Documentation for Air 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 Atmospheric Transport Module

This section provides an overall summary of the requirements for the MEPAS Atmospheric Transport Module and associated pre- and post-processors, along with the specific requirements for the module user interface (MUI). Detailed input, output, and scientific requirements are described in the sections that follow.

The purpose of the Atmospheric Transport Module is to simulate the transport, dispersion, and deposition of chemicals and radionuclides released into the atmosphere. This module will

- G1 - accept input data contained in the FRAMES Atmospheric Flux File (AFF) and Global Input Data (GID) File, as specified by the FRAMES data specifications (Whelan et al. 1997. PNNL-11748)
- G2 - be linked to a MUI that operates in Windows 95, 98, 2000, NT, ME, and XP, with the look and feel of Windows
- G3 - conduct atmospheric transport, dispersion, and deposition calculations for radionuclides and chemicals
- G4 - handle a minimum of 25 constituents per scenario
- G5 - calculate ground-level, time-varying, air concentrations and deposition rates (wet and dry) by distance and direction using a joint frequency distribution provided by the user for an area or point source
- G6 - provide as output ground-level, annual average, time-varying, air concentrations and deposition rates (wet and dry) by distance and direction into an Atmospheric Transport Output (ATO) file that is specified by the FRAMES data specifications (Whelan et al. 1997. PNNL-11748).

Input Requirements of the MEPAS Atmospheric Transport Module

The MEPAS Atmospheric Transport Module has three sources of input to conduct calculations:

- the AFF, which provides source characteristics and time-varying contaminant emission rates
- the GID file, which provides contaminant properties
- the MUI, which provides climatology, joint frequency distribution, and topographical data.

The specifications for the GID and AFF files are described in Whelan et al. 1997 (PNNL-11748).

Atmospheric Flux File Inputs

The AFF is a FRAMES data specification file that is defined as output from source modules and input to air modules. The AFF provides the MEPAS Atmospheric Transport Module with the

- area or point source type
- area of source or point exit
- height of point source
- building height for point source
- annual average air temperature for point source
- exit velocity of point source
- exit plume temperature for point source
- number of flux types (particle size types)
- time-varying, contaminant emission rates by particle size type.

Global Input Data File Inputs

The GID file is a FRAMES data specification file that contains all contaminant property data for the entire set of modules linked under FRAMES. The GID file provides the MEPAS Atmospheric Transport Module with

1. contaminant name, CAS ID, and progeny chain
2. contaminant deposition type (Gas 1, Particle 1, Particle 2, Particle 3, etc.)
3. contaminant first-order-decay/degradation half-life.

Module User Interface Inputs

The MEPAS Atmospheric Transport Module MUI is divided into three main data groups: 1) climatology, 2) joint frequency distribution, and 3) topographical data. The MUI has the following general requirements:

1. The MUI will operate in Windows 95 and will have a standard Windows look and feel.
2. The MUI will have on-line electronic help in HTML format and provide users with an easy-to-understand description of all input parameters required by the MUI, as well as an "About" tab that provides the user with title, version number, and brief description of the model.
3. The MUI will provide users with different units for the appropriate input parameters.
4. The MUI will provide a reference field for each input parameter in the MUI.

The user needs to put the data listed in the following table into the MUI (some are optional depending on user selections).

Input Data for the Atmospheric Transport Module User Interface

Climatological Data	General Joint Frequency Information	Additional Joint Frequency Distribution Data	Topographical Data
Reference weather station name	Data station name	Number, percent, or frequency of occurrence by 16 directions and 6 wind speeds for stability class A	Use of regional topographical data option
Morning mixing height	Anemometer height	Number, percent, or frequency of occurrence by 16 directions and 6 wind speeds for stability class B	Use of wind channeling model option
Afternoon mixing height	Average surface roughness	Number, percent, or frequency of occurrence by 16 directions and 6 wind speeds for stability class C	Elevation of release
Annual precipitation	Wind speed mid points	Number, percent, or frequency of occurrence by 16 directions and 6 wind speeds for stability class D	Regional surface roughness
Number of precipitation days per year	Joint frequency calms for A-G stability classes	Number, percent, or frequency of occurrence by 16 directions and 6 wind speeds for stability class E	Terrain height data (optional based on regional topographical data)
Number of thunderstorms per year	---	Number, percent, or frequency of occurrence by 16 directions and 6 wind speeds for stability class F	Wind channeling data (optional based on wind channeling model)
---	---	Number, percent, or frequency of occurrence by 16 directions and 6 wind speeds for stability class G	---

Output Requirements of the MEPAS Atmospheric Transport Module

The MEPAS Atmospheric Transport Module is required to provide its results as output to an Atmospheric Transport Output (ATO) file. The ATO is a FRAMES Air Transport Module output file that is specified by the FRAMES data specifications (Whelan et al. 1997 PNNL-11748) and may be used as input to other modules. This module is also required to produce a listing file (*.ALS file) that documents the data actually read in by the model and provides a summary of intermediate calculation and simulation results.

The MEPAS Atmospheric Transport Module provides the following data to the ATO file:

- output type (acute or chronic)
- coordinate system type (polar or Cartesian)
- spatial and temporal matrix defining time series of the regional patterns of contaminant air concentrations by particle size type
- spatial and temporal matrix defining time series of the regional patterns of deposition rates by particle size type.

The MEPAS Atmospheric Transport Module is also required to create:

- O1 - a listing file (*.ALS) using an ASCII format that echoes the input data and provides intermediate calculations and summary results.
- O2 - an error file (*.ERR) using an ASCII format at the start of the module execution. If no error occurs during simulation, this file is deleted. If an error occurs during simulation, this file will contain information on the error.

Scientific Requirements of the MEPAS Atmospheric Transport Module

Mathematical formulations and assumptions for the MEPAS Atmospheric Transport Module are contained in Droppo and Buck 1996 (PNNL-11080). Some of main computational functions of the model are

- heat-momentum plume rise formulation
- building wake dispersion formulation
- Gaussian sector-average model for annual/seasonal atmospheric transport and dispersion
- combined surface layer similarity theory model and empirical wind-tunnel model for dry deposition
- in-plume scavenging model for wet deposition
- surface layer similarity theory model for wind speed adjustments with height.

The MEPAS Atmospheric Transport Module will have the following scientific requirements:

- S1 - obey the Law of Mass Conservation
- S2 - simulate both chemicals and radionuclides
- S3 - simulate both particulate and gaseous constituents
- S4 - calculate ground-level contaminant air concentrations and deposition rates by distance and direction using a sector-averaged Gaussian approach for both area and point sources
- S5 - calculate initial plume rise (both momentum- and buoyancy-dominated) and building downwash for point sources
- S6 - consider both wet and dry deposition
- S7 - account for near-source local channel (drainage) flow for sites in complex terrain
- S8 - account for a plume intersection on local terrain heights for elevated plumes for point sources
- S9 - account for variation in concentration and deposition resulting from varying surface roughness
- S10 - adjust wind speeds for changes in height between the measurement and release site.

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Design of the MEPAS Atmospheric Transport Module

The MEPAS Atmospheric Transport Module includes models for emission from a source to the air, initial plume rise and dispersion, airborne pollutant transport and dispersion, and deposition to soils and crops. A full description of the design parameters, as well as scientific formulations for the various models, can be found in Droppo and Buck, 1996 (PNNL-11080) and can be accessed online by following this link:

- Formulations for the MEPAS Atmospheric Transport Module.

Additional design information for the Atmospheric Transport Module can be found in

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

  Input Secifications
  - AFF-Air Flux File

  Output Specifications
  - ATQ-Atmospheric Concentration File
- dictionary files for the Atmospheric Transport Module for FRAMES 2.x.

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Quality Assurance and Testing for the MEPAS Atmospheric Transport Module

The Atmospheric 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 Atmospheric 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 Atmospheric Transport Module

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