Documentation for the Computed Source Term Release 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.

Documentation for the Computed Source Term Release Module of the Multimedia Environmental Pollutant Assessment System (MEPAS)

Requirements of the MEPAS Computed Source Term Release Module

This section provides an overall summary of the requirements for the MEPAS Computed Source Term Release Module (CSTRM). The purpose of CSTRM is to calculate time-varying contaminant mass fluxes from a source as a function of time. Detailed input, output, and scientific requirements are described in the sections that follow.

Note that CSTRM was updated in 2003 to receive contaminant fluxes in the form of air deposition and overland flows. This modification allows the user to apply the module as a secondary source term. The update is documented in a separate online report.

The MEPAS CSTRM will

- G1 - have a minimum of 25 contaminants to be evaluated
- G2 - release contaminant from the waste zone to multiple transport pathways via volatization, suspension, infiltration, overland runoff, and decay/degradation loss routes
- G3 - compute contaminant mass fluxes that provide mass balance for different loss routes for each time step
- G4 - compute contaminant mass flux releases based on partitioning from the different loss routes for each time step
- G5 - compute an infiltration rate, wind erosion rate, overland runoff water flux, and overland runoff sediment erosion rate, when requested by the user
- G6 - provide as output time-varying water contaminant mass fluxes from the waste zone that meet the data specifications of the Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) software system for the infiltration and overland runoff loss routes
- G7 - provide as output time-varying air contaminant mass fluxes from the waste zone that meet the data specifications of the FRAMES software system for the volatization and suspension loss routes.

Input Requirements of the MEPAS Computed Source Term Release Module

The user enters the input data required for the MEPAS CSTRM via the module user interface (MUI). The MUI will allow the user to define the source problem and associated data. The primary input types to the MEPAS CSTRM are 1) initial contaminant mass or concentration, 2) source physical characteristics, 3) identification of loss routes, and 4) contaminant properties.

General requirements associated with the MUI are

- M1 - the graphical 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 easy-to-understand descriptions of all input parameters required
- M3 - the MUI will provide users with different units for the appropriate input parameters
- M4 - the MUI will also have an "About" tab to inform users of the title, version number, and general description of the module.

The MUI for the MEPAS CSTRM must allow the user to input all the data required for execution **(M5)**, including allowing the user to

- select the environmental media and loss routes associated with the source
- provide source characteristics associated with the environmental media and loss routes selected
- enter the initial mass or concentration data for each contaminant being evaluated
- enter key contaminant properties.

The MEPAS CSTRM has ten main data categories and each have data entry requirements. The following data are obtained from the MUI and are needed by the MEPAS CSTRM to perform its computations. The first main data category is **Options**, which allow the user to define the type of contaminated medium, release mechanisms information, and model simulation parameters. The following are the **Options** requested of the user:

- medium type for waste zone (soil/vadose, aquifer, surface impoundment)
- leaching loss route
- overland runoff loss route
- suspension loss route
- volatilization loss route
- known source and sink
- time interval and time period for simulation
- residual mass limit for simulation.

The following are the **Waste Zone** characterization data requested of the user:

- thickness of clean overburden on top of the waste zone
- thickness, width, and length of waste zone
- bulk density, moisture content, and total porosity of the waste zone
- annual average air temperature and wind speed for site
- height above ground of local wind measurement.

The following are the **Hydrology** data requested of the user:

- elevation of the Local Climatological Data (LDC) Station
- latitude and elevation of the waste zone
- Soil Conservation Service (SCS) curve number
- top soil water capacity
- annual number of days with 7.254 mm of precipitation.

The following are the **Monthly Climatology** data requested of the user for each month of the year:

- average temperature
- average precipitation
- average wind speed
- average cloud cover
- average number of precipitation
- average minimum and maximum relative humidity.

The following are the **Known Media Release** data requested of the user:

- Darcy infiltration rate(s) and associated times
- soil depth lost to water erosion rate(s) and associated times
- wind erosion rate(s) and associated times.

The following are the **Contaminant Properties** data requested of the user:

- contaminant water solubility limit
- contaminant inventory or concentration
- contaminant decay/degradation half life
- faction of volatilization release for each contaminant.

The following are the **Known Contaminant Flux** data requested of the user:

- known contaminant leaching flux rate(s) and associated time
- known contaminant overland flux rate(s) and associated time
- known contaminant suspension flux rate(s) and associated time
- known contaminant volatilization flux rate(s) and associated time
- known contaminant source/sink flux rate(s) and associated time.

The **K_d** data requested of the user includes contaminant-specific K_d and associated times. The MUI will provide an estimate of the K_d if the user selects this option **(M6)**.

The following are the **Suspension** data requested of the user:

- darcy bulk density and percent sand of the surface soil
- fraction of surface crust and roughness length
- fraction of crust and vegetation covering the soil surface
- surface roughness and the number of disturbances per month of the area
- annual maximum wind speed and Thornwaite's PEI value for the area
- any road used within the contaminated area (and whether it is paved or unpaved)
- vehicle weight, speed, number of wheels, number of trips, percent silt of road, and distance of road.

The following are the **Overland** data requested of the user:

- storm types, slope, slope length, and rain intensity for the region
- erosion, vegetation, and land practice factors.

Once the user enters this information, some intermediate calculations may be required by the MUI to feed the necessary data to the MEPAS CSTRM. These calculations are associated with the initial mass and the mass balance analysis. The user will be allowed to **(M7)**

- input user-defined contaminant mass fluxes that are inflows and outflows from the source other than the source loss routes. These are known as sources (inflow) and sinks (outflow) and are time varying. These external sources and sinks must be considered with the initial mass associated with the original source zone.
- have either MEPAS CSTRM compute all contaminant mass fluxes or have the MEPAS CSTRM compute contaminant mass fluxes for some loss routes. The user can enter known contaminant mass fluxes for other loss routes.

Note that if all contaminant mass fluxes are known for all loss routes, a different source term module must be used (FRAMES User-Defined Source Module).

The user is allowed to enter **(M8)**either user-defined water (infiltration and overland) flow rates and soil (wind, mechanical, and overland) erosion rates or have the module compute them based on source and environmental setting data. The water infiltration flow rate is required for the leaching loss route, the overland water flow rate for overland loss route, the soil erosion rate related to wind and mechanical suspension, and overland runoff loss routes.

Output Requirements of the MEPAS Computed Source Term Release Module

The MEPAS CSTRM is required to provide the following as output:

- O1 - time-varying instantaneous contaminant mass fluxes for air, soil (deposition from air) and water. These outputs must meet the specifications of the FRAMES (Whelan et al. 1997. PNNL-11748).
- O2 - the mass flux of contaminant to the air in the *.AFF file and the mass flux of contaminant to the water in the *.WFF file.

The MEPAS CSTRM provides the following data to the AFF, WFF, and SCF:

- O3 - time-varying contaminant particle and gaseous emission rates (AFF)
- O4 - time-varying contaminant infiltration and overland runoff flux rates (WFF)
- O5 - time-varying infiltration (WFF)
- O6 - time-varying wind erosion and erosion notes (AFF).

The MEPAS CSTRM is also required to

- O7 - create a list file (*.SLS) in an ASCII format that echoes the input data and provides intermediate calculations and results
- O8 - create an Error (*.ERR) File in an ASCII format at the start of the module execution.

Scientific Requirements of the MEPAS Computed Source Term Release Module

The scientific requirements for the MEPAS CSTRM are

- S1 - evaluate a minimum of 25 contaminants
- S2 - address chemical and radioactive contaminants
- S3 - maintain mass balance over time for each contaminant
- S4 - release contaminant to the appropriate transport and media via volatilization, suspension, infiltration, overland runoff, and decay/degradation loss routes
- S5 - compute progeny growth for radionuclides from decay of parent contaminant
- S6 - include source/sink as part of the waste zone loss rates and mass balance calculations
- S7 - have a minimum waste mass remaining value to determine termination of the simulation
- S8 - have a variable time step for evaluating mass loss (default is 1 year)
- S9 - compute phase distribution (soil, vapor, aqueous, organic) for each time step
- S10 - compute time-varying water flow rates (infiltration and overland runoff) based on site characteristics
- S11 - compute wind, mechanical, and overland soil erosion rates.

Other References

Remedial Action Assessment System Prototype 2.5 -- Remedial Investigation/Feasibility Study Reference Document. Draft (Baggaasen, L. M., 1993. PNL-8751).

Multimedia Environmental Pollutant Assessment System (MEPAS): Source Term Release Formulations. (Streile et al. 1996. PNNL-11248).

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Design of the MEPAS Computed Source Term Release Module

The MEPAS Computed Source Term Release Module (CSTRM) is generally the starting module for most analyses. It requires source inventories or concentrations and uses site-specific information to simulate the contaminant source releases, provides as output contaminant mass fluxes from the source, and provides input boundary conditions to the other module types (exposure, vadose, aquifer, surface water, and air). A full description of the design parameters, as well as scientific formulations for the various models, can be found in Streile et al. 1996 (PNNL-11248) and accessed online by following this link:

- Formulations for the MEPAS Computed Source Term Release Module.

Additional design information for the Computed Source Term Release Module can be found in

- Computed Source Term Release Module Help files
- specifications for the Computed Source Term Release Module for FRAMES 1.x
- Specifications for the Atmospheric Transport Module for FRAMES 1.x

  Input Secifications
  - The Computed Source Term has no Input Specificiations

  Output Specifications
  - AFF-Air Flux File
  - WFF-Water Flux File
  - SCF-Soil Concentration File
- dictionary files for the Computed Source Term Release Module for FRAMES 2.x.

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Quality Assurance and Testing for the MEPAS Computed Source Term Release Module

The Computed Source Term Release 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 Computed Source Term Release 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 Computed Source Term Release Module

Requirement	Test Case																						
---	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Y	-	-	-	-
2	-	-	-	-	-	-	-	-	-	-	-	Y	-	-	Y	Y	-	Y	Y	-	-	-	-	-
3	-	-	-	-	-	-	-	-	-	-	-	Y	-	-	-	-	-	Y	Y	-	-	-	-	-
4	-	-	-	-	-	-	-	-	-	Y	-	Y	-	-	-	-	-	-	-	-	-	-	-	-
5	-	-	-	-	-	-	-	Y	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
6	Y	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
7	-	-	-	-	-	-	-	-	Y	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
8	Y	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
9	Y	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Y	Y	-	-	-	-	-
10	Y	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
11	Y	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Y	Y	-	-	-	-	-	-	-
12	Y	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
13	Y	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
14	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Y	-	-	-	-	-	-	-	-
15	Y	Y	Y	Y	Y	Y	Y	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
16	-	-	-	-	-	-	-	Y	Y	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
17	-	-	-	-	-	-	-	-	-	Y	Y	Y	-	-	-	-	-	-	-	-	-	-	-	-
18	-	-	-	-	-	-	-	Y	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
19	Y	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
20	-	-	-	-	-	-	-	-	-	Y	-	-	-	-	-	-	-	-	-	-	-	-	-	-
21	-	-	-	-	-	-	-	-	-	-	-	-	-	Y	-	-	-	-	-	-	-	-	-	-
22	-	-	-	-	-	-	-	-	-	-	-	-	Y	Y	-	-	-	-	-	-	-	-	-	-
23	Y	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
24	Y	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
25	-	-	-	-	-	-	-	-	-	-	-	Y	-	-	-	-	-	-	-	-	-	-	-	-
26	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Y	Y	-	-
27	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Y	-
28	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Y
29	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Y	Y	Y	Y
30	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Y
31	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	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)

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