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

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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.

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Requirements of the MEPAS Vadose Zone Transport Module

This section provides an overall summary of the requirements for the MEPAS Vadose Zone Transport Module. Detailed input, output, and scientific requirements are described in the sections that follow. The purpose of the MEPAS Vadose Zone Transport Module is to simulate the migration and fate of chemical and radionuclide constituents through partially saturated porous media (i.e., vadose zones). The MEPAS Vadose Zone Transport Module will

- G1 - simulate contaminant migration for both chemicals and radionuclides through partially saturated porous media (i.e., vadose zones) and provide output consisting of instantaneous, time-varying, contaminant mass fluxes exiting the vadose zone
- G2 - have no limits on the number of constituents considered in a scenario
- G3 - operate under Windows 95 and have a user-friendly MUI with a standard Windows look and feel
- G4 - meet the module specifications for the Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES).

Input Requirements of the MEPAS Vadose Zone Transport Module

Data needed to simulate contaminant migration through a vadose zone is obtained from three sources. The previous module (i.e., source term or vadose zone) provides boundary conditions (i.e., time-varying contaminant mass fluxes entering the vadose zone, infiltration rate, and source dimensions) through the Water Flux File (WFF). The user provides the vadose zone's physical characteristics and the contaminant's distribution coefficient (Kd) through the Module User Interface (MUI) via the Global Input Data (GID) file and model pre-processor. The chemical property database provides the contaminant's chemical properties via the GID file.

General requirements for the MUI are as follows:

- 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.
- 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 following data are obtained from the WFF by the MEPAS Vadose 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:

- time-varying, instantaneous, contaminant mass (or activity) fluxes entering the vadose zone (required)
- width and length of the interface plane through which contaminant enters the vadose zone (required)
- distance from water table
- natural recharge rate
- time-varying water flux entering the vadose zone (required).

The following data are obtained from the MUI and are needed by the module to perform its computations:

- vadose zone thickness (i.e., transport distance)
- total porosity
- field capacity
- dry bulk density
- soil type coefficient
- saturated hydraulic conductivity
- longitudinal dispersivity
- constituent distribution coefficient (Kd).

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

- CASID (Chemical Abstracts Service ID 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 **(M7)** to automatically use the estimated Kd values for single constituents or automatically use estimates for all constituents.

Output Requirements of the MEPAS Vadose Zone Transport Module

The MEPAS Vadose zone transport module is required to provide the following output:

- O1 - results as a WFF
- O2 - list file (*.WLS file) that documents the data actually read in by the model and summarizes intermediate calculation results (e.g., retardation factor or decay constant) and the simulation results (peak flux and time of peak).

The following data are output to the WFF:

- time-varying, instantaneous, contaminant mass (or activity) fluxes exiting the vadose zone
- width and length of the interface plane through which the contaminant exits the vadose zone
- distance from water table
- natural recharge rate
- time-varying water flux exiting the vadose zone.

Scientific Requirements of the MEPAS Vadose Zone Transport Module

The primary scientific requirements for the MEPAS vadose zone transport module are as follows:

- S1 - obey the Law of Mass Conservation
- S2 - simulate advection in one dimension
- S3 - simulate dispersion along the flow direction
- S4 - account for the decay of radionuclides and handle the degradation of chemicals
- S5 - account for the ingrowth of progeny resulting from degradation/decay and handle decay chains with up to nine members (i.e., one parent and eight progeny)
- S6 - compute contaminant mass (or activity) fluxes exiting the vadose zone
- S7 - determine a moisture content for the vadose zone that is consistent with the infiltration rate of water entering the vadose zone and the vadose zone's physical properties. However, if the computed moisture content is less than the field capacity, use the field capacity as the moisture content.
- S8 - account for the effect of adsorption of contaminant to soil particles on travel time through the vadose zone.

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

Other References

Whelan et al., 1997 (PNNL-11748)

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Design of the MEPAS Vadose Zone Transport Module

The MEPAS Vadose Zone Transport Module simulates the migration and fate of chemical and radionuclide constituents through partially saturated porous media (i.e., vadose zones). A full description of the design parameters, as well as scientific formulations for the various models, can be found in Whelan et al. 1996 (PNNL-10907) and accessed online by following this link:

- Formulations for the MEPAS Vadose Zone Transport Module.

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

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

  Input Secifications
  - WFF-Water Flux File

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

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Quality Assurance and Testing for the MEPAS Vadose Zone Transport Module

The Vadose 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 Vadose 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 Vadose Zone Transport Module

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