

# Documentation for the Surface Water (Non-Tidal River) Transport Module of the Multimedia Environmental Pollutant Assessment System (MEPAS)

Compiled from Former Publications [PNNL-SA-32276](#) and [PNNL-11176](#)

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# Documentation for the Surface Water (Non-Tidal River) Transport Module of the Multimedia Environmental Pollutant Assessment System (MEPAS)

## 1.0 Introduction

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This documentation provides information on a component of the Multimedia Environmental Pollutant Assessment System (MEPAS), including requirements, design and specifications or formulations, and quality assurance and testing. MEPAS is an integrated impact assessment software comprising physics-based fate and transport models of air, soil, and water media. Outputs are estimates of exposures and health risk assessments for radioactive and hazardous pollutants.

MEPAS simulates the release of contaminants from a source; transport through the air, groundwater, surface water, and/or overland pathways; and transfer through food chains and exposure pathways to the exposed individual or population. For human health impacts, risks are computed for carcinogens and hazard quotients for noncarcinogens.

MEPAS is implemented on a desktop computer with a user-friendly interface that allows the user to define the problem, input the required data, and execute the appropriate models for both deterministic and probabilistic analyses.

The various MEPAS components were originally designed as a suite of tools. They have been specifically revised as objects for inclusion in the Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES), which is a software platform that allows for the linking of various modules into complete emission, transport, and exposure assessment systems ([Whelan et al., 1997](#), PNNL-11748).

Portions of this documentation may have been previously issued in reports from the Pacific Northwest National Laboratory (PNNL), operated by Battelle for the U.S. Department of Energy. All PNNL reports are issued a tracking number. Multiple numbers on the title page of this documentation indicate the numbers of these previous reports.

This documentation can be used by software engineers and testers to ensure that each component functions properly. The information can also be used by analysts and managers to better understand the component's use within FRAMES.



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# Documentation for the Surface Water (Non-Tidal River) Transport Module of the Multimedia Environmental Pollutant Assessment System (MEPAS)

## Requirements of the MEPAS Surface Water (Non-Tidal River) Transport Module

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This section provides an overall summary of the requirements for the MEPAS Surface Water Transport Module. The purpose of the MEPAS Surface Water Transport Module is to simulate the migration and fate of chemical and radionuclide constituents through non-tidal rivers. Detailed input, output, and scientific requirements are described in the sections that follow.

The MEPAS Surface Water Transport Module will

- G1 - simulate contaminant migration for both chemicals and radionuclides through non-tidal rivers and provide output consisting of instantaneous, time-varying, contaminant aqueous concentrations at a point location along the same shoreline from which contaminants entered the river
- G2 - have no limits on the number of constituents considered in a scenario
- G3 - have no restrictions on the number of point locations along the river shoreline at which concentrations are computed
- G4 - operate under Windows 95, 98, 2000, NT, ME, and XP and have a user-friendly MUI with a standard Windows look and feel.
- G5 - meet the module specifications for the Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES), described in [Whelan et al. 1997](#) (PNNL-11748).

## Input Requirements of the MEPAS Surface Water Transport Module

Data needed to simulate contaminant migration through a non-tidal river is obtained from three sources. The previous module (i.e., source term or aquifer) provides the boundary conditions (i.e., time-varying, contaminant mass fluxes entering the river and source dimensions), which are communicated to the module through the Water Flux File (WFF). The user through the module user interface (MUI) provides the river's physical characteristics, which are communicated from the MUI to the model through the Global Input Data (GID) file. A chemical property database provides the constituent chemical properties. The specifications for the WFF and GID file are described in [Whelan et al. 1997](#) (PNNL-11748).

General requirements associated with the MUI are

- M1 - The MUI will operate in Windows 95, 98, 2000, NT, ME, and XP and will have a standard Windows look and feel.
- M2 - 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.
- M3 - The MUI will provide users with a choice of units for all input parameters having dimensions associated with them.
- M4 - The MUI will include a reference feature in which the source of the specified value for each input item can be referenced if desired.
- M5 - The MUI will show the range of values allowed for each input data item, when the cursor is positioned on that item, as a scrolling message at the bottom of the screen. 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 a scrolling error message in addition to the allowed range message. Data input values within range are indicated by a green field background.
- M6 - The MUI will display the module version number, obtained from the module description (DES) file, in an "About" menu.

The MEPAS Surface Water Transport Module obtains the following data from the WFF. Those items listed as required are needed by the module to perform its computations. Other items are read in along with the required data. Because the WFF is a sequential text file, the module will read through unneeded data:

- time-varying, instantaneous, contaminant mass fluxes entering the river (required)
- width and height of the vertical rectangular area (i.e., a vertical plane along the river shoreline) through which contaminants enter the river (only the width is required)
- distance from the water table (or river surface) to the top of the rectangular area
- natural recharge rate
- time-varying, instantaneous water flux entering the river.

The following data are obtained from the MUI and are needed by the MEPAS Surface Water Transport Module to perform its computations:

- river width
- river depth (i.e., thickness of water column)
- river flow velocity
- longitudinal travel distance (i.e., x-coordinate) from the center of the source to the point at which contaminant aqueous concentrations are computed
- river discharge at the receptor location.

The MEPAS Surface Water Transport Module obtains the following data from the chemical property portion of the GID file:

- CASID
- degradation/decay half-life
- decay chain (for radionuclides)
- solubility limit.

## Output Requirements of the MEPAS Surface Water Transport Module

The MEPAS Surface Water Transport Module has the following output requirements:

- O1 - provide its results to a Water Concentration File (WCF) for contaminant aqueous concentration results
- O2 - produce a list file (\*.WLS file) that documents the data actually read in by the model and summarizes intermediate calculation results (e.g., decay constant and lateral dispersion coefficient) and the simulation results (peak concentration and time of peak).

The data provided to the WCF for contaminant aqueous concentration results include instantaneous, time-varying, contaminant aqueous concentrations for each receptor location along the shoreline.

## Scientific Requirements of the MEPAS Surface Water Transport Module

The primary scientific requirements are

- S1 - obey the Law of Mass Conservation
- S2 - simulate advection in one dimension
- S3 - simulate dispersion in one dimension (lateral or y-direction)
- S4 - account for the decay of radionuclides and be able to handle the degradation of chemicals
- S5 - account for the ingrowth of progeny resulting from degradation/decay and be able to handle decay chains with up to nine members (i.e., one parent and eight progeny)
- S6 - compute contaminant aqueous concentrations at the river (downgradient) boundary
- S7 - consider the effect of inflowing tributary or groundwater (or the withdrawl of clean water from the river) between the source and receptor on receptor concentrations.

The implementation of these requirements, in the form of mathematical formulations, is documented in [Whelan et al. 1996](#) (PNNL-10907).



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## Design of the MEPAS Surface Water (Non-Tidal River) Transport Module

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The purpose of the MEPAS Surface Water Transport Module is to simulate the migration and fate of chemical and radionuclide constituents through non-tidal rivers. The module is designed to allow for linking to subsequent media (e.g., another river section or a wetland), should these features become a requirement for a later version of the Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES). A full description of the design parameters, as well as scientific formulations for the various models, can be found in [Whelan and McDonald, 1996](#) (PNNL-11176) and accessed online by following this link:

- [Formulations for the MEPAS Surface Water \(Non-Tidal River\) Module.](#)

Additional design information for the Surface Water Transport Module can be found in

- [Surface Water Transport Module Help files](#)
- Specifications for the Surface Water Transport Module for FRAMES 1.x
  - Input Specifications*
    - [WEF](#)-Water Flux File
  - Output Specifications*
    - [WCF](#)-Water Concentration File
- [Dictionary files](#) for the Surface Water Transport Module for FRAMES 2.x.



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## Quality Assurance and Testing for the MEPAS Surface Water (Non-Tidal River) Transport Module

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The Surface Water Transport Module was developed under a quality assurance (QA) program that looked at the software life cycle: requirements analysis, design, programming, modification, testing, and implementation. Quality is defined as the ability 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 through attention to details.

The program was designed to be compatible with similar processes used by our clients. For example, our QA process compares favorably with that in the U.S. Environmental Protection Agency Directive 2182, *System Design and Development Guidance* (EPA.1997. Directive 2182). It also compares favorably with the Office of Civilian Radioactive Waste Management's *Quality Assurance Requirements and Description, Supplement I, Software* (OCRWM.1995).

Part of the QA program involves testing each component to ensure that it satisfies its requirements. The [requirements](#) section of this documentation provides a list of requirements for the MEPAS Surface Water Transport Module. A test plan was developed with test cases that addressed these requirements. The following table shows how these requirements were addressed in testing.

**Testing Matrix for the MEPAS Surface Water Transport Module**

Requirement	Test Case						
	1	2	3	4	5	6	7
---							
1	Y	-	-	-	-	-	-
2	Y	-	-	-	-	-	-
3	Y	-	-	-	-	-	-
4	Y	Y	Y	Y	-	-	-
5	Y	-	-	-	-	-	-
6	-	Y	-	-	-	-	-
7	Y	-	-	-	-	-	-
8	-	-	-	-	Y	-	-
9	-	-	-	-	-	-	-
10	-	-	-	-	-	-	-
11	-	-	-	-	-	Y	-
12	Y	-	-	-	-	-	-
13	Y	-	-	-	-	-	-
14	-	-	-	-	-	-	Y
15	Y	-	-	-	-	-	-
16	Y	-	-	-	-	-	-
17	-	-	-	-	-	-	-
18	Y	-	-	-	-	-	-
19	Y	-	-	-	-	-	-
20	Y	-	-	-	-	-	-

Since test packages can be affected by coding changes in different versions, the tests (including the documents they generate) are packaged with the FRAMES Install.

For additional information on the QA program, including testing, see the following documents:

- *An Approach to Ensuring Quality in Environmental Software* ([Gelston et al., 1998](#). PNNL-11880)

