Documentation for the Chronic Exposure Module of the Multimedia Environmental Pollutant Assessment System (MEPAS)

Compiled from Former Publications PNNL-SA-32274 and PNL-10523

With Contributions From

P. J. Chamberlain
D. L. Strenge

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 Chronic Exposure Module of the Multimedia Environmental Pollutant Assessment System (MEPAS)

Design of the MEPAS Chronic Exposure Module

The MEPAS Chronic Exposure Module is designed to take time-varying, contaminant concentrations in environmental media (i.e., groundwater, surface water, air, and soil) and generate average contaminant concentrations in exposure media at the point of exposure or contact with receptors. The total time frame over which the environmental media concentrations occur is divided into discrete exposure intervals (which may or may not overlap) as determined by the user, and an average concentration is determined for each of these intervals. A full description of the design parameters, as well as scientific formulations for the various models, can be found in Strenge and Chamberlain, 1995 (PNL-10523) and accessed online by following this link:

- Formulations for the MEPAS Chronic Exposure Module.

Additional design information for the Chronic Exposure Module can be found in

- Chronic Exposure Module Help files
- Specifications for the Chronic Exposure Module for FRAMES 1.x

  Input Specifications
  - ATQ-Atmospheric Concentration File
  - WCF-Water Concentration File
  - SCF-Soil Concentration File

  Output Specifications
  - EPF-Exposure Pathway File
- dictionary files for the Chronic Exposure Module for FRAMES 2.x.

Documentation for the Chronic Exposure 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 Chronic Exposure Module of the Multimedia Environmental Pollutant Assessment System (MEPAS)

LEGAL NOTICE

Documentation for the Chronic Exposure Module of the Multimedia Environmental Pollutant Assessment System (MEPAS)

Quality Assurance and Testing for the MEPAS Chronic Exposure Module

The Chronic Exposure 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 Chronic Exposure 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 Chronic Exposure Module

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

Documentation for the Chronic Exposure Module of the Multimedia Environmental Pollutant Assessment System (MEPAS)

Requirements of the MEPAS Chronic Exposure Module

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

The MEPAS Chronic Exposure Module will

- G1 - compute chemical and radionuclide contaminant concentrations in the exposure medium at the point of exposure or contact with receptors for all exposure pathways shown in the table following the list, except for external exposure to radionuclides in outdoor air from a passing plume. The values are averaged for each interval of a set of exposure duration intervals specified by the user. For external exposure to radionuclides in outdoor air, the module is required to take the dose equivalence values produced by the atmospheric transport module and perform the averaging.
- G2 - allow up to 25 constituents to be considered in a scenario.
- G3 - meet the module specifications for the Framework for Risk Analysis in Mulimedia Environmental Systems (FRAMES).

MEPAS Chronic Exposure Module Exposure Pathways by Transport or Source Medium

Exposure Pathway	Transport or Source Medium			
---	Ground Water	Surface Water	Atmosphere	Soil
Ingestion of drinking water	Yes	Yes	No	No
Dermal contact with water while showering	Yes	Yes	No	No
Inadvertent ingestion of water while showering	Yes	Yes	No	No
Ingestion of leafy vegetables	Yes	Yes	Yes	Yes
Ingestion of other vegetables	Yes	Yes	Yes	Yes
Ingestion of meat	Yes	Yes	Yes	Yes
Ingestion of milk	Yes	Yes	Yes	Yes
Ingestion of fin fish	No	Yes	No	No
Ingestion of shellfish	No	Yes	No	No
Inadvertent ingestion of water while swimming	No	Yes	No	No
Dermal contact with water while swimming	No	Yes	No	No
Dermal contact with sediment during shoreline use	No	Yes	No	No
Inadvertent ingestion of sediment during shoreline use	No	Yes	No	No
Inadvertent ingestion of soil	No	No	Yes	Yes
Dermal contact with soil	No	No	Yes	Yes
Indoor inhalation of volatile chemicals released from shower water	Yes	Yes	No	No
Indoor inhalation of volatile chemicals released from other domestic water uses	Yes	Yes	No	No
Inhalation of outdoor air from a passing plume	No	No	Yes	No
Inhalation of resuspended soil particles	No	No	Yes	Yes
External exposure to radionuclides while swimming	No	Yes	No	No
External exposure to radionuclides while boating	No	Yes	No	No
External exposure to radionuclides in sediment during shoreline use	No	Yes	No	No
External exposure to radionuclides in soil	No	No	Yes	Yes
External exposure to radionuclides in outdoor air from a passing plume	No	No	Yes	No

Input Requirements of the MEPAS Chronic Exposure Module

Data needed to compute contaminant concentrations in an exposure medium are obtained from three sources. The previous module in the scenario (i.e., a transport or source module) provides the boundary conditions (i.e., time-varying, contaminant concentrations in the source or transport medium). The boundary conditions are communicated to the module through the Water Concentration File (WCF) for groundwater and surface water transport pathways, the Atmospheric Transport Output (ATO) file for the air pathway, and the Soil Concentration File (SCF) for contaminants at a contaminated soil source.

Through the MUI, the user provides exposure pathways to consider, the time discretization and exposure duration information, and the physical characteristics of the exposure media (as needed). The input data supplied through the MUI is communicated to the model through the Global Input Data (GID) file and the model pre-processor.

The chemical property database provides contaminant chemical properties (e.g., water purification factors, bioaccumulation factors, food chain transfer factors, etc.). The GID file is also used to store the contaminant chemical property data.

Thus, the general input requirement **(I1)** for the Chronic Exposure Module is to accept input from the WCF, ATO, SCF, and GID files and the module pre-processor.

There are also 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 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 by the MUI.
- 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 allow the user to input exposure control data (start time for the exposure calculations, maximum ending time for the exposure calculations, and number of time intervals for evaluation), which will apply globally to all four source and transport media. The duration of each time interval is equal to the exposure duration, which is defined by the user for each of the four source and transport media.
- M7(a) - The MUI will allow the user to select the exposure pathways to be included in the analysis. Only those pathways that make sense for the current scenario will be available as options to the user. For example, if the groundwater medium is the only medium being considered, then dermal contact while swimming is not an available exposure pathway and should either be grayed out or not shown at all. The allowed exposure pathways for each medium are tabled above.
- M7(b) - The MUI will allow the non-functional text boxes to be displayed as unchecked, even if the user had checked them previously. This will make it clear to the user that only their selections will be performed by the model.

The MUI must also allow the user to define additional parameters needed in the analysis. These parameters include the following:

- M8 - When, and only when, an exposure pathway involving soils is selected, the user will be allowed to select from two methods for defining the surface soil leach rate constants. Under Option 1, the user provides leach rate constants for each contaminant (including progeny). Under Option 2, the user provides soil characterization data and distribution coefficients, and the program calculates the leach rate constant. For this option the MUI requires input of surface soil thickness (i.e., effective depth of mixing), surface soil moisture content, soil dry bulk density infiltration rate, and contaminant distribution coefficient (Kd) for each contaminant (including progeny).
- M9 - The MUI will allow specification of the exposure duration for the exposed individual in the scenario, with separate values specified for groundwater, surface water, atmospheric, and measured soil exposures.
- M10 - When atmospheric transport is the source of contamination, the MUI will display the X,Y coordinates entered by the user on the General Input screen to specify the exposure location relative to the release point. The General Input screen is the screen on which the user selects the model to be used.
- M11 - The exposure module will also provide an option to customize the exposure data specific to each exposure pathway. The MUI will access a default parameter file and populate the data fields under a separate menu item.
- M12 - The user will be allowed to access the parameters under the Customize menu and change the values for the current exposure scenario. The values will be saved for retrieval and display when the MUI is next entered.

The user will have access **(M13)** to the following parameter sets:

- soil aerial density, plant retention fraction, and crop yields
- animal feed, water, and soil intake rates
- translocation factors to edible parts of plants
- fraction of animal feed and water that is contaminated
- delay times between harvest and consumption for farm products
- crop growing periods for four sources of contamination (groundwater, surface water, atmospheric deposition, and initial soil contamination)
- resuspension factors and mass loading factor
- indoor air factors to relate domestic water concentration to indoor air concentration for volatile chemicals, radon, and all other constituents.

Addition input requirements are as follows:

- I2 - obtain data from the WCF whenever a groundwater or surface water exposure pathway is selected. These data will include time-varying, instantaneous, aqueous concentrations for each contaminant (including progeny).
- I3 - The MEPAS Chronic Exposure Module will obtain data from the SCF whenever a soil exposure pathway is selected. These data will include the initial, instantaneous, total soil concentration on a bulk-volume basis (i.e., total mass of contaminant per bulk volume of soil) for each contaminant (including progeny).
- I4 - The MEPAS Chronic Exposure Module will obtain data from the ATO file whenever an atmospheric exposure pathway is selected.

The module obtains the following data from the ATO file:

- time-varying, annual average, airborne concentrations for each contaminant and all pollutant types (i.e., gaseous, particle 1, etc.)
- time-varying, annual average, deposition flux rates for each contaminant and all pollutant types
- time-varying, annual average dose equivalent for external radiation exposure to outdoor air in a passing plume for each radioactive contaminant and all pollutant types.

As needed, the following data are obtained **(I5)** from the chemical properties database:

- water treatment purification factor
- degradation/decay half-life
- transfer factors for animal feed to meat and milk
- soil-to-plant transfer factors
- deposition velocity from air
- bioaccumulation factors (for fin fish and shellfish)
- octanol-water partition coefficient (Kow)
- Henry's law constant.

Output Requirements of the MEPAS Chronic Exposure Module

The exposure module has the following output requirements:

- O1 - produce an Exposure Pathway File (EPF) that contains the average exposure medium concentration to the EPF in the specified format for each selected exposure pathway (except for external radiation exposure to outdoor air), specified time interval, contaminant (including progeny), and exposure location. Allow multiple exposure locations only for the atmospheric transport analysis.
- O2 - produce a listing file (*.ELS file) in ASCII format that documents the data actually read in by the model and summarizes intermediate calculation results (e.g., computed leach rate constants for agricultural soil, etc.).
- O3 - write the average radiation dose (Sv) to the EPF file in the specified format, if the ATO file data are in Sv, for the external radiation exposure to outdoor air pathway, specified time interval, contaminant (including progeny), and exposure location. If the ATO file data are not in Sv, write results in intake concentration units (Bq/m^3).

Scientific Requirements of the MEPAS Chronic Exposure Module

The scope of the exposure analysis is determined by the transport or source modules connected to the exposure module (e.g., atmospheric transport, aquifer) and by the selections the user makes in the MUI. The mathematical formulations for this module are provided in Strenge and Chamberlain, 1995 (PNL-10523).

The contaminant concentration in the source or transport medium is the starting point for the exposure analysis. Except for the atmospheric transport medium, this concentration is an instantaneous value. For the atmospheric transport medium, the concentrations are averaged over a 1-year period and the deposition rates are annual average values. The transport medium may or may not be the medium of exposure. For example, the groundwater transport pathway generates estimates of contaminant concentration in the groundwater at the well. In this case, the well water is also the medium of exposure, although some modifications to the concentration are possible during transfer through the treatment plant and distribution system to the individuals exposed during domestic water uses. When the well water is used to irrigate agricultural crops, the exposure medium is not the well water, but the foods produced. For agricultural pathways, models are used to estimate the transfer of pollutants from the irrigation water to the food consumed by humans.

The processes affecting the transfer of contaminants from the transport or source medium to the exposure medium are defined in the following list of scientific requirements for the exposure module:

- S1 - include the reduction of contaminant concentrations from processing at a water supply treatment plant as an option for all exposure pathways involving the domestic use of contaminated water.
- S2 - consider the loss of contaminants, through degradation/decay or other processes, from the water distribution system during transport to a domestic use or irrigation location for all exposure pathways involving the domestic or agricultural use of contaminated water.
- S3 - consider the loss of contaminants, through degradation/decay or other processes, from plants after harvest but before consumption by animals or exposed individuals for all pathways involving agricultural crops.
- S4 - consider the accumulation of contaminants in agricultural soil over time for all pathways involving agricultural crops.
- S5 - consider the processes of deposition to plant surfaces, to agricultural soil with root uptake by plants and animal feed, and to agricultural soil with animal ingestion of soil (in conjunction with feed intake) for all pathways involving atmospheric transport.
- S6 - consider the process of atmospheric deposition to residential soil for evaluation of soil exposure pathways (external ground exposure, soil ingestion, soil dermal contact, and inhalation of resuspended contaminants) for all pathways involving atmospheric transport.
- S7 - evaluate using the resuspension factor method air concentrations resulting from atmospheric deposition to soil followed by resuspension (because the contaminant soil concentrations have dimensions of mass of contaminant per unit area). Evaluate measured contaminant concentrations in soil using a mass loading factor because contaminant soil concentrations have dimensions of mass of contaminant per unit mass of soil.
- S8 - evaluate radioactive decay explicitly for all processes modeled that involve periods of time, provided the decay has not been previously evaluated by an earlier component. Include in the decay production and decay of progeny radionuclides when chain decay is involved.
- S9 - consider the use of irrigation water for food and animal feed production, and use of water as an animal drinking water source, for all groundwater and surface water analyses.
- S10 - consider the processes of irrigation water deposited on plant surfaces and agricultural soil, with root uptake by plants and animal feed and animal ingestion of soil (in conjunction with feed intake), for all groundwater and surface water analyses.
- S11 - use special models for tritium and carbon-14. Tritium occurs in the environment and food chain as tritiated water, and carbon-14 occurs as carbon dioxide. Because water and carbon dioxide are normal constituents in biological systems, these contaminants do not behave in biological systems like trace pollutants, hence the need for special models to calculate tritium and carbon-14 accumulation and transfer to agricultural products.
- S12 - evaluate exposures for the measured soil transport with the soil concentration being defined at the start of the analysis (as opposed to being represented as an average value over a period of time). The change in initial soil concentration with time is accounted for by loss from the soil for radioactive decay, leaching, and by other processes as described by the soil loss rate constant for the constituent.

Other References

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

Documentation for the Chronic Exposure Module of the Multimedia Environmental Pollutant Assessment System (MEPAS)
