Documentation for the Saturated Zone Transport Module of the Multimedia Environmental Pollutant Assessment System (MEPAS)

Compiled from Former Publications PNNL-SA-32275 and PNNL-10907

With Contributions From

J. P. McDonald
C. Sato
G. Whelan

Work supported by various clients, including

U.S. Army Corps of Engineers
Engineer Research and Development Center
Vicksburg, Mississippi

U.S. Department of Energy
Office of Environmental Management
Washington, D.C.

U.S. Environmental Protection Agency
Office of Research and Development, Ecosystems Research Division
Athens, Georgia

U.S. Environmental Protection Agency
Office of Air and Radiation, Office of Indoor Air and Radiation
Washington, D.C.

U.S. Nuclear Regulatory Commission
Office of Nuclear Regulatory Research
Washington, D.C.

Work conducted by

Pacific Northwest National Laboratory
Richland, Washington 99352

Documentation for the Saturated Zone Transport Module of the Multimedia Environmental Pollutant Assessment System (MEPAS)

LEGAL NOTICE

Documentation for the Saturated Zone Transport Module of the Multimedia Environmental Pollutant Assessment System (MEPAS)

Documentation for the Saturated Zone Transport Module of the Multimedia Environmental Pollutant Assessment System (MEPAS)

1.0 Introduction

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.

Documentation for the Saturated Zone Transport Module of the Multimedia Environmental Pollutant Assessment System (MEPAS)

Requirements of the MEPAS Saturated Zone Transport Module

This section provides an overall summary of the requirements for the MEPAS Saturated Zone Transport Module. Detailed input, output, and scientific requirements are described in the sections that follow.

The purpose of the MEPAS Saturated Zone Transport Module is to simulate the migration and fate of chemical and radionuclide constituents through saturated porous media (e.g., aquifers). Input to the module consists of time-varying contaminant mass (or activity) fluxes entering the aquifer, the physical characteristics of the aquifer itself, and the constituent properties. Output consists of time-varying contaminant mass fluxes exiting the aquifer or time-varying contaminant aqueous concentrations at a point within the aquifer.

Currently, contaminant mass fluxes entering the aquifer can originate from a source term within the aquifer or from a vadose zone. The aquifer's physical characteristics are entered through a module user interface (MUI), and constituent properties are obtained from a constituent property database. The output contaminant mass fluxes can be used as input to a river module, and contaminant aqueous concentrations can be used as input to an exposure module. In addition, the output contaminant mass fluxes or aqueous concentrations also can serve as the endpoint of the simulation.

The MEPAS Saturated Zone Transport Module will

- G1 - simulate contaminant migration for both chemicals and radionuclides through saturated porous media (e.g., aquifers) and provide output consisting of instantaneous, time-varying, contaminant mass fluxes exiting the aquifer or instantaneous, time-varying, contaminant aqueous concentrations at a point location within the aquifer
- G2 - have no limits on the number of constituents considered in a scenario
- G3 - have no restrictions on the number of point locations within the saturated zone 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 FRAMES.

Input Requirements of the MEPAS Saturated Zone Transport Module

Data needed to simulate contaminant migration through a saturated zone are obtained from three sources. The previous module (i.e., source term or vadose zone) provides the boundary conditions (i.e., time-varying, contaminant mass fluxes entering the aquifer, water flux from the previous medium or source term, and source dimensions). These conditions are communicated to the module through the Water Flux File (WFF). Through the MUI, the user provides the aquifer?s physical characteristics and the constituent?s distribution coefficient (Kd). The former are communicated from the MUI to the model through the A chemical property database provides the constituents' chemical properties. Global Input Data file (GID) and the model's pre-processor. The GID file is also used to store the chemical property data. The specifications for the WFF and GID file are described in Whelan et al. 1997 (PNNL-11748).

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

- M1 - the MUI will operate in Windows 95, 98, 2000, NT, ME, and XP, with the look 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 it requires.
- 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 the user desires.
- 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 following data are obtained from the WFF by the MEPAS Saturated Zone Transport Module. Those items listed as required are needed by the module to perform its computations. Other items are read and simply reported to the output WFF to meet the WFF specifications:

- time-varying, instantaneous solute fluxes entering the aquifer (required)
- width and length of the horizontal interface plane (i.e., a plane at the water table) through which solute enters the aquifer, if the previous medium is a vadose zone (required)
- width and height of the vertical interface plane (i.e., a plane perpendicular to the water table) through which solute enters the aquifer, if the previous medium is a saturated zone (required)
- distance from the water table to the top of the interface plane (should be zero if the previous medium is a vadose zone, otherwise is greater than or equal to zero if the previous medium is a saturated zone) (required)
- natural recharge rate
- time-varying, instantaneous water flux entering the aquifer (required when the previous medium is a vadose zone).

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

- medium thickness
- total porosity
- effective porosity
- dry bulk density
- Darcian groundwater flow velocity
- longitudinal dispersivity (i.e., x-dispersivity)
- lateral dispersivity (i.e., y-dispersivity)
- vertical dispersivity (i.e., z-dispersivity)
- longitudinal travel distance (i.e., x-coordinate) from the center of the source to the point at which solute concentrations are computed or to the plane through which solute fluxes are computed
- lateral distance (i.e., y-coordinate) from the center of the source to the point at which solute concentrations are computed
- vertical distance (z-coordinate) from the upper surface of the aquifer (e.g., water table) to the point at which concentrations are computed
- constituent distribution coefficient (Kd)
- percentage of the input contaminant mass flux that actually enters the aquifer

The MEPAS Saturated Zone Transport Module obtains the following data from the chemical property section of the GID file:

- CASID (Chemical Abstracts Service Identification Number)
- decay/degradation half-life
- decay chain (for radionuclides)
- solubility limit
- carbon-matter partition coefficient (Koc) (for organics)

The MUI provides users with an estimate of the Kd for each contaminant based on soil property data entered by the user. The Kd values are computed according to Strenge and Peterson, 1989 (PNL-7145). The following soil property data are needed for this estimate:

- percentage of sand
- percentage of silt
- percentage of clay
- percentage of organic matter
- percentage of iron and aluminum
- pH of the pore water
- carbon-matter partition coefficient (obtained from the chemical database).

In addition to allowing the user to enter their own Kd values, the MUI provides the user with options to automatically use the estimated Kd value for single constituents or automatically use estimates for all constituents.

Output Requirements of the MEPAS Saturated Zone Transport Module

The MEPAS Saturated Zone Transport Module is required to provide its results as output to a WFF (for contaminant mass flux results) or Water Concentration File (WCF) (for contaminant aqueous concentration results). The module is also required to produce a listing file (*.WLS file) that documents the data actually read in by the model and provides a summary of intermediate calculation results (e.g., retardation factor and decay constant) and the simulation results (peak flux or concentration and time of peak).

The following data are provided as output to the WFF for contaminant mass flux results:

- instantaneous, time-varying, contaminant mass fluxes exiting the aquifer
- width and height of the vertical interface plane (i.e., a plane perpendicular to the water table) through which contaminant exits the aquifer
- distance from the water table to the top of the vertical interface plane through which contaminant exits the aquifer
- natural recharge rate
- time-varying, instantaneous water flux exiting the aquifer through the vertical interface plane.

Data provided as output to the WCF for contaminant aqueous concentration results include instantaneous, time-varying, contaminant aqueous concentrations for each receptor location in the aquifer.

Scientific Requirements of the MEPAS Saturated Zone Transport Module

The primary scientific requirements for the MEPAS Saturated Zone Transport Module are

- obey the Law of Mass Conservation
- simulate advection in one dimension
- simulate dispersion in three dimensions
- account for the decay of radionuclides and be able to handle the degradation of chemicals
- account for the ingrowth of progeny resulting from decay/degradation and be able to handle decay chains with up to nine members (i.e., one parent and eight progeny)
- compute solute fluxes exiting the aquifer when the aquifer is not the last transport medium in the scenario
- compute solute concentrations at the aquifer (downgradient) boundary when the aquifer is the last transport medium in the scenario
- account for the effect of adsorption of contaminant to soil particles on travel time through the aquifer
- account for the effect of water flowing into the aquifer from a vadose zone on contaminant aqueous concentrations in the aquifer, especially near the source (i.e., handle both near-field and far-field cases)

The implementation of these requirements, in the form of mathematical formulations, are documented in Whelan et al. 1996 (PNNL-10907). However, their section of the document is out-of-date with respect to the effect of inflowing water from the vadose zone. The current technique to handle both near-field and far-field cases is described only in project quality assurance documentation.

Documentation for the Saturated Zone Transport Module of the Multimedia Environmental Pollutant Assessment System (MEPAS)

Design of the MEPAS Saturated Zone Transport Module

The migration and fate of contaminants through the groundwater are described by a three-dimensional, advective-dispersive equation for solute transport. The results are based on semianalytical solutions (i.e., solutions that require numerical integration) that are well established in the scientific literature. The Saturated Zone Transport Module accounts for the major mechanisms of constituent mobility (i.e., adsorption/desorption), persistence (i.e., degradation or decay), advection, and hydrodynamic dispersion.

A full description of the design parameters, as well as scientific formulations for the various mechanims, can be found in Whelan et al., 1996 (PNNL-10907) and can be accessed online by following this link:

- Multimedia Environmental Pollutant Assessment System (MEPAS): Ground Water Pathway Formulations.

Additional design information for the Saturated Zone Transport Module can be found in

- Saturated Zone Transport Module Help files
- Specifications for the Saturated Zone Transport Module for FRAMES 1.x

  Input Secifications
  - WFF-Water Flux File

  Output Specifications
  - WFF-Water Flux File
  - WCF-Water Concentration File
- dictionary files for the Saturated Zone Transport Module for FRAMES 2.x.

Documentation for the Saturated Zone Transport Module of the Multimedia Environmental Pollutant Assessment System (MEPAS)

Quality Assurance and Testing for the MEPAS Saturated Zone Transport Module

The Saturated Zone 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 Saturated Zone 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 Saturated Zone Transport Module

Requirement	Test Case												
---	1	2	3	4	5	6	7	8	9	10	11	12	13
1	Y	-	-	-	-	-	-	-	-	-	-	-	-
2	Y	-	-	-	-	-	-	-	-	-	-	-	-
3	-	-	-	-	-	-	-	-	-	-	-	-	-
4	Y	-	-	-	-	-	-	-	-	-	-	-	-
5	-	-	-	-	-	-	-	-	-	-	-	-	-
6	Y	-	-	-	-	-	-	-	-	-	-	-	-
7	-	-	-	-	-	-	-	-	-	-	-	-	-
8	Y	-	-	-	-	-	-	-	-	-	-	-	-
9	Y	-	-	-	-	-	-	-	-	-	-	-	-
10	Y	-	-	-	-	-	-	-	-	-	-	-	-
11	-	-	-	-	-	-	-	-	-	-	-	-	-
12	-	-	-	-	-	-	-	-	-	-	-	-	-
13	-	-	-	-	-	-	-	-	-	-	-	-	-
14	Y	-	-	-	-	-	-	-	-	-	-	-	-
15	Y	-	-	-	-	-	-	-	-	-	-	-	-
16	-	-	-	-	-	-	-	-	-	-	-	-	-
17	-	-	-	-	-	-	-	-	-	-	-	-	-
18	Y	-	-	-	-	-	-	-	-	-	-	-	-
19	Y	-	-	-	-	-	-	-	-	-	-	-	-
20	Y	-	-	-	-	-	-	-	-	-	-	-	-
21	Y	-	-	-	-	-	-	-	-	-	-	-	-
22	Y	-	-	-	-	-	-	-	-	-	-	-	-
23	Y	-	-	-	-	-	-	-	-	-	-	-	-
24	Y	-	-	-	-	-	-	-	-	-	-	-	-
25	Y	-	-	-	-	-	-	-	-	-	-	-	-
26	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)