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**US Army Corps of Engineers**
Waterways Experiment Station

# Development of a Multimedia Exposure Assessment Model for Evaluating Ecological Risk of Exposure to Military-Related Compounds (MRCs) at Military Sites

*by Patrick N. Deliman, WES*
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WES



Prepared for Headquarters, U.S. Army Corps of Engineers

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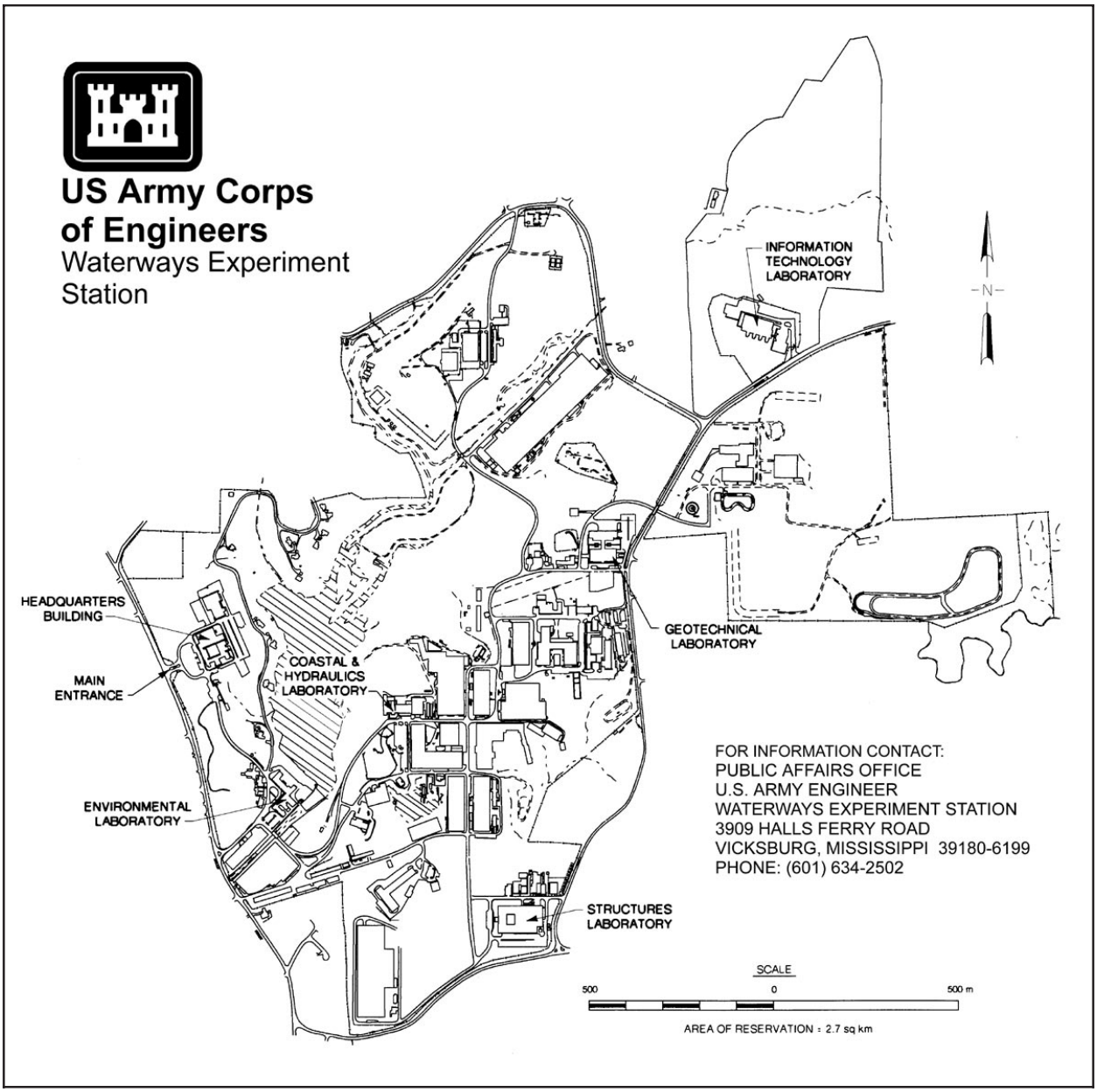


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# Preface

The work reported herein was conducted by the U.S. Army Engineer Waterways Experiment Station (WES) for Headquarters, U.S. Army Corps of Engineers (HQUSACE). Funding was provided by the HQUSACE Installation Restoration Research Program (IRRP), Fate and Effects Thrust Area, Work Unit entitled Fate and Transport of Military Unique Contaminants in Soil, Sediment, and Water Ecosystems. Dr. Clem Myer was the IRRP Coordinator at the Directorate of Research and Development, HQUSACE. The IRRP Program Manager was Dr. M. John Cullinane, WES.

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The work was conducted under the general supervision of Dr. Mark S. Dortch, Chief, WQCMB, Dr. Richard E. Price, Chief, EPED, and Dr. John Harrison, Director, EL.

At the time of publication of this report, Director of WES was Dr. Robert W. Whalin, and WES Commander was COL Robin R. Cababa, EN.

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# 1 Introduction

## Background

Contamination to air, surface water, and groundwater from military-related compounds (MRCs) has been of increasing concern in the past several years due to the closing of munition plants and bases. MRCs usually refer to some type of explosive compound or to a by-product of such. However, some radioactive materials may also be classified as MRCs.

Because of the many mediums, or multimedia, available for the spread of contamination (air, surface water, groundwater, etc.), the effects of the contamination on ecological units from each of the primary modes of exposure need to be evaluated via the specific protocol of the exposure routes.

The assessment of the exposure to ecological units from the many mediums through the use of an exposure model is desirable to determine the risk associated with exposure to MRCs from these media. This assessment is valuable for permitting and planning activities as well as for possible cleanup operations of contaminated sites should the risk to an ecological unit become too great.

Ideally, when a general idea of the level of risk associated with an exposure is desired, the use of a screening-level model will maximize the amount of information provided while minimizing the amount of effort required to obtain the necessary information to make an assessment of risk. A screening-level model refers to the use of simplified, quantitative, predictive methods that minimize time and effort for implementation. Simplification is achieved by making assumptions that reduce complexity of the predictive mathematical formulations and input data requirements.

The intent here was to evaluate the existing multimedia exposure assessment models and determine which models would lend themselves easily to modification to handle the assessment of ecological risk of exposure from military unique compounds. The primary MRCs addressed in this report are 2,4,6-trinitrotoluene (TNT), hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX), and octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine

(HMX). Also in this report is a brief section on radioactive contaminants such as plutonium, americium, etc.

## Objectives

The objectives of this report are to provide a review of the screening-level risk assessment models evaluated in this study and to discuss the modifications of the selected model in order to allow it to address the assessment of ecological risk of exposure to military unique compounds.

# 2 Review of Exposure Assessment Models

A review of existing exposure assessment models was conducted to meet the requirements of the Fate and Effects Research Program for a screening-level multimedia exposure assessment model for MRCs. A literature research effort was conducted to determine the most useful exposure assessment models for this task. The research turned up numerous models which were narrowed to nine potential candidates based on their use as a screening-level tool. The models that were ultimately considered as potential candidates are shown in Table 1.

**Table 1**
**List of Exposure Assessment Models Evaluated**

| |
|---|
| MEPAS (Buck et al. 1995) |
| FRAMES[1] |
| MULTIMED (Health and Welfare Canada 1992) |
| MULTIMED-DP (Salhotra et al. 1993) |
| RESRAD-CHEM (EPA 1995) |
| MMSOILS (EPA 1995) |
| PIRANHA (Burns 1992) |
| PCGEMS (Access EPA 1993) |
| PRÉCIS (Sandia National Laboratories 1994) |

[1] Personal Communication, 1997, Gene Whelan, Pacific Northwest National Laboratory, Richland, WA.

## Model Histories and Backgrounds

### MEPAS

The Multimedia Environmental Pollutant Assessment System (MEPAS) was developed by Pacific Northwest Laboratory for the U.S. Department of Energy (DOE) Office of Environment, Safety, and Health. It was derived from the Remedial Action Priority System (RAPS) and is comprised of a set of computer programs used to prioritize hazardous,

radioactive, and mixed-waste sites based on their potential impact on human health. MEPAS is applicable to a wide range of environmental management and regulatory applications. The model can be applied to inactive as well as to active air and water release sites. The model itself uses a simplified contaminant-transport and exposure algorithm encapsulated into a user-friendly shell containing an extensive database of approximately 476 contaminants. MEPAS is an integrated system of analytical, semi- analytical, and empirically based mathematical models that simulate the release of contaminants from sources, migration and fate of these contaminants through various environmental media, concentrations at designated receptor locations, and health effects to specified sensitive receptors caused by exposure to these contaminants. It was designed to address long-term average environmental conditions resulting from release to the environment from point and area sources. MEPAS does not address acute exposures to environmental contamination.

## FRAMES

The Framework for Risk Analysis and Management of Environmental Systems (FRAMES) was developed by Pacific Northwest National Laboratory for the DOE. FRAMES is an object-oriented model that is still under development. Within FRAMES will reside a collection of computer algorithms that will simulate the following elements of a transport, exposure, and risk-assessment system: contaminant source and release to environment (including surface hydrology), overland transport, vadose-zone transport, saturated-zone transport, atmospheric transport, surface water transport, food-supply transport (including animals and plants to humans), intake computation, and health impacts. In FRAMES, each of the above-listed elements, and many that are not listed, can and will be represented by separate modules. FRAMES utilizes three types of files: primary data communication files which transfer information between modules, global input data files where all user input is stored, and other data files which allow for imported data files, exported data files, and maintained databases.

Within FRAMES, data transfer linkages are designed to avoid data redundancy, to provide dynamic linked modules (modules are linked as the direct result of user selection), and to provide a framework/user interface that allows for relatively easy inclusion of additional modules and models, promotes access to national databases, minimizes data-exchange requirements, and allows for unlimited access to data.

## MULTIMED

The Multimedia Exposure Assessment Model (MULTIMED) was developed by the Center for Exposure Assessment Modeling (CEAM) of the U.S. Environmental Protection Agency (USEPA). It simulates the movement of contaminants leaching from a waste disposal facility or from

contaminated soils. It is comprised of several modules that predict concentrations at a receptor due to transport in the subsurface, surface water, or air. The model is accompanied by a preprocessor, PREMED, and a postprocessor, POSTMED. The preprocessor guides the user in the creation of a Subtitle D input file, while the postprocessor is used to generate plots of data obtained from the simulation.

The model calculates contaminant concentrations in groundwater, surface water, and air resulting from emissions from hazardous waste sites. The hydrologic and atmospheric pathways are addressed independently with no transfer of contaminant between the two pathways.

### MULTIMED-DP

The Multimedia Exposure Assessment Model - Daughter Products (MULTIMED-DP) is essentially the same as the MULTIMED except that it can be used to simulate the transport and fate of first- and second-generation transformation (daughter) products that migrate from a waste source through the unsaturated and saturated zones to a down gradient receptor well.

### RESRAD-CHEM

The Residual Radioactivity (RESRAD) model was developed in the early 1980s by Argonne National Laboratory for the DOE. It was initially developed to calculate site-specific residual radioactive material guidelines and radiation dose/risk to an onsite individual at a radioactively contaminated site. The RESRAD code has been continuously updated and improved to now include chemical contaminants (RESRAD-CHEM).

The pathways considered by this model include direct external exposure, dust inhalation, exposure to radon, and ingestion of plant foods, meat, milk, aquatic foods, water and soil. The model has a built-in capability to do sensitivity analysis on input parameters, and it also has the capability to do uncertainty analysis on input parameters and databases using the Latin Hypercube Sampling (LHS) technique.

### MMSOILS

The MMSOILS model was developed by Tetra Tech, Inc., for the USEPA. MMSOILS is a methodology for estimating the human exposure and health risk associated with releases of contamination from hazardous waste sites. The methodology addresses the transport of a chemical through groundwater, surface water, soil, the atmosphere, and aquatic/terrestrial food chains. For multimedia exposure, the model provides estimates of human exposure through individual pathways and cumulative exposure through all pathways considered. The risk associated with the

total exposure dose is calculated based on the chemical-specific toxicity data.

The human exposure pathways considered include soil ingestion, air inhalation of volatile compounds and particulate matter, dermal contact, ingestion of drinking water, consumption of fish, consumption of plants grown on contaminated soil, and consumption of animals that grazed on contaminated pastures. For multimedia exposure, the methodology provides estimates of human exposure through individual pathways and cumulative exposure through all pathways considered.

## PIRANHA

The Pesticide and Industrial chemical Risk ANalysis and Hazard Assessment (PIRANHA) model was developed by the USEPA. PIRANHA is a computer-based system for applying the ecotoxicological and environmental sciences to ecological risk assessment. PIRANHA includes a Geographic Information System (GIS-) based facility for locating biological resources potentially at risk from pesticide and industrial chemicals, a toxicological inferencing program for species-to-species extrapolation of acute toxicity, models for predicting ambient chemical exposures in aquatic and agro-ecosystems, and bioaccumulation models for fauna.

The PIRANHA model can use up to three sub-models during the course of analysis. These sub-models are the Pesticide and Root Zone Model (PRZM), the Exposure Analysis Modeling System (EXAMS), and the Food and Gill Exchange of Toxic Substances (FGETS) model.

The PRZM is a one-dimensional, dynamic, compartmental model for simulating vertical chemical movement in unsaturated soil systems within and immediately below the plant root zone. It allows the user to simulate movement of potentially toxic chemicals, particularly pesticides, that are applied to the soil or to plant foliage. Dynamic simulations allow for the consideration of pulse loads, the prediction of peak events, and the estimation of time-varying mass emission or concentration profiles.

The EXAMS model is an interactive computer program intended to give decision-makers access to a responsive, general, and controllable tool for readily deriving and evaluating the behavior of synthetic chemicals in the environment. The model estimates exposure, fate, and persistence following release of an organic chemical into an aquatic ecosystem.

The FGETS model simulates the bioaccumulation of nonmetabolized organic chemicals in fish. The model is formulated in such a way that its parameterization does not rely upon specific toxicokinetic studies but, rather, depends on physical and chemical properties of the compounds that can be estimated by other models and on ecological, morphological, and physiological characteristics of the fish that can be obtained from computerized databases.

### PCGEMS

The Graphical Exposure Modeling System PC (PCGEMS) is a stand-alone version of the Graphical Exposure Modeling System (GEMS) for use on a PC. GEMS began development in 1981 by the USEPA. PCGEMS supports exposure and risk assessments by providing access to single medium and multimedia fate and exposure models, physical-chemical property estimation techniques, statistical analysis, graphics and mapping programs with related data on environments, sources, receptors, and populations. PCGEMS is an easily learned interface to various models, programs, and data needed for exposure and risk assessments. Currently, PCGEMS contains associated environmental and 1980 population data encompassing most of the United States.

The PCGEMS allows the use of mathematical algorithms to calculate an estimate of pollutant concentration based on a number of environmental factors. It also allows the use of several screening-level models that predict chemical partitioning, the separation of components of a chemical mixture, among the environmental media. These models include media-specific capabilities for modeling pollutant releases to the atmosphere, surface water, soil, and groundwater.

### PRÉCIS

The Probabilistic Risk Evaluation and Characterization Investigation System (PRÉCIS) was developed by Sandia National Laboratory for the DOE. The software aids site investigators in performing probabilistic risk assessments to quantify risk to human and environmental receptors (with associated uncertainty) resulting from site contamination, in determining risk-based action or cleanup levels, and in prioritizing data needs for characterization. It can be used to estimate dose and action or cleanup levels for radionuclides, risks and toxicity effects from hazardous chemicals, and action or cleanup levels for hazardous chemicals. The software incorporates a user-friendly Graphical User Interface (GUI) and is available in versions for Windows 3.1®, Windows NT®, Windows 95®, and Macintosh®.

## Exposure Model Pathways and Features

The candidate models have various features and pathways which are summarized in Table 2. A more detailed comparison of the models, which includes comparison of such features as uncertainty analysis, partitioning, ability to simulate transformation products, etc., is shown in Table 3.

## Table 2
## Pathway/Feature Comparison of Candidate Multimedia Models

| Pathway/ Feature | Model | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | PCGEMS | MEPAS | MULTIMED | MULTIMED-DP | MMSOILS | PIRANHA | FRAMES | RESRAD-CHEM | PRÉCIS |
| **Transport Media** | | | | | | | | | |
| Air | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| Groundwater | Y | Y | Y | Y | Y | N | Y | Y | Y |
| Soil | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| Surface water | Y | Y | Y | Y | Y | Y | Y | N | Y |
| **Source Type** | | | | | | | | | |
| Underground storage tank | N | Y | N | N | Y | N | Y | N | [1] |
| Surface water | Y | Y | N | N | Y | N | Y | N | [1] |
| Landfill | Y | Y | Y | Y | Y | N | Y | Y | [1] |
| Stack | Y | Y | N | N | N | N | Y | N | [1] |
| Soil | Y | Y | N | N | Y | Y | Y | Y | [1] |
| Road | N | N | N | N | N | N | N | N | [1] |
| **General Features** | | | | | | | | | |
| User interface | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| Default data | Y | Y | N | N | Y | Y | Y | | Y |
| Risk assessment | Y | Y | N | N | Y | Y | Y | Y | Y |
| Toxics | Y | Y | Y | Y | Y | Y | Y | Y | Y |
| Nutrients | N | N | N | N | N | N | N | N | N |
| **GW Pathways** | | | | | | | | | |
| Model type | Flow/Trans | Flow/Trans | Flow/Trans | Flow/Trans | Flow/Trans | N/A | Flow/Trans | Flow/Trans | Transport |
| Zone | Both | Both | Both | Both | Both | N/A | Both | Both | Both |
| Degradation | Y | Y | Y | Y | Y | N/A | Y | Y | — |
| Retardation | Y | Y | Y | Y | Y | N/A | Y | Y | — |
| Dispersion | Y | Y | Y | Y | Y | N/A | Y | N | — |
| **NPS Pathways** | | | | | | | | | |
| Watershed | Agricultural/ Undeveloped | Agricultural/ Landfill | Landfill | Landfill | Landfill | Agricultural | Agricultural/ Landfill | Landfill | Agricultural |
| Watersheds | Single | Single | Single | Single | Single | Single | Single | Single | Single |
| Events | Continuous | — | Both | Both | Continuous | Continuous | — | Annual average | Annual average |
| Sediment transport | Y | Y | N | N | Y | N | Y | Y | N |
| Adsorption | Y | N | N | N | N | Y | N | N | Y |
| Volatilization | Y | N | Y | Y | Y | Y | N | N | N |

*(Continued)*

**Table 2 (Concluded)**

| Pathway/ Feature | Model | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | PCGEMS | MEPAS | MULTIMED | MULTIMED-DP | MMSOILS | PIRANHA | FRAMES | RESRAD-CHEM | PRÉCIS |
| **SW Pathways** | | | | | | | | | |
| Water body type | Lake/River/ Estuary | River | River | River | Lake/ River | Lake/River | River | N/A | Stream/ Pond |
| Degradation | Y | N | Y | Y | Y | Y | N | N/A | — |
| Adsorption | Y | N | Y | Y | Y | Y | N | N/A | — |
| Volatilization | Y | N | Y | Y | Y | Y | N | N/A | N |
| **Air Pathways** | | | | | | | | | |
| Release mechanism | Y | Y | Y | Y | Y | Y | Y | Y | N |
| Dilution/ transport | Y | Y | Y | Y | Y | Y | Y | Y | — |
| Washout | N | Y | N | N | N | N | Y | N | N |
| Deposition | Y | Y | N | N | Y | Y | Y | Y | — |
| Complex terrain | Y | Y | N | N | N | N | Y | N | N |
| Wake effects | Y | Y | N | N | N | N | Y | Y | N |
| Degradation | Y | Y | Y | Y | N | N | Y | Y | — |

Note: GW = Groundwater, NPS = Non-Point Source, SW = Surface Water
[1] Calculations are based on time since material was placed.

## Selection of Screening-Level Model for Simulating MRCs

Based on a model's overall capability as a screening-level tool for evaluating MRCs, the ease with which adaptations or modules could be made to an existing model without significant code modification, and the relative ease-of-use or user-friendliness of the final product, risk assessment models were chosen as the building blocks for the creation of a module which contains the primary process descriptions for the fate of target MRCs. The models that were chosen for the adaptation to simulate MRCs were FRAMES and MEPAS.

### Evaluation of MEPAS database for existing MRCs

The MEPAS risk assessment model's database was analyzed to determine the current chemical property/risk association values of any existing MRCs. The MEPAS database contained information for TNT, RDX, and HMX. The existing information contained in the MEPAS database on each of these three chemicals is presented in Table 4.

## Table 3
## Detailed Comparison of Potentially Useful Multimedia Models

| Property | Model | | | | | | |
|---|---|---|---|---|---|---|---|
| | **MEPAS** | **MULTIMED** | **MULTIMED-DP** | **RESRAD-CHEM** | **MMSOILS** | **FRAMES** | **PIRANHA** |
| Uncertainty estimation | N (Sum[3] is available separately as option) | Y (Monte Carlo) | Y (Monte Carlo) | Y | Y | Y | Y |
| Screening level | Y | Y | Y | Y | Y | Y | Y |
| Assessment level | Y | Y | Y | Y | Y | Y | Y |
| Risk estimation | Y | Y | Y | Y | Y | Y | Y |
| Applicable to NAPLs[1] | N | N | N | N | N | N | N |
| Homogeneous medium | Y | Y | Y | Y | Y | Y | N/A |
| Heterogeneous medium | N | N | N | N | N | N | N/A |
| Overland transport | Y (modified curve-number technique) | N | N | N | Y | Y | Y |
| Sediment transport | Y (Universal Soil Loss Eqn.) | N | N | Y | Y | Y | N |
| Evapo-transpiration | Y (Penman Method with Correction Factor) | Y | Y | Y | Y | Y | Y |
| Groundwater transport | 1-D advective, 3-D dispersive | 1-D advective, 3-D dispersive | 1-D advective, 3-D dispersive | 1-D advection only | 1-D advective, 3-D dispersive | 1-D | N/A |
| Surface-water transport | 1-D advection & 2-D dispersion | 0-D complete mixing | 0-D complete mixing | 0-D complete mixing (onsite pond) | 1-D advection & dispersion | 1-D | Y |
| Atmospheric transport (far field) | Gaussian Plume model | Gaussian Plume model | Gaussian Plume model | Gaussian Plume model | Gaussian Plume model | Gaussian Plume model | — |
| Atmospheric transport (near field) | N | N | N | Y (0-D complete mixing) | Y (0-D complete mixing) | N | — |
| Unsat. zone flow | 1-D SS or Dynamic | 1-D | 1-D | 1-D | 1-D | 1-D SS or Dynamic | N/A |
| Maximum unsat. layers | 5 | 20 | 20 | — | — | 5 | N/A |
| Sat. zone flow | Constant & uniform (1-D) | Constant & uniform (1-D) | Constant & uniform (1-D) | Constant & uniform (1-D) | Constant & uniform (1-D) | Constant & uniform (1-D) | N/A |
| Maximum sat. layers | 1 | 1 | 1 | — | — | 1 | N/A |
| Surface-water flow | 2-D steady state | 1-D steady state | 1-D steady state | Surface hydrology | 1-D steady state | 2-D steady state | Steady state |
| Multi-porosity | N | N | N | N | N | N | N |
| Multi-pathway | Y | Y | Y | Y | Y | Y | Y |
| Transformation products | Y | N | Y | Y | N | Y | Y |
| Linear partitioning | Y | Y | Y | Y | Y | Y | Y |
| Non-linear partitioning | N | N | N | N | N | N | N |
| Multiple sources per simulation | Y | N | N | N | N | Y | — |

***(Continued)***

## Table 3 (Concluded)

| Property | Model | | | | | | |
|---|---|---|---|---|---|---|---|
| | MEPAS | MULTIMED | MULTIMED-DP | RESRAD-CHEM | MMSOILS | FRAMES | PIRANHA |
| Multiple contaminants per simulation | Y | N | N | Y | Y | Y | Y |
| PC platform | Y | Y | Y | Y | Y | Y | Y |
| Workstation platform | Y | N | N | N | — | Y | Y |

[1] NAPL = Non-aqueous phase liquid

## Table 4
## MEPAS Database Parameters for TNT, RDX, and HMX

| Property/Parameter | TNT Value | RDX Value | HMX Value |
|---|---|---|---|
| **Physical Properties** | | | |
| Molecular weight (g/mole) | 227.1 | 222.1 | 296.2 |
| Vapor pressure (mm HG @ 25 °C) | 8.99E-08 | 4.08E-04 | 8.40E-04 |
| Henry's Law constant (atm $m^3$/mole @ 25 °C) | 1.37E-04 | 8.30E-06 | 3.53E-06 |
| Water solubility (mg/L @ 25 °C) | 480.00 | 38.40 | 2.63 |
| Carbon matter partition coefficient (ml/g) | 17.80 | 1.01E+03 | 2.40 |
| Octanol-water partition coefficient (ml/g) | 77.60 | 1.91E+03 | 3.90 |
| Aqueous skin permeability (cm/hr) | 0.00 | 0.00 | 0.00 |
| **Environmental Half-times** | | | |
| In air (days) | 0.00 | 0.00 | 0.00 |
| In groundwater (days) | 0.00 | 0.00 | 0.00 |
| In surface water (days) | 5.78E-01 | 6.63 | 17.70 |
| In soil (days) | 0.00 | 2.52E+06 | 1.17E+06 |
| **Environmental Transfer Factors** | | | |
| Bioaccumulation in fish (L/kg) | 0.00 | 0.00 | 0.00 |
| Bioaccumulation in shellfish (L/kg) | 0.00 | 0.00 | 0.00 |
| Soil-to-plant transfer factor | 0.00 | 0.00 | 0.00 |
| Feed-to-animal meat transfer factor (d/kg) | 0.00 | 0.00 | 0.00 |
| Feed-to-cow milk transfer factor (d/L) | 0.00 | 0.00 | 0.00 |
| Grout diffusion coefficient ($cm^2$/sec) | 5.00E-08 | 5.00E-08 | 5.00E-08 |
| Water purification factor (mg/kg/day) | 1.00 | 1.00 | 1.00 |
| Deposition velocity (m/sec) | 0.00 | 0.00 | 0.00 |
| Atmospheric deposition class | 6 | 6 | 6 |
| **Toxicities and Slope Factors** | | | |
| Inhalation slope factor (mg/kg/day) | 3.00E-02 | 0.11 | 0.00 |
| Ingestion slope factor (mg/kg/day) | 3.00E-02 | 0.11 | 0.00 |
| Inhalation reference dose (mg/kg/day) | 5.00E-04 | 3.00E-02 | 5.00E-02 |
| Ingestion reference dose (mg/kg/day) | 5.00E-04 | 3.00E-02 | 5.00E-02 |
| Gastro-intestinal absorption factor | 0.00 | 0.00 | 0.00 |
| Skin absorption fraction from soil | 0.00 | 0.00 | 0.00 |

## Proposed revisions to the MEPAS database for TNT, RDX, and HMX

Evaluation of some of the most current data and analyses available led to recommended changes to parameters in the MEPAS database. Table 5 shows the environmental data (Townsend and Myers 1996) where changes to the MEPAS database are suggested for TNT, RDX, and HMX.

**Table 5**
**Literature Values for Key TNT, RDX, and HMX Environmental Data**

| Property | TNT Value | RDX Value | HMX Value |
|---|---|---|---|
| Vapor pressure (mm Hg @ 25 °C) | 5.51E-06 | 4.03E-09 | 3.33E-14 |
| Henry's Law constant (atm $m^3$/mole @ 25 °C) | 1.10E-08 | 1.96E-11 | 2.60E-15 |
| Water solubility (mg/L @ 25 °C) | 100.00 | 45.00 | 5.00 |
| Carbon matter partition coefficient (ml/g) | 524.81 | 7.76 - 269.15[1] | 3.47 - 676.08[1] |
| Octanol-water partition coefficient (ml/g) | 72.4 - 114.8[1] | 7.2 - 7.4[1] | 1.15 - 1.82[1] |
| Environmental half-time in groundwater (days) | 28 - 360[1] | | |

[1] Denotes range of values cited in literature (Townsend and Myers 1996)

Brannon et al. (in preparation) studied the behavior of TNT and its mono and diamino transformation products in a surface and aquifer soil under both aerobic and anoxic conditions and determined the sorption coefficients for these compounds. Table 6 shows the distribution coefficients (also called adsorption coefficients) obtained for TNT and the transformation products 4ADNT, 2ADNT, 2,4-DANT, and 2,6-DANT under aerobic conditions for a surface and an aquifer soil. The properties of the soils which were used in the Brannon study are shown in Table 7.

**Table 6**
**Distribution Coefficients ($K_d$) for TNT and its Transformation Products Obtained Under Aerobic Conditions in a Surface and an Aquifer Soil (from Brannon et al. in preparation)**

| | Sharkey Clay Surface Soil | | | LAAP Aquifer Soil | | |
|---|---|---|---|---|---|---|
| Compound | $K_d$, ml/g | Std. Error | $r^2$ | $K_d$, ml/g | Std. Error | $r^2$ |
| TNT | 2.2 | 0.12 | 0.99 | 0.23 | 0.02 | 0.99 |
| 4ADNT | 4.0 | 0.22 | 0.99 | 0.22 | 0.04 | 0.86 |
| 2ADNT | 5.5 | 0.26 | 0.99 | 0.31 | 0.05 | 0.92 |
| 2,4-DANT | 2.1 | 0.27 | 0.94 | 0.08 | 0.02 | 0.79 |
| 2,6-DANT | 5.5 | 0.48 | 0.97 | 0.09 | 0.002 | 0.99 |

**Table 7**
**Soil Properties (from Brannon et al. in preparation)**

| Soil | TOC[1], % | % Sand | % Silt | % Clay | CEC meq/100g[2] |
|---|---|---|---|---|---|
| Sharkey clay | 2.4 | 13.8 | 37.5 | 48.7 | 38.9 |
| LAAP SP-SM Sandy silt | 0.015 | 92.5 | 2.5 | 5.0 | 3.6 |

[1] Total organic carbon
[2] Cation exchange capacity expressed in milliequivalents per 100 grams soil

Equation 1 shows the theoretical linear, reversible equilibrium partitioning coefficient relationship

$$K_d = \frac{C_p}{C_d} \tag{1}$$

where

$K_d$ = distribution coefficient, $L^3/M$
$C_p$ = mass of chemical sorbed per mass of solid, $M/M$
$C_d$ = dissolved chemical mass per unit volume of liquid, $M/L^3$
$M$ = mass
$L$ = length

The MEPAS model allows the user four options when specifying the adsorption coefficient $K_d$. If the adsorption coefficient is known to the user, then that value may be used directly within MEPAS from the "Worksheet" menu and by selecting template 2.7-"Adsorption Coefficients ($K_d$)". From this worksheet, the user may directly enter the adsorption coefficient. The second option is applicable if the user does not know the adsorption coefficient but does know the fraction of organic carbon ($f_{oc}$) and the organic carbon partition coefficient ($K_{oc}$). In this case, Equation 2 (Karickhoff 1979) may be used for most nonpolar organics to determine the adsorption coefficient ($K_d$).

$$K_d = f_{oc} * K_{oc} \tag{2}$$

where

$f_{oc}$ = fraction of organic carbon
$K_{oc}$ = organic carbon partition coefficient, ml/g.

The third option applies if the user knows the $f_{oc}$ but does not know the $K_{oc}$. In this case, the user can estimate $K_d$ from Equation 2 but use the value of $K_{oc}$ obtained from the MEPAS environmental database for the chemical constituent of concern. The $K_{oc}$ is readily obtainable for a particular constituent from the MEPAS environmental database. The complete listing of data for a constituent is obtained by selecting the "Site" option from the MEPAS main menu, then selecting the "Edit Site" option. This brings up the "Site Summary" menu where the user may select the "Constituent Source Defined" option and press Enter twice. The fourth option is to use the default values which MEPAS provides in the case where the user does not know the $f_{oc}$ nor the $K_{oc}$. In this case, MEPAS will calculate a suggested value based on the user's description of the soil properties (percentage of sand, silt, clay and organic matter) and the following relationship between the soil properties and the $f_{oc}$ as proposed by Whelan et al. (1987):

$$f_{oc} = (0.005 * \%\ sand + 0.4 * \%\ silt + 2.0 * \%\ clay + 57.735 * \%\ om)\ 10^{-4} \quad (3)$$

where

$\%sand$ = percentage of sand component of soil

$\%silt$ = percentage of silt component of soil

$\%clay$ = percentage of clay component of soil

$\%om$ = percentage of organic matter in the soil

In order to provide the user with a more realistic estimated value of $K_d$ for TNT, the MEPAS database was updated using the information in Tables 6 and 7 from Brannon et al. (in preparation) for TNT in Sharkey clay. Rearranging Equation 2 to solve for the value $K_{oc}$ yields Equation 4:

$$K_{oc} = \frac{K_d}{f_{oc}} \quad (4)$$

When Equation 4 is solved, it provides a $K_{oc}$ value of 91.67 ml/g. The $K_{oc}$ value obtained in this manner is a factor of 5.0 of the MEPAS database original default value for TNT of 17.80 ml/g. The original $K_{oc}$ value in the MEPAS database was referenced to the USEPA's GEMS VP-1,2,K methods.

The data from Tables 6 and 7 for LAAP aquifer soil were not used in the calculation of $K_{oc}$ from Equation 4 because the fraction of organic carbon in the aquifer soil is less than 0.5 percent. Typically, nonlinearity occurs on a plot of $f_{oc}$ versus $K_d$ for $f_{oc}$ values less than 0.5 percent (Rebhun et al. 1992). The $f_{oc}$ formulation in MEPAS is essentially

unaffected by this nonlinearity because it uses Equation 3 to obtain a value for $f_{oc}$, which allows the fraction of organic matter to be weighted among the other components of sand, silt, and clay.

With a new value of $K_{oc}$ for TNT, a revised value for the octanol-water partition coefficient ($K_{ow}$) can now be derived for the MEPAS database. Karickhoff (1984) noted that predictions of $K_{oc}$ based on values of $K_{ow}$ are much more reliable than those based on solubility (McGrath 1995). The Multimedia Modeling Environmental Database Editor (MMEDE), a database support program supplied with MEPAS, can estimate values of $K_{oc}$ based on solubility or $K_{ow}$. MMEDE contains $K_{oc}$ estimation routines for pesticides, aromatics, assorted chemicals, and s-triazines for a total of seven methods of estimation (Warren and Strenge 1994). For the aromatic compound TNT, one of two methods can be chosen to estimate $K_{oc}$. The first is the GEMS Method K-2 (also termed the Lyman 4-10 method) which is as follows:

$$\log K_{oc} = \log K_{ow} - 0.21 \tag{5}$$

where

$K_{ow}$ = octanol-water partition coefficient, ml/g.

The other method is the Lyman Method 4-9

$$\log K_{oc} = 0.937 * (\log K_{ow}) - 0.006 \tag{6}$$

Rearranging Equation 6 above and solving for $K_{ow}$ based on a $K_{oc}$ value of 91.67 ml/g, yields a value for $K_{ow}$ of 126.05 ml/g. This value is slightly out of the range of 72.4 -114.8 ml/g compiled and presented by Townsend and Myers (1996). For comparison, solving the Lyman 4-10 equation for $K_{ow}$ yields a value of 148.67 ml/g.

Table 8 summarizes the revisions made to the MEPAS database for TNT. There are no published recent studies with estimated or measured partition coefficients for RDX and HMX. There are some studies with RDX and HMX which are currently on-going and with preliminary results of $K_d$. Therefore, Table 8 shows the values that were changed in the MEPAS database using the data from Townsend and Myers (1996) for RDX and HMX.

## Table 8
## Revisions to the MEPAS Database for TNT, RDX, and HMX

| Property | TNT Value | RDX Value | HMX Value |
|---|---|---|---|
| Vapor pressure (mm Hg @ 25 °C) | 5.51E-06[1] | 4.03E-09 | 3.33E-14 |
| Henry's law constant (atm $m^3$/mole @ 25 °C) | 1.10E-08[1] | 1.96E-11 | 2.60E-15 |
| Water solubility (mg/L @ 25 °C) | 100.0[1] | 45.00 | 5.00 |
| Carbon matter partition coefficient (ml/g) | 91.67[2] | 100.0[4] | 3.47[5] |
| Octanol-water partition coefficient (ml/g) | 126.05[3] | 7.2[4] | 1.82[5] |
| Environmental half-time in groundwater (days) | 360[1] | | |

[1] Data from Townsend and Myers (1996)
[2] Value derived from Brannon et al. (in preparation)
[3] Lyman Method 4-9, data from Warren and Strenge (1994)
[4] Obtained from latest available values listed in Table A2 of Townsend and Myers (1996)
[5] Obtained from latest available values listed in Table A3 of Townsend and Myers (1996)

# 3 Process Descriptions for the Fate of Target MRCs

Process descriptions for explosive compounds are poorly developed because specific reaction mechanisms and their interrelations are poorly understood (McGrath 1995). This section describes the processes affecting the fate of military explosive compounds and radionuclides in the environment. This section will concentrate more on explosive rather than radioactive compounds, since the processes affecting explosive compounds in the environment have not been well studied nor analyzed in as great detail as radioactive compounds. Processes affecting groundwater transport of explosives include, but are not limited to, advection, hydrodynamic dispersion, adsorption, biodegradation, abiotic transformations, solubility, volatilization, and chemical reactions.

## Factors Affecting Contaminant Transport

Darcy's law states that the rate of flow through a porous medium is directly proportional to the difference in head and inversely proportional to the length of the flow path. The mathematical representation of Darcy's law is

$$\nu = \left(\frac{-k\rho g}{\mu}\right)\left(\frac{dh}{dl}\right) \tag{7}$$

where

$\nu$ = specific discharge, L/t

$k$ = intrinsic permeability, $L^2$

$\rho$ = fluid density, $M/L^3$

$g$ = acceleration due to gravity, $L/t^2$

$\mu$ = dynamic viscosity, $ML^{-1}t^{-1}$

$dh/dl$ = hydraulic gradient, L/L

$L$ = length

$t$ = time

$M$ = mass

If one desires to use the groundwater terminology where hydraulic conductivity is used instead of permeability, then Equation 7 can be rewritten using a term for hydraulic conductivity as

$$\nu = -K\frac{dh}{dl} \tag{8}$$

where

$$K = \frac{k\rho g}{\mu} \tag{9}$$

and

$K$ = hydraulic conductivity, $L/t$

The general partial differential advection-dispersion equation (Freeze and Cherry 1979) describing three-dimensional solute transport in a porous, saturated, homogeneous, and isotropic medium under steady-state flow, and assuming that Darcy's law applies, is

$$\frac{\partial C}{\partial t} = \left[\frac{\partial}{\partial x}\left(D_x\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z\frac{\partial C}{\partial z}\right)\right] - \left[\frac{\partial}{\partial x}\left(\bar{\nu}_x C\right) + \frac{\partial}{\partial y}\left(\bar{\nu}_y C\right) + \frac{\partial}{\partial z}\left(\bar{\nu}_z C\right)\right] - \left(\frac{\rho_b}{n}\right)\left(\frac{\partial S}{\partial t}\right) \tag{10}$$

where

$C$ = mass of solute per unit volume of solution, $M/L^3$

$D_x$ = dispersion coefficient in the $x$ direction, $L^2/t$

$D_y$ = dispersion coefficient in the $y$ direction, $L^2/t$

$D_z$ = dispersion coefficient in the $z$ direction, $L^2/t$

$\bar{\nu}_x$ = average linear velocity in the $x$ direction, L/t

$\bar{v}_y$ = average linear velocity in the *y* direction, L/t

$\bar{v}_z$ = average linear velocity in the *z* direction, L/t

$\rho_b$ = bulk mass density of the porous medium, $M/L^3$

$n$ = porosity

$S$ = the mass of chemical constituent adsorbed on a unit mass of solid of the porous medium, M/M

This equation is the basic fundamental principle to all transport modeling efforts. The source term is added to the equation to handle the effects of retardation of solute transport through adsorption, chemical reaction, biological transformation, or radioactive decay.

### Advection

Advection is the process by which a compound is transported primarily due to the bulk motion of flowing groundwater. In Equation 10, that portion of transport due to advection is

$$-\left[\frac{\partial}{\partial x}\left(\bar{v}_x C\right)+\frac{\partial}{\partial_y}\left(\bar{v}_y C\right)+\frac{\partial}{\partial z}\left(\bar{v}_z C\right)\right]$$

Advection is applicable to the transport of both military energetic compounds and radioactive materials.

### Hydrodynamic dispersion

Hydrodynamic dispersion is the process by which the contaminant is transported by variations in the microscopic velocity within each pore channel and from one channel to the next. It is caused by the mechanical mixing during fluid advection and the molecular diffusion due to the thermal-kinetic energy of the solute particles. Dispersion caused by the mechanical mixing of a solute due to fluid movement is called mechanical dispersion. Molecular diffusion is usually of concern only at low velocities. Unlike molecular diffusion, mechanical dispersion is usually of greater concern because it has more pronounced effects on the transport of a solute. In Equation 10 that portion of transport due to dispersion is

$$\left[\frac{\partial}{\partial x}\left(D_x \frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(D_y \frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(D_z \frac{\partial C}{\partial z}\right)\right]$$

Dispersion can be an important transport mechanism for both radioactive and energetic military compounds.

### Adsorption

Adsorption is the process by which molecules adhere to a surface with which they come into contact. Adsorption depends on the type of clay, the initial ratio of adsorbed mole fractions, and the concentration of solute in suspension.

### Biotransformation

Biotransformation is the process by which a substance is modified into another substance(s) by the activities of living organisms (e.g., bacteria and fungi). A more specific form of biotransformation is biodegradation. Biodegradation is the metabolic breakdown of materials into simpler components by living organisms. These other components can, at times, be more detrimental to the environment than the original material. Biotransformation of military specific radioactive material is not likely to occur.

### Abiotic transformation

Abiotic transformation is the process by which a chemical substance in the environment is modified by nonbiological mechanisms. This usually includes polymerization, oxidation-reduction reactions, and hydrolysis. If abiotic transformation of substances at or near the surface is considered, then this would include the process of photolysis.

Polymerization is the reaction process by which the molecules of a monomer combine to form larger molecules with a molecular weight greater than that of the original monomer, resulting in a molecule with repeated structural units.

The oxidation-reduction reaction is an oxidizing chemical change where an element's positive valence is increased (electron loss) and an accompanied simultaneous element's valence is reduced (electron gain). Stated another way, a reaction in which one reactant is oxidized (loses electrons) and one reactant is reduced (gains electrons).

Hydrolysis is the reaction between any substance and the hydrogen and hydroxyl ions found in water.

Photolysis is the process by which ultraviolet energy from sunlight is used to break the chemical bonds of a substance and form a modified substance(s).

### Solubility

Solubility is the mass of a chemical substance that will dissolve in a unit volume of solution under specified conditions of temperature and pressure. Solubility is a critical parameter in modeling an explosive contaminant's environmental fate and transport (McGrath 1995). Many explosive compounds and their derivatives are present as crystalline solids in the subsurface where they can dissolve slowly and leach into groundwaters.

### Volatilization

Volatilization is the process by which a chemical substance, either in solid or aqueous phase, undergoes a transfer of mass to the vapor phase due to high temperatures and/or low pressures weakening the chemical bonds which hold the substance together in its solid or aqueous phase. Individual components of the substance with low boiling points or melting points usually separate first, followed by components of next higher boiling/melting point order until an equilibrium point is reached where little or no more components are removed. For most common explosives, volatilization is relatively insignificant due to the high boiling point or melting point of the compounds involved.

## Energetic Military Compounds

### Fate of TNT

The major factors affecting fate and transport of TNT in the subsurface include abiotic transformations, sorption, diffusion, advection, hydrodynamic dispersion, and biodegradation (McGrath 1995). Recent research indicates that biotic transformations are even more pronounced than abiotic transformations (Townsend and Myers 1996). Some of these processes are more active and prominent than others, and some may not even have a mentionable role for a particular system.

*a. Transformation of TNT.* McCormick, Feeherry, and Levinson (1976) discovered that TNT transforms under both aerobic and anaerobic conditions. Depending on the reducing potential of the system, one to three of the nitro groups could be reduced to amino groups. The transformation pathway of TNT was studied by Kaplan and Kaplan (1982) who suggested the routes depicted in Figure 1. Several studies have shown higher production of 4-amino-2,6-dinitrotoluene (4A-DNT) than 2-amino-4,6-dinitrotoluene (Olin, Myers, and Townsend 1996). Townsend and Myers (1996) indicated that the preferred reduction route is TNT $\rightarrow$ 4A-DNT $\rightarrow$ 2,4-diamino-6-nitrotoluene (2,4-DANT).

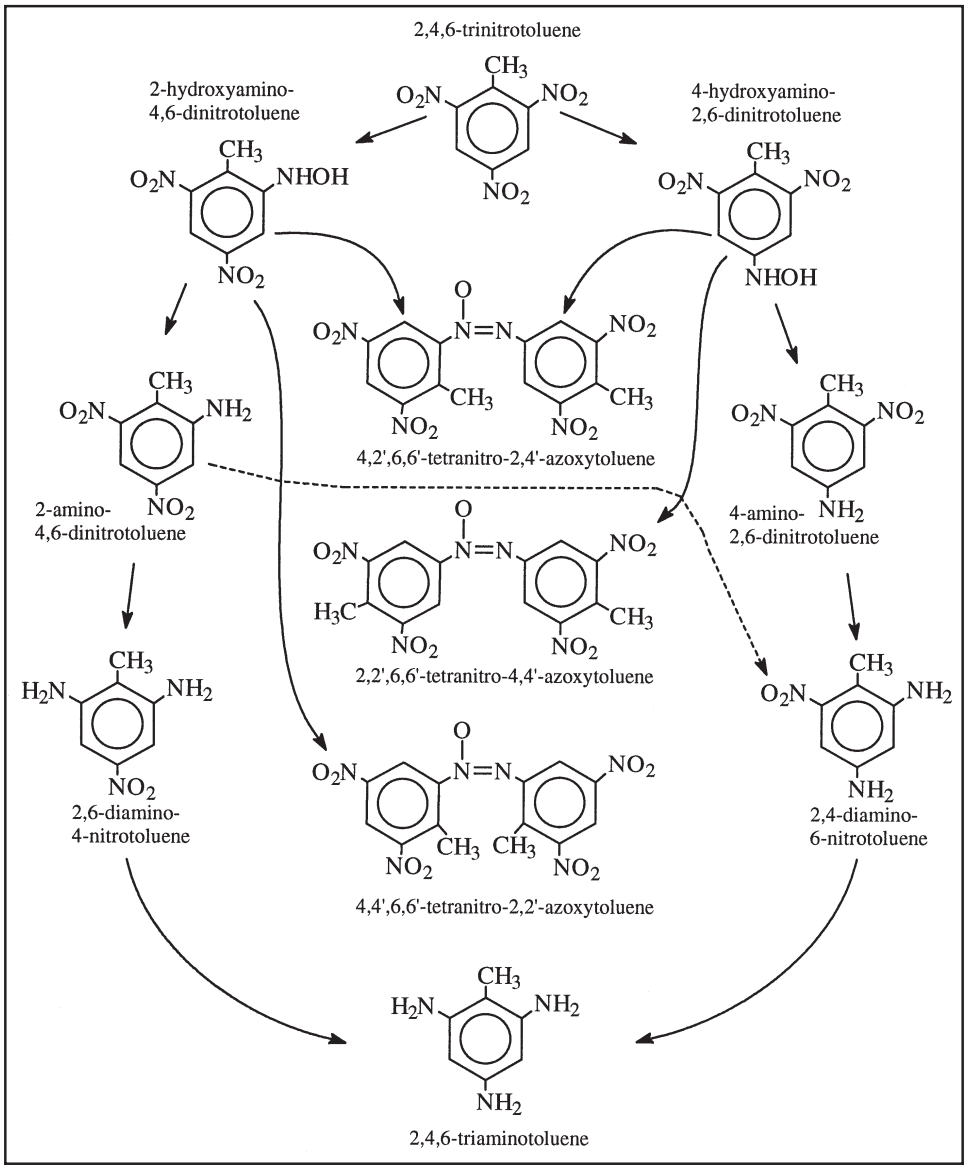


Figure 1. TNT transformation pathway diagram (McGrath 1995) (after Kaplan and Kaplan 1982)

TNT transformations in unsterilized soils are far more extensive than those in sterilized soils, indicating that the abiotic transformation component is small compared to the biotic transformation component (Townsend and Myers 1996). Studies have indicated that TNT transformations are significantly enhanced under anaerobic conditions (Townsend and Myers 1996).

*b. Sorption of TNT.* The determination of sorption parameters for TNT is often made difficult because of the formation of transformation products such as 4A-DNT, 2A-DNT, 2,4-DANT, and 2,6-DANT (Brannon and Myers 1997). Cosolute effects on the sorption of TNT were studied by Ainsworth et al. (1993), and their data suggest that

TNT and RDX utilize at least a fraction of the same sorption sites. Competition by these solutes for sorption sites reduces the sorption of individual solutes as compared with their single solute sorption values (Townsend and Myers 1996). In addition to competition among cosolutes, competition for sorption sites among TNT and its transformation products occurs (Townsend and Myers 1996). Studies have reported distribution coefficients for TNT in the range 0.0 to 56 ml/g (Townsend and Myers 1996).

## Fate of RDX

The major factors affecting the fate and transport of RDX in the subsurface are abiotic transformation, advection, sorption, diffusion, hydrodynamic dispersion, and biodegradation.

*a*. *Transformation of RDX*. The transformation of RDX has not been well documented because of the lack of microanalytical procedures for measuring the transformation products (Townsend and Myers 1996). A scheme for the biodegradation of RDX was proposed by McCormick, Cornell, and Kaplan (1981). In their proposed scheme (shown in Figure 2), RDX degrades through a series of nitro group reductions to a point where ring fragmentation occurs. This study found that RDX degradation occurred only under anaerobic conditions; however, a recent study by Myers et al. (in preparation) showed RDX degradation occurring under both aerobic and anaerobic conditions. Reports on the transformation of RDX have shown that RDX transformation is much less significant than TNT transformation.

*b*. *Sorption of RDX*. In a study by Ainsworth et al. (1993), cosolute effects on the sorption of RDX suggest that RDX and TNT compete for the same sorption sites. Distribution coefficients for RDX have been reported as being measured in the range from 0.0 to 6.75 ml/g (Townsend and Myers 1996).

## Transformation of HMX

The transformation of HMX has little study, but those studies that have been performed reported distribution coefficients in the range 0.0 to 13.25 ml/g (Townsend and Myers 1996). Like RDX, HMX transformation is much less significant than that of TNT.

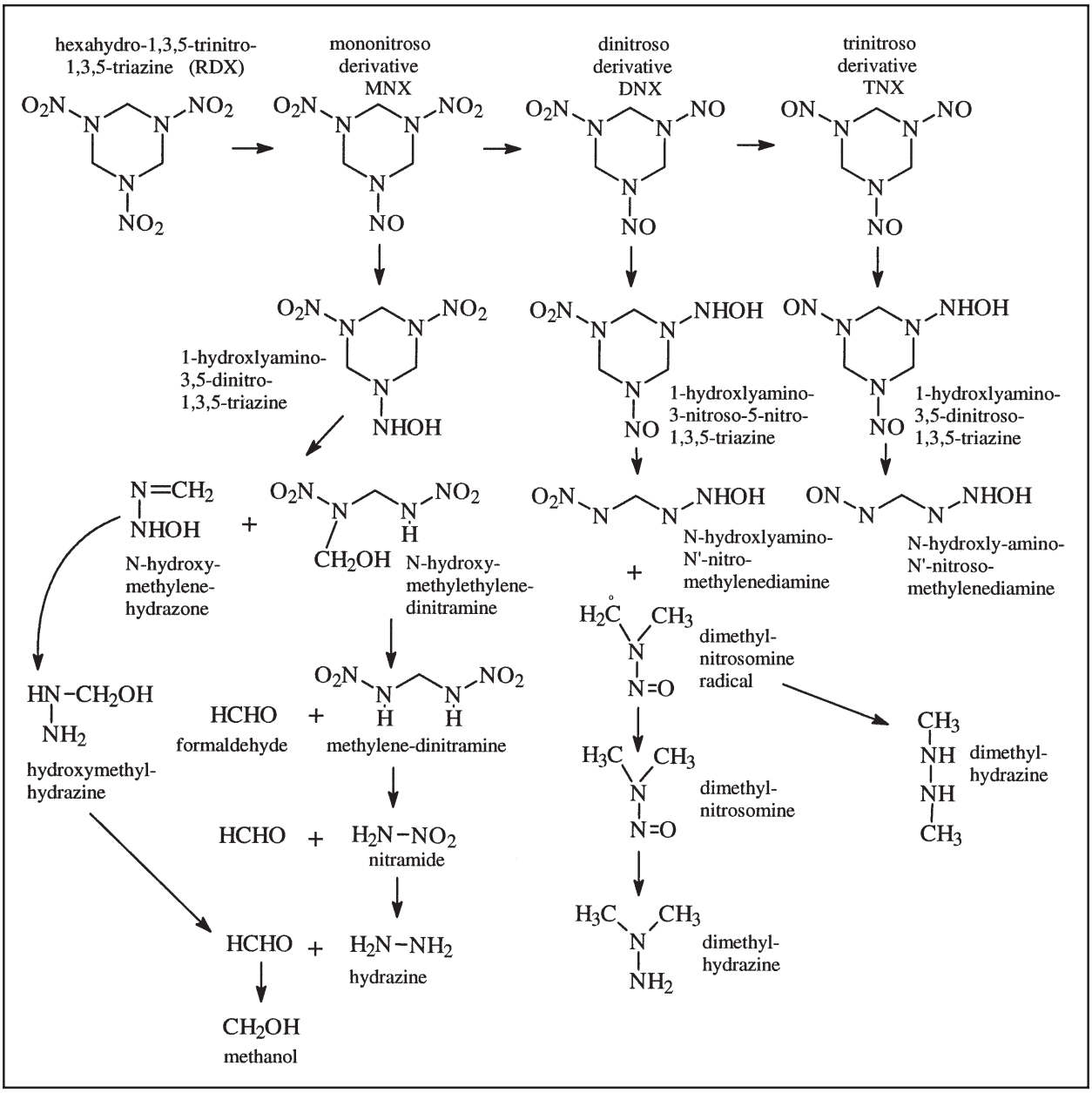


Figure 2. RDX biodegradation scheme (McGrath 1995) (after McCormick, Cornell, and Kaplan 1981)

# Radioactivity

## Radioactive decay process

Radioactive decay is an exponential rate process in which the number of atoms likely to decay in a given amount of time is proportional to the number of atoms present. This is expressed mathematically as a first-order differential equation in the form,

$$-\frac{dN}{dt} = kN \tag{11}$$

where

$N$ = number of atoms

$dN/dt$ = instantaneous time rate of change of the number of atoms

$k$ = decay constant

Integrating Equation 11 above will provide the number of atoms at any time

$$N(t) = N_0 e^{-kt} \tag{12}$$

where

$N(t)$ = number of atoms at time $t$

$N_0$ = number of atoms present at time equal zero

$e$ = base of the natural logarithm

$k$ = decay constant

$t$ = time

Equation 12 can also be expressed in terms of half-life, which is the amount of time required for one-half of the number of atom nuclei to decay. The relation between the decay constant and half-life is as follows,

$$k = \frac{\log_e 2}{t_{1/2}} \tag{13}$$

where

$k$ = decay constant

$t_{½}$ = half-life

Using the relation between the decay constant and the half-life, Equation 12 can be rewritten in the following form

$$N(t) = N_0(0.5)^{\frac{t}{t_{½}}} \quad (14)$$

where

$N(t)$ = number of atoms at time $t$

$N_0$ = initial number of atoms at time equal zero

$t$ = time

$t_{½}$ = half-life

## Radioactive modes of decay

Radioactive decay occurs through four primary decay modes. These primary radioactive decay modes include alpha decay, beta decay, positron decay, and electron capture. Each of these types of radioactive decay can create a newly formed nucleus with an excess of energy which is usually released by emitting one or more gamma rays. The measurement of the gamma rays is useful in identifying the type of radioactivity present since the gamma rays have high energy which is characteristic of the particular radioactive nucleus.

*a*. *Alpha decay.* Alpha particles are stable entities, identical to a helium-4 nucleus, which consist of two protons and two neutrons. Alpha decay is a type of radioactive disintegration caused when an unstable atomic nucleus dissipates excess energy by spontaneously ejecting an alpha particle. The following is an example of alpha decay:

$$^{241}\text{Am} \rightarrow {}^{237}\text{Np} + \alpha$$

where americium-241 decays to form neptunium-237, and $\alpha$ represents the release of an alpha particle.

*b*. *Beta decay.* When the nucleus of an atom has too many neutrons, the most likely course of decay is that the nucleus will emit an electron. Historically, electrons that are released in this manner are referred to as beta particles or rays, having been named before they were identified as electrons. The following is an example of beta decay:

$$^{239}\text{Np} \rightarrow {}^{239}\text{Pu} + \beta^-$$

where neptunium-239 decays into plutonium-239, and $\beta^-$ represents the release of a beta particle (or electron).

*c*. *Positron decay*. When the nucleus of an atom has too few neutrons it may acquire another neutron by ejecting a positive electron, or positron. This relieves the nucleus of one unit of positive charge. An example of this kind of radioactive decay is the following:

$$^{11}C \rightarrow {}^{11}B + \beta^+$$

where carbon-11 decays into boron-11, and $\beta^+$ represents the release of a positron. The positron is composed of antimatter and is very short-lived because of its existence in a world composed of matter. When a positron meets an ordinary electron the two particles annihilate each other and release their energy as two gamma rays of 0.5 megaelectron volts (MeV) each. Positron radioactivity is always accompanied by the emission of gamma rays of 0.5 MeV in addition to any other gamma rays which may be emitted.

*d*. *Electron capture*. Another way that the nucleus of an atom with too few neutrons may gain a neutron is to capture one of the negatively charged electrons orbiting about the nucleus. An electron from an inner shell of an atom is absorbed by the nucleus. In the process, a proton is converted into a neutron, and the atomic number is decreased by one. An example of this type of radioactive decay is as follows:

$$^{7}Be + e^- \rightarrow {}^{7}Li$$

where beryllium-7 decays to form lithium-7.

## Radioactive elements associated with MRCs and their fate

Some of the radioactive elements used or created in the manufacture of nuclear weapons include, but are not limited to, such elements as uranium-233, 234, 235, 238, 239; neptunium-237, 239; plutonium-238, 239, 240, 241, 242; americium- 241; thorium-232; and tritium (a radioactive isotope of hydrogen).

*a*. *Fate of plutonium*. Plutonium is a silvery-white radioactive metal that exists as a solid under normal conditions. Small amounts of plutonium occur naturally, but by-far the majority has been produced by man in nuclear reactors. Plutonium is produced when uranium absorbs an atomic particle. Plutonium has several isotopes, some of the most common being plutonium-238 and plutonium-239, where plutonium-239 is the primary source of nuclear-weapon-grade plutonium. Because plutonium is radioactive, it constantly decays,

releasing energy and forming new products. The energy released is called alpha radiation because of the release of alpha particles. The new products of the plutonium decay process are called daughter products. Daughter products are radioactive as well, and they, too, continue to decay until a nonradioactive daughter is formed. Plutonium-238 has a half-life of approximately 90 years and that of plutonium-239 is 24,000 years (ATSDR 1990).

A review of the MEPAS database for data on plutonium is presented in Table 9. A search through literature for justification of any changes to the database found none. The daughter products for five of the plutonium isotopes used in the MEPAS database are shown in Table 10.

*b*. *Fate of tritium*. Tritium ($^{3}H$) is a radioactive isotope of hydrogen and is used in the manufacture of nuclear weapons as well as in the nuclear power industry. Tritium undergoes beta decay and forms helium-3 ($^{3}He$) as the daughter product which is stable (i.e., nonradioactive). Tritium is one of the weakest beta emitters known, and the range of the beta particles emitted is approximately 5 mm in air or 0.005 mm in water and soft tissue (DOE primer on tritium safe handling practices). All chemical reactions involving hydrogen can also be performed with tritium, sometimes at a higher rate if the tritium concentration is high enough to catalyze the reaction.

A review of literature about tritium provided no justification for changes to the MEPAS database for tritium environmental parameters. The MEPAS database information is shown in Table 11.

## Table 9
## Existing MEPAS Database Information on Plutonium

| Property | Value | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | $^{234}Pu$ | $^{235}Pu$ | $^{236}Pu$ | $^{237}Pu$ | $^{238}Pu$ | $^{239}Pu$ | $^{240}Pu$ | $^{241}Pu$ | $^{242}Pu$ |
| **Physical Data** | | | | | | | | | |
| Molecular weight (g/mole) | 234 | 235 | 236 | 237 | 238 | 239 | 240 | 241 | 242 |
| Half-life (days) | 3.67E-01 | 1.76E-02 | 1.04E+03 | 4.53E+01 | 3.20E+04 | 8.79E+06 | 2.39E+06 | 5.25E+03 | 1.37E+08 |
| **Dose Factors** | | | | | | | | | |
| Ingestion dose factor (rem/pCi) | 3.79E-11 | 6.36E-12 | 1.17E-06 | 4.44E-10 | 3.20E-06 | 3.54E-06 | 3.54E-06 | 6.84E-08 | 3.36E-06 |
| Inhalation dose factor (rem/pCi) | 2.74E-08 | 2.28E-12 | 1.45E-04 | 1.97E-09 | 3.92E-04 | 4.29E-04 | 4.29E-04 | 8.25E-06 | 4.11E-04 |
| Dermal dose factor (rem/pCi) | 1.00E-07 | 1.00E-09 | 5.60E-04 | 5.60E-09 | 3.20E-03 | 3.60E-03 | 3.60E-03 | 6.90E-05 | 3.40E-03 |
| Air immersion factor (rem/hr per pCi/$m^3$) | 3.79E-11 | 5.21E-11 | 8.45E-14 | 2.68E-11 | 6.49E-14 | 5.64E-14 | 6.32E-14 | 9.65E-16 | 5.33E-14 |
| Ground exposure factor (rem/hr per pCi/$m^2$) | 8.34E-13 | 1.15E-12 | 1.31E-14 | 6.18E-13 | 1.11E-14 | 4.89E-15 | 1.07E-14 | 2.57E-17 | 8.88E-15 |
| Water immersion factor (rem/hr per pCi/L) | 8.48E-11 | 1.16E-10 | 1.97E-13 | 6.03E-11 | 1.51E-13 | 1.28E-13 | 1.48E-13 | 2.16E-15 | 1.24E-13 |
| **Environmental Transfer Factors** | | | | | | | | | |
| Bioaccumulation in fish (L/kg) | 2.50E+02 | 2.50E+02 | 2.50E+02 | 2.50E+02 | 2.50E+02 | 2.50E+02 | 2.50E+02 | 2.50E+02 | 2.50E+02 |
| Bioaccumulation in shellfish (L/kg) | 1.00E+02 | 1.00E+02 | 1.00E+02 | 1.00E+02 | 1.00E+02 | 1.00E+02 | 1.00E+02 | 1.00E+02 | 1.00E+02 |
| Soil-to-plant transfer factor (d/kg) | 5.00E-05 | 5.00E-05 | 5.00E-05 | 5.00E-05 | 5.00E-05 | 5.00E-05 | 5.00E-05 | 5.00E-05 | 5.00E-05 |
| Feed-to-animal meat transfer factor (d/kg) | 5.00E-07 | 5.00E-07 | 5.00E-07 | 5.00E-07 | 5.00E-07 | 5.00E-07 | 5.00E-07 | 5.00E-07 | 5.00E-07 |
| Feed-to-cow milk transfer factor (d/L) | 1.00E-07 | 1.00E-07 | 1.00E-07 | 1.00E-07 | 1.00E-07 | 1.00E-07 | 1.00E-07 | 1.00E-07 | 1.00E-07 |
| Grout diffusion coefficient ($cm^2$/sec) | 0.0 | 0.0 | 0.0 | 0.0 | 5.00E-13 | 5.00E-13 | 5.00E-13 | 5.00E-13 | 0.0 |
| Water purification factor | 0.0 | 0.0 | 0.0 | 0.0 | 7.00E-01 | 7.00E-01 | 7.00E-01 | 7.00E-01 | 0.0 |
| Deposition velocity (m/sec) | 1.00E-03 | 1.00E-03 | 1.00E-03 | 1.00E-03 | 1.00E-03 | 1.00E-03 | 1.00E-03 | 1.00E-03 | 1.00E-03 |
| Atmospheric deposition class | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| **Toxicities and Slope Factors** | | | | | | | | | |
| Inhalation slope factor (risk/pCi) | 0.0 | 0.0 | 1.34E-08 | 0.0 | 2.74E-08 | 2.78E-08 | 2.78E-08 | 2.81E-10 | 2.64E-08 |
| Ingestion slope factor (risk/pCi) | 0.0 | 0.0 | 7.68E-11 | 0.0 | 2.95E-10 | 3.16E-10 | 3.15E-10 | 5.20E-12 | 3.00E-10 |
| External exposure (risk/yr per pCi/g) | 1.76E-07 | 2.56E-07 | 2.32E-11 | 1.23E-07 | 1.15E-10 | 1.26E-11 | 1.87E-11 | 7.85E-12 | 1.55E-11 |
| Gastro-intestinal absorption factor | 0.0 | 0.0 | 0.0 | 0.0 | 1.00E-03 | 1.00E-03 | 1.00E-03 | 1.00E-03 | 0.0 |
| Skin absorption fraction from soil | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

## Table 10
## MEPAS Plutonium Decay Products

| Isotope | Decay Product 1 | Decay Product 2 | Decay Product 3 | Decay Product 4 | Decay Product 5 |
|---|---|---|---|---|---|
| $^{238}Pu$ | $^{234}U$ | $^{230}Th$ | $^{226}Ra$ | $^{222}Rn$ | $^{210}Pb$ |
| $^{239}Pu$ | $^{235}U$ | $^{231}Pa$ | $^{227}Ac$ | $^{227}Th$ | $^{223}Ra$ |
| $^{240}Pu$ | $^{236}U$ | $^{232}Th$ | | | |
| $^{241}Pu$ | $^{241}Am$ | $^{237}Np$ | $^{233}Pa$ | $^{233}U$ | $^{229}Th$ |
| $^{242}Pu$ | $^{238}U$ | $^{234}Th$ | $^{234}U$ | $^{230}Th$ | $^{226}Ra$ |

## Table 11
## Existing MEPAS Database Information on Tritium

| Property | Value |
|---|---|
| **Physical Data** | |
| Molecular weight (g/mole) | 20 |
| Vapor pressure (mm Hg) | 2.38E+01 |
| Henry's Law constant (atm $m^3$/mole) | 6.00E-07 |
| Half-life (days) | 4.49E+03 |
| **Dose Factors** | |
| Ingestion dose factor (rem/pCi) | 6.30E-11 |
| Inhalation dose factor (rem/pCi) | 6.30E-11 |
| Dermal dose factor (rem/pCi) | 6.30E-11 |
| Air immersion factor (rem/hr per pCi/$m^3$) | 0.0 |
| Ground exposure factor (rem/hr per pCi/$m^2$) | 0.0 |
| Water immersion factor (rem/hr per pCi/L) | 0.0 |
| **Environmental Transfer Functions** | |
| Bioaccumulation in fish (L/kg) | 1.00E+00 |
| Bioaccumulation in shellfish (L/kg) | 1.00E+00 |
| Soil-to-plant transfer factor (d/kg) | 0.0 |
| Feed-to-animal meat transfer factor (d/kg) | 0.0 |
| Feed-to-cow milk transfer factor (d/L) | 0.0 |
| Grout diffusion coefficient ($cm^2$/sec) | 5.00E-08 |
| Water purificiation factor | 1.00E+00 |
| Deposition velocity (m/sec) | 0.0 |
| Atmospheric deposition class | 4 |
| **Toxicities and Slope Factors** | |
| Inhalation slope factor (risk/pCi) | 9.59E-14 |
| Ingestion slope factor (risk/pCi) | 7.15E-14 |
| External exposure (risk/yr per pCi/g) | 0.0 |
| Gastro-intestinal absorption factor | 1.00E+00 |
| Skin absorption fraction from soil | 0.0 |

c. *Fate of uranium.* Uranium is a heavy, silvery-white metal that has 16 isotopes, all of which are radioactive. Naturally occurring uranium nominally contains 99.28305 percent by weight $^{238}U$, 0.7110 percent $^{235}U$, and 0.0054 percent $^{234}U$ (Hammond 1995). Uranium-238 is of particular importance because it can be readily converted through a series of decay reactions into plutonium. Acids dissolve the metal, but it is unaffected by alkalis.

A review of the MEPAS database for data on uranium is shown in Table 12. The radioactive decay products of uranium from the MEPAS decay database are shown in Table 13. A literature search found no additional data to warrant any changes to these databases for uranium.

d. *Fate of neptunium.* Neptunium is an actinide series metal with silvery appearance and 15 isotopes. The radio-isotope $^{237}Np$ is obtained as a by-product from nuclear reactors in the production of plutonium.

The MEPAS database contains information on 3 of the 15 isotopes of neptunium which is presented in Table 14. The decay products from the MEPAS database for $^{237}Np$ are shown in Table 15. A review of literature on neptunium found no justification for changes to the MEPAS database for this element.

## Table 12
## Existing MEPAS Database Information on Uranium

| Property | Isotope | | | | | | |
|---|---|---|---|---|---|---|---|
| | $^{232}U$ | $^{233}U$ | $^{234}U$ | $^{235}U$ | $^{236}U$ | $^{238}U$ | $^{239}U$ |
| **Physical Data** | | | | | | | |
| Molecular weight (g/mole) | 232 | 233 | 234 | 235 | 236 | 238 | 239 |
| Half-life (days) | 2.63E+04 | 5.79E+07 | 8.93E+07 | 2.57E+11 | 8.55E+09 | 1.63E+12 | 1.63E-02 |
| **Dose Factors** | | | | | | | |
| Ingestion dose factor (rem/pCi) | 1.31E-06 | 2.89E-07 | 2.83E-07 | 2.66E-07 | 2.69E-07 | 2.55E-07 | 7.73E-11 |
| Inhalation dose factor (rem/pCi) | 6.59E-04 | 1.35E-04 | 1.32E-04 | 1.23E-04 | 1.25E-04 | 1.18E-04 | 3.74E-11 |
| Dermal dose factor (rem/pCi) | 3.00E-05 | 6.20E-06 | 6.10E-06 | 5.60E-06 | 5.80E-06 | 5.50E-06 | 0.0 |
| Air immersion factor (rem/hr per pCi/$m^3$) | 1.88E-13 | 2.17E-13 | 1.02E-13 | 9.59E-11 | 6.66E-14 | 4.53E-14 | 2.90E-11 |
| Ground exposure factor (rem/hr per pCi/$m^2$) | 1.35E-14 | 9.53E-15 | 9.96E-15 | 1.97E-12 | 8.65E-15 | 7.34E-15 | 6.84E-13 |
| Water immersion factor (rem/hr per pCi/L) | 4.29E-13 | 4.84E-13 | 2.33E-13 | 2.11E-10 | 1.54E-13 | 1.06E-13 | 6.49E-11 |
| **Environmental Transfer Factors** | | | | | | | |
| Bioaccumulation in fish (L/kg) | 5.00E+01 | 5.00E+01 | 5.00E+01 | 5.00E+01 | 5.00E+01 | 5.00E+01 | 5.00E+01 |
| Bioaccumulation in shellfish (L/kg) | 6.00E+01 | 6.00E+01 | 6.00E+01 | 6.00E+01 | 6.00E+01 | 6.00E+01 | 6.00E+01 |
| Soil-to-plant transfer factor (d/kg) | 3.50E-03 | 3.50E-03 | 3.50E-03 | 3.50E-03 | 3.50E-03 | 3.50E-03 | 3.50E-03 |
| Feed-to-animal meat transfer factor (d/kg) | 2.00E-04 | 2.00E-04 | 2.00E-04 | 2.00E-04 | 2.00E-04 | 2.00E-04 | 2.00E-04 |
| Feed-to-cow milk transfer factor (d/L) | 6.00E-04 | 6.00E-04 | 6.00E-04 | 6.00E-04 | 6.00E-04 | 6.00E-04 | 6.00E-04 |
| Grout diffusion coefficient ($cm^2$/sec) | 0.0 | 1.00E-11 | 1.00E-11 | 1.00E-11 | 1.00E-11 | 1.00E-11 | 1.00E-11 |
| Water purification factor | 0.0 | 7.00E-11 | 7.00E-01 | 7.00E-01 | 7.00E-11 | 7.00E-11 | 7.00E-11 |
| Deposition velocity (m/sec) | 1.00E-03 | 1.00E-03 | 1.00E-03 | 1.00E-03 | 1.00E-03 | 1.00E-03 | 1.00E-03 |
| Atmospheric deposition class | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| **Toxicities and Slope Factors** | | | | | | | |
| Inhalation slope factor (risk/pCi) | 5.29E-08 | 1.41E-08 | 1.40E-08 | 1.30E-08 | 1.32E-08 | 1.24E-08 | 0.0 |
| Ingestion slope factor (risk/pCi) | 8.12E-11 | 4.48E-11 | 4.44E-11 | 4.52E-11 | 4.21E-11 | 4.27E-11 | 0.0 |
| External exposure (risk/yr per pCi/g) | 3.42E-11 | 1.06E-09 | 2.14E-11 | 2.63E-07 | 1.72E-11 | 1.50E-11 | 1.32E-07 |
| Gastro-intestinal absorption factor | 0.0 | 5.00E-02 | 5.00E-02 | 5.00E-02 | 5.00E-02 | 5.00E-02 | 5.00E-02 |
| Skin absorption fraction from soil | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

## Table 13
## MEPAS Uranium Decay Products

| Isotope | Decay Product 1 | Decay Product 2 | Decay Product 3 | Decay Product 4 | Decay Product 5 |
|---|---|---|---|---|---|
| $^{233}U$ | $^{229}Th$ | $^{225}Ra$ | $^{225}Ac$ | | |
| $^{234}U$ | $^{230}Th$ | $^{226}Ra$ | $^{222}Rn$ | $^{210}Pb$ | $^{210}Po$ |
| $^{235}U$ | $^{231}Pa$ | $^{227}Ac$ | $^{227}Th$ | $^{223}Ra$ | |
| $^{236}U$ | $^{232}Th$ | | | | |
| $^{237}U$ | $^{234}Th$ | $^{234}U$ | $^{230}Th$ | $^{226}Ra$ | $^{222}Rn$ |

**Table 14**
**Existing MEPAS Database Information on Neptunium**

| Property | Isotope | | |
|---|---|---|---|
| | $^{237}$Np | $^{238}$Np | $^{239}$Np |
| **Physical Data** | | | |
| Molecular weight (g/mole) | 237 | 238 | 239 |
| Half-life (days) | 7.82E+08 | 2.12E+00 | 2.36E+00 |
| **Dose Factors** | | | |
| Ingestion dose factor (rem/pCi) | 4.44E-06 | 4.00E-09 | 3.26E-09 |
| Inhalation dose factor (rem/pCi) | 5.40E-04 | 3.70E-08 | 2.51E-09 |
| Dermal dose factor (rem/pCi) | 4.50E-03 | 0.0 | 4.30E-09 |
| Air immersion factor (rem/hr per pCi/m$^3$) | 1.37E-11 | 3.62E-10 | 1.02E-10 |
| Ground exposure factor (rem/hr per pCi/m$^2$) | 3.82E-13 | 7.05E-12 | 2.17E-12 |
| Water immersion factor (rem/hr per pCi/L) | 3.08E-11 | 7.83E-10 | 2.27E-10 |
| **Environmental Transfer Factors** | | | |
| Bioaccumulation in fish (L/kg) | 2.50E+02 | 2.50E+02 | 2.50E+02 |
| Bioaccumulation in shellfish (L/kg) | 4.00E+02 | 4.00E+02 | 4.00E+02 |
| Soil-to-plant transfer factor (d/kg) | 2.35E-03 | 2.35E-03 | 2.35E-03 |
| Feed-to-animal meat transfer factor (d/kg) | 5.50E-05 | 2.00E-04 | 2.00E-04 |
| Feed-to-cow milk transfer factor (d/L) | 5.00E-06 | 6.00E-04 | 6.00E-04 |
| Grout diffusion coefficient (cm$^2$/sec) | 5.00E-13 | 5.00E-13 | 5.00E-13 |
| Water purification factor | 7.00E-01 | 7.00E-01 | 7.00E-01 |
| Deposition velocity (m/sec) | 1.00E-03 | 1.00E-03 | 1.00E-03 |
| Atmospheric deposition class | 1 | 3 | 3 |
| **Toxicities and Slope Factors** | | | |
| Inhalation slope factor (risk/pCi) | 3.45E-08 | 4.68E-12 | 2.41E-12 |
| Ingestion slope factor (risk/pCi) | 2.95E-10 | 4.56E-12 | 4.27E-12 |
| External exposure (risk/yr per pCi/g) | 7.56E-07 | 1.95E-06 | 2.42E-07 |
| Gastro-intestinal absorption factor | 1.00E-03 | 1.00E-03 | 1.00E-03 |
| Skin absorption fraction from soil | 0.0 | 0.0 | 0.0 |

**Table 15**
**MEPAS Neptunium Decay Products**

| Isotope | Decay Product 1 | Decay Product 2 | Decay Product 3 |
|---|---|---|---|
| $^{237}$Np | $^{233}$Pa | $^{233}$U | $^{229}$Th |

*e. Fate of americium.* Americium is a silvery-white metal of the actinide series. It is a synthetic chemical element, undetected in nature. All isotopes of americium are unstable, with the most important isotope being $^{241}$Am which is readily available in large quantities from the production of plutonium. Americium reacts with oxygen and with hydrogen forming americium dioxide ($AmO_2$) and americium hydride ($AmH_2$), respectively.

The MEPAS database contains data on eight of the isotopes of americium which are presented in Table 16. The decay products from the MEPAS database for three of the radio-isotopes of americium are shown in Table 17. A review of literature on americium found no justification for changes to the MEPAS database for this element.

*f. Fate of thorium.* Thorium is silvery-white metal of the actinide series with 25 known isotopes, all of which are unstable. Thorium is slowly attacked by water and does not dissolve readily in most common acids.

The MEPAS database contains data on 7 of the 25 isotopes of thorium, presented in Table 18. The decay products from the MEPAS database for six of the radio-isotopes of thorium are shown in Table 19. A review of literature on thorium found no justification for changes to the MEPAS database for this element.

## Table 16
## Existing MEPAS Database Information on Americium

| Property | Isotope | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | $^{237}$Am | $^{238}$Am | $^{239}$Am | $^{240}$Am | $^{241}$Am | $^{242}$Am | $^{242M}$Am | $^{243}$Am |
| **Physical Data** | | | | | | | | |
| Molecular weight (g/mole) | 237 | 238 | 239 | 240 | 241 | 242 | 242 | 243 |
| Half-life (days) | 5.07E-02 | 6.81E-02 | 4.96E-01 | 2.12E+00 | 1.58E+05 | 6.70E-01 | 5.55E+04 | 2.70E+06 |
| **Dose Factors** | | | | | | | | |
| Ingestion dose factor (rem/pCi) | 6.59E-11 | 1.32E-10 | 9.88E-10 | 2.53E-09 | 3.64E-06 | 1.41E-09 | 2.12E-06 | 3.62E-06 |
| Inhalation dose factor (rem/pCi) | 2.39E-11 | 8.58E-10 | 4.59E-10 | 1.84E-09 | 4.44E-04 | 5.85E-08 | 5.14E-04 | 4.40E-04 |
| Dermal dose factor (rem/pCi) | 1.00E-08 | 4.00E-08 | 1.00E-07 | 8.00E-07 | 3.70E-03 | 3.30E-07 | 3.50E-03 | 3.70E-03 |
| Air immersion factor (rem/hr per pCi/m$^3$) | 2.27E-10 | 5.77E-10 | 1.38E-10 | 6.66E-10 | 1.09E-11 | 8.19E-12 | 2.83E-13 | 2.90E-11 |
| Ground exposure factor (rem/hr per pCi/m$^2$) | 4.72E-12 | 1.13E-11 | 2.46E-12 | 1.31E-11 | 3.65E-13 | 2.08E-13 | 3.39E-14 | 7.12E-13 |
| Water immersion factor (rem/hr per pCi/L) | 4.98E-10 | 1.25E-09 | 3.07E-10 | 1.44E-09 | 2.50E-11 | 1.83E-11 | 6.96E-13 | 6.58E-11 |
| **Environmental Transfer Factors** | | | | | | | | |
| Bioaccumulation in fish (L/kg) | 2.50E+02 | 2.50E+02 | 2.50E+02 | 2.50E+02 | 2.50E+02 | 2.50E+02 | 2.50E+02 | 2.50E+02 |
| Bioaccumulation in shellfish (L/kg) | 1.00E+03 | 1.00E+03 | 1.00E+03 | 1.00E+03 | 1.00E+03 | 1.00E+03 | 1.00E+03 | 1.00E+03 |
| Soil-to-plant transfer factor (d/kg) | 1.03E-04 | 1.03E-04 | 1.03E-04 | 1.03E-04 | 1.03E-04 | 1.03E-04 | 1.03E-04 | 1.03E-04 |
| Feed-to-animal meat transfer factor (d/kg) | 3.50E-06 | 3.50E-06 | 3.50E-06 | 3.50E-06 | 3.50E-06 | 3.50E-06 | 3.50E-06 | 3.50E-06 |
| Feed-to-cow milk transfer factor (d/L) | 4.00E-07 | 4.00E-07 | 4.00E-07 | 4.00E-07 | 4.00E-07 | 4.00E-07 | 4.00E-07 | 4.00E-07 |
| Grout diffusion coefficient (cm$^2$/sec) | 0.0 | 0.0 | 0.0 | 0.0 | 5.00E-13 | 5.00E-13 | 5.00E-13 | 5.00E-13 |
| Water purification factor | 0.0 | 0.0 | 0.0 | 0.0 | 7.00E-01 | 7.00E-01 | 7.00E-01 | 7.00E-01 |
| Deposition velocity (m/sec) | 1.00E-03 | 1.00E-03 | 1.00E-03 | 1.00E-03 | 1.00E-03 | 1.00E-03 | 1.00E-03 | 1.00E-03 |
| Atmospheric deposition class | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| **Toxicities and Slope Factors** | | | | | | | | |
| Inhalation slope factor (risk/pCi) | 0.0 | 0.0 | 0.0 | 0.0 | 3.85E-08 | 1.04E-11 | 3.49E-08 | 3.82E-08 |
| Ingestion slope factor (risk/pCi) | 0.0 | 0.0 | 0.0 | 0.0 | 3.28E-10 | 1.47E-12 | 2.92E-10 | 3.27E-10 |
| External exposure (risk/yr per pCi/g) | 1.41E-06 | 4.05E-06 | 7.38E-07 | 4.72E-06 | 4.59E-09 | 5.76E-09 | 9.45E-09 | 2.43E-08 |
| Gastro-intestinal absorption factor | 0.0 | 0.0 | 0.0 | 0.0 | 1.00E-03 | 1.00E-03 | 1.00E-03 | 1.00E-03 |
| Skin absorption fraction from soil | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

## Table 17
## MEPAS Americium Decay Products

| Isotope | Decay Product 1 | Decay Product 2 | Decay Product 3 | Decay Product 4 | Decay Product 5 |
|---|---|---|---|---|---|
| $^{241}$Am | $^{237}$Np | $^{233}$Pa | $^{233}$U | $^{229}$Th | $^{225}$Ra |
| $^{242M}$Am | $^{242}$Am | $^{242}$Cm | $^{238}$Pu | $^{234}$U | $^{230}$Th |
| $^{243}$Am | $^{239}$Pu | $^{235}$U | $^{231}$Pa | $^{227}$Ac | $^{227}$Th |

## Table 18
## Existing MEPAS Database Information on Thorium

| Property | Isotope | | | | | | |
|---|---|---|---|---|---|---|---|
| | $^{227}$Th | $^{228}$Th | $^{229}$Th | $^{230}$Th | $^{231}$Th | $^{232}$Th | $^{234}$Th |
| **Physical Data** | | | | | | | |
| Molecular weight (g/mole) | 227 | 228 | 229 | 230 | 231 | 232 | 234 |
| Half-life (days) | 1.87E+01 | 6.99E+02 | 2.68E+06 | 2.81E+07 | 1.06E+00 | 1.41E-10 | 2.41E+01 |
| **Dose Factors** | | | | | | | |
| Ingestion dose factor (rem/pCi) | 3.81E-08 | 3.96E-07 | 3.53E-06 | 5.48E-07 | 1.35E-09 | 2.73E-06 | 1.37E-08 |
| Inhalation dose factor (rem/pCi) | 1.62E-05 | 3.42E-04 | 2.15E-03 | 3.26E-04 | 8.77E-10 | 1.64E-03 | 3.50E-08 |
| Dermal dose factor (rem/pCi) | 5.70E-05 | 1.80E-03 | 1.70E-02 | 2.50E-03 | 6.80E-10 | 1.40E-02 | 3.90E-08 |
| Air immersion factor (rem/hr per pCi/m$^3$) | 6.51E-11 | 1.23E-12 | 5.09E-11 | 2.33E-13 | 6.94E-12 | 1.16E-13 | 1.65E-11 |
| Ground exposure factor (rem/hr per pCi/m$^2$) | 1.38E-12 | 3.13E-14 | 1.14E-12 | 9.99E-15 | 2.47E-13 | 7.34E-15 | 3.64E-13 |
| Water immersion factor (rem/hr per pCi/L) | 1.43E-10 | 2.73E-12 | 1.14E-10 | 5.24E-13 | 1.57E-11 | 2.64E-13 | 3.58E-11 |
| **Environmental Transfer Factors** | | | | | | | |
| Bioaccumulation in fish (L/kg) | 1.00E+02 | 1.00E+02 | 1.00E+02 | 1.00E+02 | 1.00E+02 | 1.00E+02 | 1.00E+02 |
| Bioaccumulation in shellfish (L/kg) | 5.00E+02 | 5.00E+02 | 5.00E+02 | 5.00E+02 | 5.00E+02 | 5.00E+02 | 5.00E+02 |
| Soil-to-plant transfer factor (d/kg) | 3.00E-05 | 3.00E-05 | 3.00E-05 | 3.00E-05 | 3.00E-05 | 3.00E-05 | 3.00E-05 |
| Feed-to-animal meat transfer factor (d/kg) | 6.00E-06 | 6.00E-06 | 6.00E-06 | 6.00E-06 | 6.00E-06 | 6.00E-06 | 6.00E-06 |
| Feed-to-cow milk transfer factor (d/L) | 5.00E-06 | 5.00E-06 | 5.00E-06 | 5.00E-06 | 5.00E-06 | 5.00E-06 | 5.00E-06 |
| Grout diffusion coefficient (cm$_2$/sec) | 1.00E-12 | 1.00E-12 | 1.00E-12 | 1.00E-12 | 0.0 | 1.00E-12 | 1.00E-12 |
| Water purification factor | 7.00E-01 | 7.00E-01 | 7.00E-01 | 7.00E-01 | 0.0 | 7.00E-01 | 7.00E-01 |
| Deposition velocity (m/sec) | 1.00E-03 | 1.00E-03 | 1.00E-03 | 1.00E-03 | 1.00E-03 | 1.00E-03 | 1.00E-03 |
| Atmospheric deposition class | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| **Toxicities and Slope Factors** | | | | | | | |
| Inhalation slope factor (risk/pCi) | 4.31E-09 | 9.45E-08 | 7.60E-08 | 1.72E-08 | 1.10E-12 | 1.93E-08 | 1.90E-11 |
| Ingestion slope factor (risk/pCi) | 4.04E-11 | 6.29E-11 | 5.65E-11 | 3.75E-11 | 1.79E-12 | 3.28E-11 | 1.93E-11 |
| External exposure (risk/yr per pCi/g) | 1.74E-07 | 5.28E-06 | 5.94E-08 | 4.40E-11 | 2.09E-09 | 1.97E-11 | 5.71E-08 |
| Gastro-intestinal absorption factor | 2.00E-04 | 2.00E-04 | 2.00E-04 | 2.00E-04 | 0.0 | 2.00E-04 | 2.00E-04 |
| Skin absorption fraction from soil | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

## Table 19
## MEPAS Thorium Decay Products

| Isotope | Decay Product 1 | Decay Product 2 | Decay Product 3 | Decay Product 4 | Decay Product 5 |
|---|---|---|---|---|---|
| $^{227}$Th | $^{223}$Ra | | | | |
| $^{228}$Th | $^{224}$Ra | | | | |
| $^{229}$Th | $^{225}$Ra | $^{225}$Ac | | | |
| $^{230}$Th | $^{226}$Ra | $^{222}$Rn | $^{210}$Pb | $^{210}$Po | |
| $^{232}$Th | $^{228}$Ra | $^{228}$Th | $^{224}$Ra | | |
| $^{234}$Th | $^{234}$U | $^{230}$Th | $^{226}$Ra | $^{222}$Rn | $^{210}$Pb |

# 4 Summary and Recommendations

A review of existing exposure assessment models was performed, and a multimedia exposure assessment model for evaluating ecological risk of exposure to military-related compounds at military sites has been developed. The MEPAS model developed by Pacific Northwest Laboratory for the U.S. DOE was selected, with changes made to its environmental database. The model is applicable to TNT, HMX, RDX, and several radioactive contaminants such as plutonium and americium. The model is primarily intended as a screening-level tool to aid in identifying an ecological risk from an MRC. The model can be applied to inactive as well as active air and water release sites.

The model itself uses a simplified contaminant-transport and exposure algorithm encapsulated into a user-friendly shell. The model is an integrated system of analytical, semi-analytical, and empirically based mathematical models that simulate the release of contaminants from sources, migration and fate of these contaminants through various environmental media, concentrations at designated receptor locations, and health effects to specified sensitive receptors caused by exposure to these contaminants.

The model focuses on addressing long-term average environmental conditions resulting from release to the environment from point and area sources. Inherent in the design of the model is the lack of the capability to address acute exposures to environmental contamination.

Recommendations for model improvement include future studies to address toxicities (such as reference doses), slope factors (such as ingestion slope factor), and environmental transfer factors (such as bioaccumulation). These areas need to be addressed to determine values that are more specific to ecological units. Most of the parameters from these areas were not modified for this study and could potentially be of significant importance in determining the risk of exposure to an ecological unit from MRCs. Additionally, future applications of the model to specific ecological units are needed to gather a more complete understanding of the model's strengths and limitations.

# References


Access EPA. (1993). USEPA 220-b-93-008, U.S. Government Printing Office, Washington, DC.

Ainsworth, C. C., Harvey, S. D., Szecsody, J. E., Simmons, M. A., Cullinan, V. I., Resch, C. T., and Mong, G. H. (1993). "Relationship between the leachability characteristics of unique energetic compounds and soil properties," Final Report, Project Order No. 91PP1800, U.S. Army Biomedical Research and Development Laboratory, Fort Detrick, Frederick, MD.

ATSDR. (1990). "Plutonium ATSDR public health statement, December 1990." Agency for Toxic Substances and Disease Registry, Atlanta, GA.

Brannon, J. M., and Myers, T. E. (1997). "Review of fate and transport processes of explosives," Technical Report IRRP-97-2, U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.

Brannon, J. M., Myers, T. E., Pennington, J. C., and Hayes, C. A. "Fate of TNT and its major transformation products in a surface and aquifer soil" (in preparation), U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.

Buck, J. W., Castleton, K. J., Whelan, G., McDonald, J. P., Droppo, J. G., Sato, C., Strenge, D. L., and Streile, G. P. (1995). *Multimedia environmental pollutant assessment system (MEPAS) application guidance*, Pacific Northwest Laboratory, Richland, WA.

Burns, L. A. (1992). *Pesticide and industrial chemical risk analysis and hazard assessment*, Environmental Research Laboratory, U.S. Environmental Protection Agency, Athens, GA.

Freeze, R. A., and Cherry, J. A. (1979). *Groundwater*. Prentice-Hall, Englewood Cliffs, NJ.

Hammond, C. R. (1995). *CRC handbook of chemistry and physics*, CRC Press, Cleveland, OH.

Health and Welfare Canada. (1992). *Review and assessment of two multimedia exposure models: MEPAS and MULTIMED*, Intera Information Technologies Corp., Environmental Sciences Division, Nepean, Ontario, Canada.

Kaplan, D. L., and Kaplan, A. M. (1982). "Thermophilic biotransformations of 2,4,6-trinitrotoluene under simulated composting conditions," *Applied and Environmental Microbiology* 44(3), 757-60.

Karickhoff, S. W. (1979). "Sorption of hydrophobic pollutants on natural sediments," *Water Research* 13, 241-48.

_____. (1984). "Organic pollutant sorption in aquatic systems," *Journal of Hydraulic Engineering* 110(6), 707-35.

McCormick, N. G., Cornell, J. H., and Kaplan, A. M. (1981). "Biodegradation of hexahydro-1,3,5-trinitro-1,3,5-riazine," *Applied and Environmental Microbiology* 42(5), 817-23.

McCormick, N. G., Feeherry, F. E., and Levinson, H. S. (1976). "Microbial transformation of 2,4,6-trinitrotoluene and other nitroaromatic compounds," *Applied and Environmental Microbiology* 31, 949-58.

McGrath, C. J. (1995). "Review of formulations for processes affecting the subsurface transport of explosives," Technical Report IRRP-95-2, U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.

Myers, T. E., Brannon, J. M., Pennington, J. C., Townsend, D. M., Davis, W. M., Ochman, M. K., Hayes, C. A., and Myers, K. F. "Laboratory studies of soil sorption/transformation kinetics for explosives" (in preparation), U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.

Olin, T. J., Myers, T. E., Townsend, D. M. (1996). "2,4,6-trinitrotoluene (TNT) transformation/sorption in thin-disk soil columns under anaerobic conditions," Technical Report IRRP-96-6, U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.

Rebhun, M., Kalabo, R., Grossman, L., Manka, J., and Rav-Acha, C. (1992). "Sorption of organics on clay and synthetic and synthetic humic-clay complexes simulating aquifer processes," *Water Resources* 26 (1), 79-84.

Ruiz, C. E. "Application of sorption walls for site remediation" (in preparation), U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.

Salhotra, A. M., Mineart, P., Sharp-Hansen, S., Allison, T., Johns, R., and Mills, W. (1993). "MULTIMED, the multimedia exposure assessment model for evaluating the land disposal of wastes — model theory,"

NTIS Report PB93-186 252/AS, National Technical Information Service, Springfield, VA.

Sandia National Laboratories. (1994). *Précis user's manual*, Sandia National Laboratories, Albuquerque, NM.

Townsend, D. M., and Myers, T. E. (1996). "Recent developments in formulating model descriptors for subsurface transformation and sorption of TNT, RDX, and HMX," Technical Report IRRP-96-1, U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.

Warren, B. R., and Strenge, D. L. (1994). *Multimedia-modeling environmental database editor (MMEDE) user manual*, Pacific Northwest Laboratory, Richland, WA.

Whelan, G., Strenge, D. L., Droppo, J. G., Jr., Steelman, B. L., and Buck, J. W. (1987). *The remedial action priority system (RAPS): mathematical formulations*, DOE/RL/87-09, PNL-6200, Pacific Northwest Laboratory, Richland, WA.

U.S. Department of Energy. (1994). *Primer on tritium safe handling practices*, DOE Handbook 1079-94, U.S. Department of Energy, Washington, DC.

U.S. Environmental Protection Agency (1995). *Benchmarking analysis of three multimedia models: RESRAD, MMSOILS, and MEPAS*, Argonne National Laboratory, Pacific Northwest National Laboratory, Tetra Tech, Inc., U.S. Environmental Protection Agency, and University of Tennessee.

# Bibliography

Burns, L. A., “Exposure analysis modeling system user’s guide for EXAMS II version 2.94," U.S. Environmental Protection Agency, Athens, GA.

Montgomery, J. H., and Welkom, L. M. (1991). *Groundwater chemicals desk reference*, Lewis Publishers, Chelsea, MI.

Montgomery, J. H. (1991). *Groundwater chemicals desk reference volume 2*, Lewis Publishers, Chelsea, MI, 832-34.

Price, C. B., and Brannon, J. M. (1995). “Transformation of 2,4,6-trinitrotoluene under controlled Eh/Ph conditions,” Technical Report IRRP-95-5, U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.

Townsend, D. M., Myers, T. E., and Adrian, D. D. (1995). “2,4,6-trinitrotoluene (TNT) transformation/sorption in thin-disk soil columns,” Technical Report IRRP-95-4, U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.

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This report describes several multimedia exposure assessment models and discusses their applicability for use in evaluating ecological risk of exposure to military-related compounds (MRCs). The risk of exposure to MRCs by ecological units is of vital importance because of the unique characteristics of certain military specific compounds. This assessment of risk is valuable for permitting and planning activities as well as for possible cleanup operations of contaminated sites should the risk to an ecological unit become too great. The requirement that the model be a screening-level model was made to allow for the use of simplified, quantitative, predictive methods that minimize time and effort for implementation in order to quickly obtain the necessary information needed to make a judgment of risk to an ecological unit. The MRCs of primary concern addressed in this report are 2,4,6-trinitrotoluene (TNT), hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX), and octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX). Briefly discussed is the risk of exposure to radioactive compounds.

This report presents a discussion of the selection of an existing screening-level model and the modifications made to allow for the evaluation of ecological risk of exposure to the primary MRCs of concern at military sites (i.e., TNT, RDX, and HMX).

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