUMMM user interface is written using MS-Visual Basic 6.0. The module is written in Borland C++ version 3.0.

## 5.0 Testing Approach and Results

The test procedure summary includes as a minimum the date, name of tester, and version. The target requirements should be clearly identified. Other information that is helpful and may be appropriate to add to the test procedure summary is start time, end time, and location of the test. If there are any regulations or change request documentations related to the test, then that information should also be noted in the summary of the test procedure.

### **Pass/Fail Test Criteria**

Test criteria should be defined before testing. A standard set of nomenclature needs to be identified and documented. The standardization explanation needs to be archived with the test procedures so that future assessors can fully understand the testing measurement employed. An explanation of what success/failure means is critical for the defensiveness of the test.

### **Test Procedure Components:**

A log of the test should be documented containing information on the steps that demonstrate the requirement, expected results, and requirement specific criteria used to determine a pass or fail finding. Related comments and documentation should also be captured. It is very valuable to identify the documents used to support the understanding and expectation of the requirement (e.g., statement of work, users guide, help file). This identification of related documentation helps to tie together a quality documentation package of procedures for future readers.

When designing the flow of a testing procedure, there are several types of requirements that can be grouped to facilitate testing, including functional requirements, data flow, calculations, output checks, and user-scenario cases.

- **Functional Requirements**—Functions that exist in each component of the system, based on client requirements.
- **Data Flow**—Flow of information between users, database tables, modules, displays, and the output produced.
- **Calculations**—Any processing of module/display values, including units conversions. Any data transformation should be documented and tested for the system.
- **Outputs Check**—Confirmation of the correct generation of the output products.
- **Additional Scenarios**—Scenarios that are developed to provide some holistic assessment of cases that may be possible and relevant to expected use of the product.

Other information, such as prerequisite requirements, inputs, and assumptions, can also be collected and should be documented, if they exist.

Other supporting tools should be considered, where appropriate. Tools such as change tracking and automated testing are helpful in sustaining a quality testing process.

## 5.1 Test Sequence

Requirements for delaying the execution of an MC run until a user-defined Time occurs are summarized in the Requirements Section of this document and are succinctly presented in Table 5.1. The requirements are written as concise, fundamental, testable requirements.

**Table 5.1.** Summary of Requirements for Delaying the Execution of an MC Run Until a User-Defined Time Occurs

<b>Requirement Number</b>	<b>Requirement</b>
1	Confirm that the modified SUMMM should function as before and meet all previous requirements.
2	Allow the user to not delay the MC simulations.
3	Allow the user to delay the starting time of the MC simulations up to 23 hours by allowing for a user-defined starting time.
4	Start the simulations at the user-defined time.

To confirm that the software meets the requirements listed in Table 5.1, the following test case was developed to confirm the performance delaying an MC application. Only one test case was necessary to prove that the modifications to the SUMMM user interface were successful.

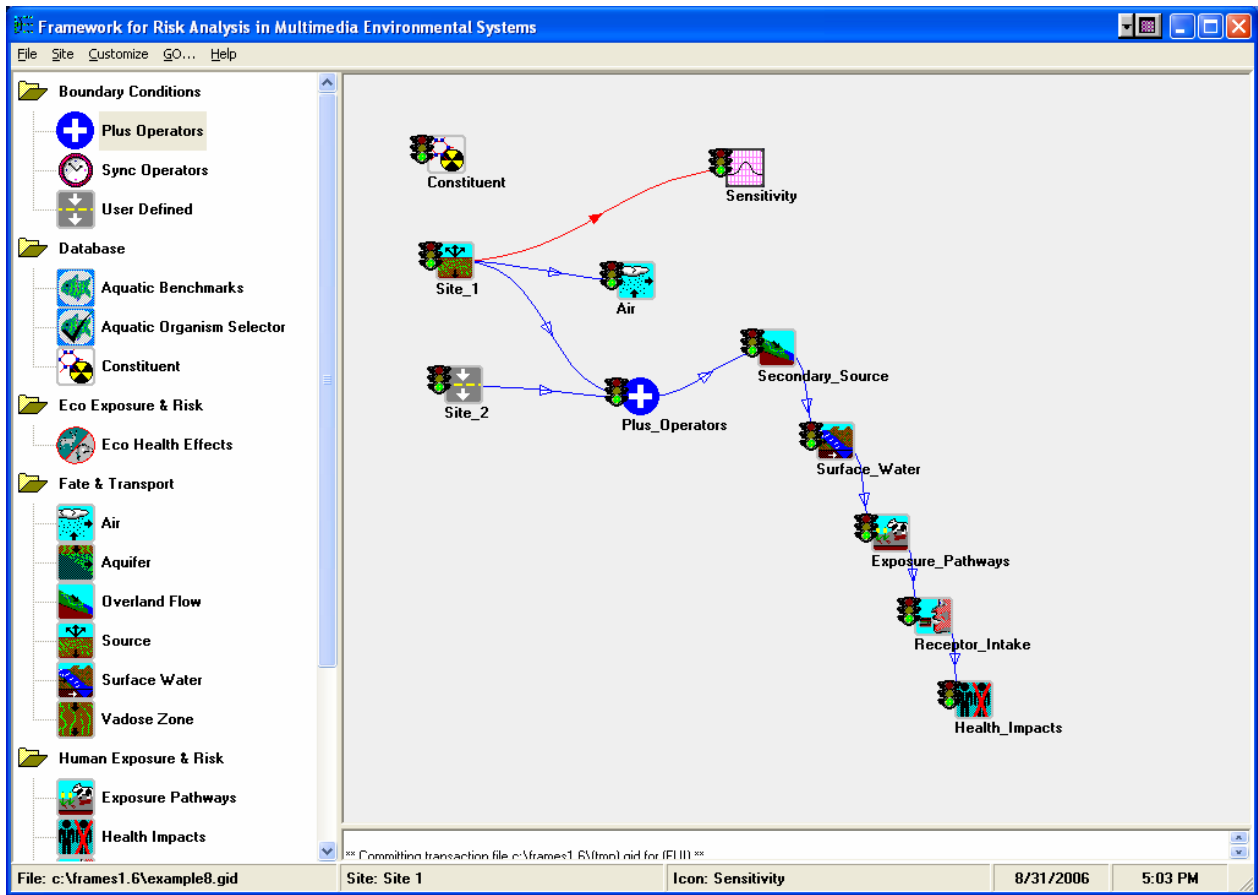
## 5.2 Test Case Example 8

### 5.2.1 Description

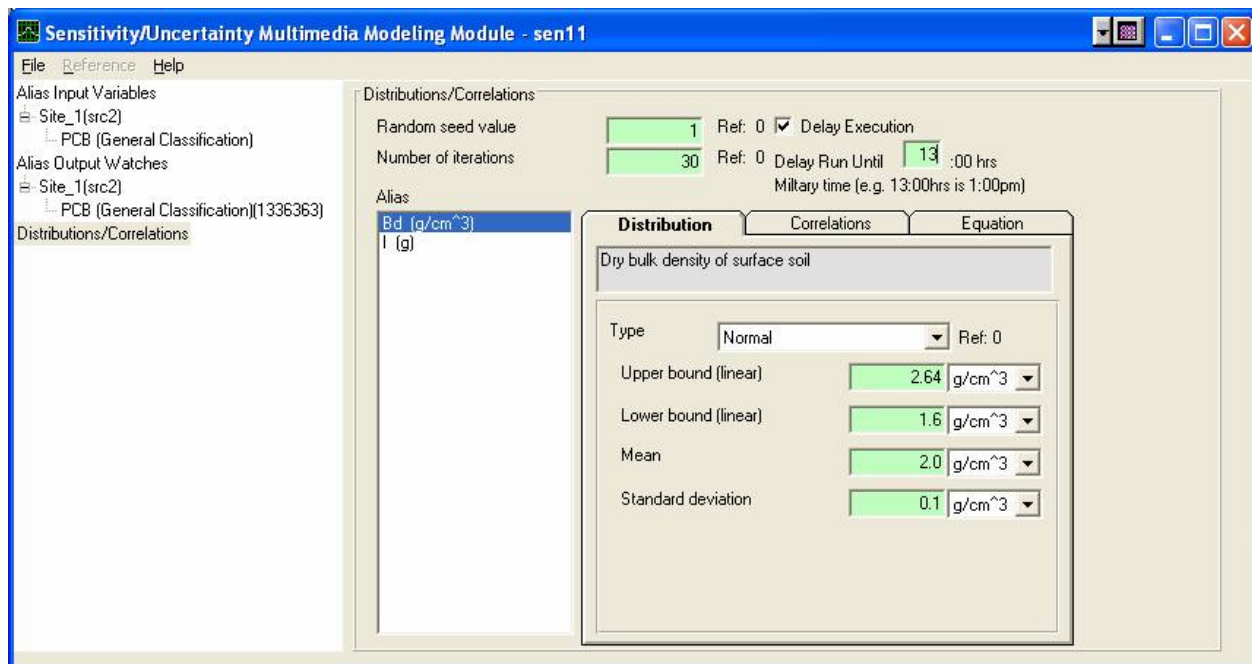
The purpose of this test case is to test the general functionality of delaying the start of an MC simulation until a user-defined time. The SUMMM user interface has been modified to allow the user to specify a start time in terms of military time. This test case will examine and test Requirements 1 and 4. Figure 5.1 presents the Conceptual Site Model, associated with Example 8. The test is to see if the MC application executes when specified. There are no output results to inspect for accuracy.

### 5.2.2 Input Data

The input data for this test case are documented in Figure 5.2. The “Delay Execution” option was chosen, and the MC application was delayed until 1 pm (1300 hours military time).



**Figure 5.1.** Conceptual Site Model (CSM) Testing the Fundamental Requirements of 1 through 4 for Testing the Option to Delay an MC Run Until a User-Defined Time



**Figure 5.2.** SUMMM User Interface Depicting the User-Defined Input to Delay an Execution Until 1 pm (1300 hours military time)

### 5.2.3 Expected Results

The following results are expected: At 1 pm (1300 hours military time), the SUMMM will execute its MC simulations

### 5.2.4 Conducting the Test

The following are the steps that were used to test the appropriate behavior of the modifications to the SUMMM user interface to delay the execution of the MC application.

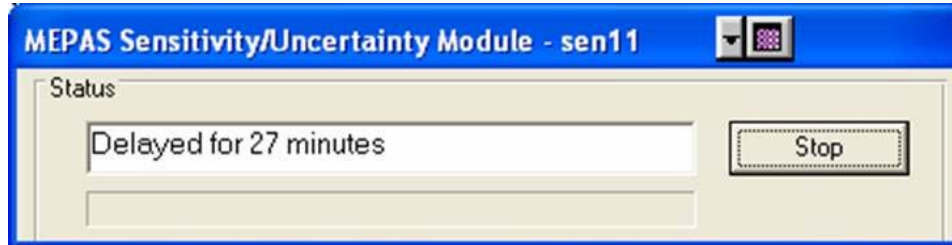
- 1 Open Example8.gid.
- 2 Add a sensitivity icon to the diagram.
- 3 Attach an arrow from the source (Site\_1) to the SUMMM module.
- 4 Choose the SUMMM module for the sensitivity icon.
- 5 In the sensitivity interface, select src2 Site\_1 Dry Bulk Density and Inventory Quantity, PCB,<sup>(a)</sup> and add Bd and I as the aliases, respectively.
- 6 Choose the (src2 Site\_1) under the Alias Output Watches.
- 7 Choose Adsorbed Constituent Flux at year(s) # (, #...) for PCB (General Classification) (1336363), and add an alias of Ca.
- 8 Choose Distribution/Correlations from the tree control.

(a) PCB = polychlorinated biphenyl

- 9 Set the distributions and statistical parameters for Bd and I.
- 10 Do not choose “Delay Execution.”
- 11 Choose Files, save and exit.
- 12 Right-click on the SUMMM icon and “Run Model.” The behavior should be as in previous versions.
- 13 Choose “Delay Execution” in the user interface, and delay the execution until 1 pm (1300 hours military time) by inputting 13.
- 14 Choose Files, save and exit.
- 15 Right-click on the SUMMM icon and “Run Model.” A screen should appear that tells the user the number of minutes before the execution will begin. After the execution begins, the behavior should be as in previous versions.

## 5.2.5 Results

When the user-defined information was input, as specified in Figure 5.2, and Steps 1 through 15 in Section 5.2.4 were implemented, the program returned a message, indicating a delay of 27 minutes, as illustrated by Figure 5.3. As the computer’s clock approached 1 pm, the screen, as identified in Figure 5.3, also approached zero minutes. When zero minutes occurred, the MC simulation was successfully executed as if there was no delay.



**Figure 5.3.** Message that is Automatically Generated, Indicating the Time Remaining in Minutes Before the MC Application is Executed

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<http://www.epa.gov/athens/research/modeling/supermuseum/supermuseum.html>

### 6.1 Documentation for the FRAMES-3MRA Technology Software System

Volume 1: *Overview of the FRAMES-HWIR Technology Software System*. 1998. PNNL-11914, Vol. 1, Pacific Northwest National Laboratory, Richland, Washington.

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