

# Documentation for the Chemical Database Editor 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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# Documentation for the Chemical Database Editor of the Multimedia Environmental Pollutant Assessment System (MEPAS)

## Requirements of the MEPAS Chemical Database Editor

This section provides an overall summary of the requirements for the MEPAS Chemical Database Editor. Detailed input and scientific requirements are described in the sections that follow.

The purpose of the Chemical Database Editor is to provide information on constituents used to simulate the transport, dispersion, and deposition of chemicals and radionuclides released into the atmosphere. This module will

- G1 - operate within the Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES), described in [Whelan et al., 1997](#) (PNNL-11748).
- G2 - allow the user to create, access, and save a chemical database (.mdb file)
- G3 - operate in Windows 95, 98, NT, ME, and XP
- G4 - not require modifications to any existing components that run under FRAMES (for example, GENII and MEPAS).

## Input Requirements of the MEPAS Chemical Database Editor

The user interface for the MEPAS Chemical Database Editor will have the following put requirements:

- I1 - allow the user to select an existing database from a list of available databases (in the FRAMES database format) to be used for an analysis
- I2 - allow the user to select a constituent for viewing or editing
- I3 - allow the user to select constituents from a list ordered by name or Chemical Abstract Service Identification Number (CASID)
- I4 - allow the user to change any property value associated with the constituent
- I5 - allow the user to print a paper copy or write to a file a report of properties for one or more constituents
- I6 - provide help information about the parameters in the database
- I7 - provide error messages to the user when inappropriate values are provided for any parameter (as determined by ranges defined within the database)
- I8 - allow the user to assign references to each property value added or modified
- I9 - allow the user to add new references or select from previous references
- I10 - allow the user to select or deselect constituents to be included in an analysis
- I11 - allow the user to view constituents grouped by chemical groups (e.g., polycyclic aromatic hydrocarbons)
- I12 - allow the user to add or delete contaminants from the database.

## Scientific Requirements of the MEPAS Chemical Database Editor

The MEPAS Chemical Database Editor has the scientific requirement (S1) to provide property estimation methods for selected properties.



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## Design of the MEPAS Chemical Database Editor

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The purpose of the Chemical Database Editor is to provide information on constituents used to simulate the transport, dispersion, and deposition of chemicals and radionuclides released into the atmosphere. Design information for the Chemical Database Editor can be found in

- Chemical Database Editor Help files
- [Dictionary files](#) for the Chemical Database Editor for FRAMES 2.x.

### Other References

- *Concepts of a Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES)*. ( [Whelan et al. 1997](#). PNNL-11748).



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## Quality Assurance and Testing for the MEPAS Chemical Database Editor

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The Chemical Database Editor 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 Chemical Database Editor. 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 Chemical Database Editor**

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