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Development Center

# **Validation Applications of the Training Range Environmental Evaluation and Characterization System (TREECS™)**

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## Final report

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**Abstract:** The Training Range Environmental Evaluation and Characterization System (TREECS™) is being developed for the Army with varying levels of capability to forecast the fate of and risk from munitions constituents (MC), such as high explosives (HE), within and transported from firing/training ranges to surface water and groundwater. The overall objective is to provide environmental specialists with tools to assess the potential for migration of MC into surface water and groundwater systems and to assess range management strategies to protect human and environmental health.

TREECS™ includes two tiers of analysis. Tier 1 consists of screening-level methods that assume highly conservative, steady-state MC loading and fate. Tier 1 requires minimal data input requirements and can be easily and quickly applied to assess the potential for migration into surface water and groundwater. Tier 2 provides time-varying analyses, since it does not make the highly conservative assumptions of steady-state (time-invariant) conditions with no MC loss or degradation as used for Tier 1. The Tier 2 soil model solves mass balance equations for both solid and non-solid phase MC with dissolution. Additionally, MC residue loadings to the range soil can vary from year to year based on munitions use. Thus, media concentrations computed with Tier 2 should be closer to reality.

As with any model, validation applications are needed to gain confidence in using the model. Validation applications involve comparing model-predicted results against data measured from the modeled site so that the model can be evaluated in terms of representing real-world conditions. Tier 2 of TREECS™ was applied to four sites at four different Army installations for validation purposes. This report describes the results of those applications with comparisons of computed and observed MC concentrations in surface water and groundwater.

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## Preface

The Training Range Environmental Evaluation and Characterization System (TREECS™) was funded by the U.S. Army's Environmental Quality and Installations (EQI) Research Program. The TREECS™ applications reported herein were conducted by Dr. Mark Dortch of MSD Engineering Consulting under a sub-contract to Los Alamos Technical Associates (LATA); LATA was under contract to the U.S. Army Engineer Research and Development Center (ERDC). This report was written by Dr. Dortch. Peer review of this report was conducted by Dr. Billy Johnson and Jeffrey Gerald of the Water Quality and Contaminant Modeling Branch (WQCMB), Environmental Processes and Effects Division (EPED), Environmental Laboratory (EL), ERDC.

Dr. Johnson was the overall leader of the TREECS™ project. The study was conducted under the general direction of Dr. Beth Fleming, Director, EL; Dr. Warren Lorrentz, Chief, EPED; and Dr. Patrick Deliman, acting Chief WQCMB and Technical Directory of Environmental Modeling for ERDC. John Ballard was Program Manager of the EQI Program. Dr. Elizabeth Ferguson was Director of the EQI Program.

Dr. Jeffery P. Holland was Director of ERDC. COL Kevin J. Wilson was Commander. This report is approved for limited distribution only.

## Unit Conversion Factors

| Multiply             | By            | To Obtain       |
|----------------------|---------------|-----------------|
| acres                | 4,046.873     | square meters   |
| cubic feet           | 0.02831685    | cubic meters    |
| degrees Fahrenheit   | $(F-32)/1.8$  | degrees Celsius |
| feet                 | 0.3048        | meters          |
| miles (U.S. statute) | 1,609.347     | meters          |
| pounds (mass)        | 0.45359237    | kilograms       |
| English tons         | 907.2         | kilograms       |
| slugs                | 14.59390      | kilograms       |
| square feet          | 0.09290304    | square meters   |
| square miles         | 2.589998 E+06 | square meters   |

## List of Acronyms, Symbols, and Abbreviations

|                   |   |
|-------------------|---|
| AOI               | area of interest  |
| Cu                | copper  |
| DoD               | Department of Defense   |
| DODIC             | Department of Defense Identification Code                                   |
| EL                | Environmental Laboratory  |
| EPED              | Environmental Processes and Effects Division                                |
| ERDC              | Engineer Research and Development Center                                    |
| FRAMES            | Framework for Risk Analysis in Multimedia Environmental Systems             |
| $f_{oc}$          | fraction of organic carbon of sediment solids                               |
| HGCT              | Hydro-Geo-Characteristics Toolkit   |
| HE                | high explosives   |
| KClO <sub>4</sub> | potassium perchlorate   |
| $K_d$             | sediment – water MC partitioning distribution coefficient, L/kg             |
| MC                | munitions constituents  |
| MEPAS             | Multimedia Environmental Pollutant Assessment System                        |
| MIDAS             | Munition Items Disposition Action System                                    |
| MOA               | memorandum of agreement   |
| MW                | molecular weight  |
| NRCS              | Natural Resources Conservation Service                                      |
| ORAP              | Operational Range Assessment Program  |
| Pb                | lead  |
| Plus-SG           | Plus operator for surface water and groundwater                             |
| POC               | Proof-of-concept (application)  |
| ppb               | parts per billion   |
| ppm               | parts per million   |
| RDX               | Royal Demolition eXplosive, 1,3,5-trinitro-1,3,5-triazine, a high explosive |
| RECOVERY          | Contaminant fate and transport model for surface water and sediments        |
| RTC               | range and training complex  |
| SAFRs             | small arms firing ranges  |
| Sb                | antimony  |
| SCS               | Soil Conservation Service   |
| TNT               | 2,3,6-trinitrotoluene, a high explosive                                     |
| TREECS™           | Training Range Environmental Evaluation and Characterization System         |
| TSS               | total suspended solids concentration  |
| USEPA             | U.S. Environmental Protection Agency  |
| USLE              | Universal Soil Loss Equation  |
| USMA              | U.S. Military Academy   |
| WFF               | water flux file used in FRAMES  |

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|      |                                |
|------|--------------------------------|
| WSS  | Web Soil Survey Web-based tool |
| WWII | World War II                   |
| Zn   | zinc                           |

# 1 Introduction

## Background

The Training Range Environmental Evaluation and Characterization System (TREECS™) is being developed for the Army with varying levels of capability to forecast the fate of munitions constituents (MC), such as high explosives (HE) and metals, within and transported from firing/training ranges to surface water and groundwater. The overall purpose is to provide environmental specialists with tools to assess the potential for MC migration into surface water and groundwater systems and to assess range management strategies to ensure protection of human health and the environment. In addition to the Army, these tools could potentially be used by other services within the Department of Defense (DoD).

TREECS™ is accessible from the World Wide Web (<http://el.erdcl.usace.army.mil/treecs/>) and presently has two tiers for assessments. Tier 1 consists of screening-level methods that require minimal data input requirements and can be easily and quickly applied to assess the potential for MC migration into surface water and/or groundwater at concentrations exceeding protective health benchmarks at receptors' locations. Assumptions, such as steady-state conditions, are made to provide conservative or worst case estimates for potential receptor media concentrations under Tier 1. If a potential concern is indicated by a Tier 1 analysis, then there would be cause to proceed to Tier 2 to obtain a more definitive assessment. The formulations for the Tier 1 modeling approach are presented by Dortch et al. (2009).

Tier 2 assessment methods require more detailed site data and more knowledge and skill to apply, but can be applied by local environmental staff that have a moderate understanding of multi-media fate and transport. The Tier 2 approach allows time-varying analyses of both the solid and non-solid phases of MC with dissolution. A time-varying analysis should provide more accurate predictions with generally lower concentrations due to mediating effects of transport phasing and dampening. The Tier 2 modeling approach is described by Dortch et al. (2011a). Tiers 1 and 2 focus on contaminant stressors and human and ecological health end point metrics.

## Scope

This report describes validation applications of the Tier 2 modeling approach. The details of the Tier 2 modeling approach are not repeated in this report, but they can be found in the report by Dortch et al. (2011a). Model validation is the process of evaluating the ability of a model to reasonably represent real-world conditions of the modeled system. Validation involves comparing model-predicted results to observed (measured) field data. Successful validations, in which the model results compare reasonably well to observations, help build confidence in using a model to make predictions or forecasts for other systems.

Validation applications for four Army installations are reported herein. These include: Fort A.P. Hill, Virginia; Massachusetts Military Reservation (MMR), Massachusetts; U.S. Military Academy, West Point, New York; and Fort Jackson, South Carolina. A chapter is devoted to each installation and the associated validation applications. Within each of these chapters, the installation and application site conditions are briefly described. Estimations for model inputs are next explained, followed by comparison of modeled and observed results. The last chapter contains a summary of conclusions.

## 2 Fort A.P. Hill Application

### Site description

Fort A.P. Hill was used for the TREECS™ Tier 1 and Tier 2 proof-of-concept (POC) applications during model development (Dortch et al. 2010, 2011b). The results of the Tier 2 POC application to Fort Hill are compared herein to recently measured field concentrations of MC. The field measurements were obtained under Phase II of the Army's Operational Range Assessment Program (ORAP). All observed data were collected around the 2010 time frame and were provided to ERDC by the U.S. Army Public Health Command (Provisional), Army Institute of Public Health.

As described by E.A. Engineering, Science, and Technology, Inc. (EA) (2006), Fort A.P. Hill occupies 75,794 acres in the eastern portion of Caroline County, Virginia. Bisected by U.S. Route 301, the installation is located approximately 20 miles southeast of Fredericksburg, Virginia (see Figure 1). Fort A.P. Hill was established as an Army training facility in 1941 for use in troop and artillery training on land purchased by the federal government. Today, Fort A.P. Hill is a training and maneuver center focused on providing realistic joint and combined arms training. The installation is used year-round for military training of both active and reserve troops of the Army, Navy, Marines, and Air Force, as well as other government agencies. Fort A.P. Hill currently conducts training in 128 training areas. There are 98 firing ranges and three impact areas. Other information regarding this installation as well as the ORAP Phase I assessment can be found in the EA report (2006). Other site description and characterization information required for the modeling is discussed in the Tier 1 and Tier 2 POC application reports by Dortch et al. (2010 and 2011b).

The area of interest (AOI) consisted of the main impact area as shown in Figure 2. The modeled MC of interest included RDX, TNT, lead, copper, and potassium perchlorate,  $KClO_4$ . The two explosives are the result of firing live large- and medium-caliber weapons. The two metals result primarily from small arms firing ranges (SAFRs), which are outside the AOI, but a single AOI was used to represent all sources of MC.

White Lake on Beverly Run was selected as the target surface water body, and a hypothetical receptor well located about 4,000 m down-gradient from the AOI was selected for the target groundwater well (see Figure 1).

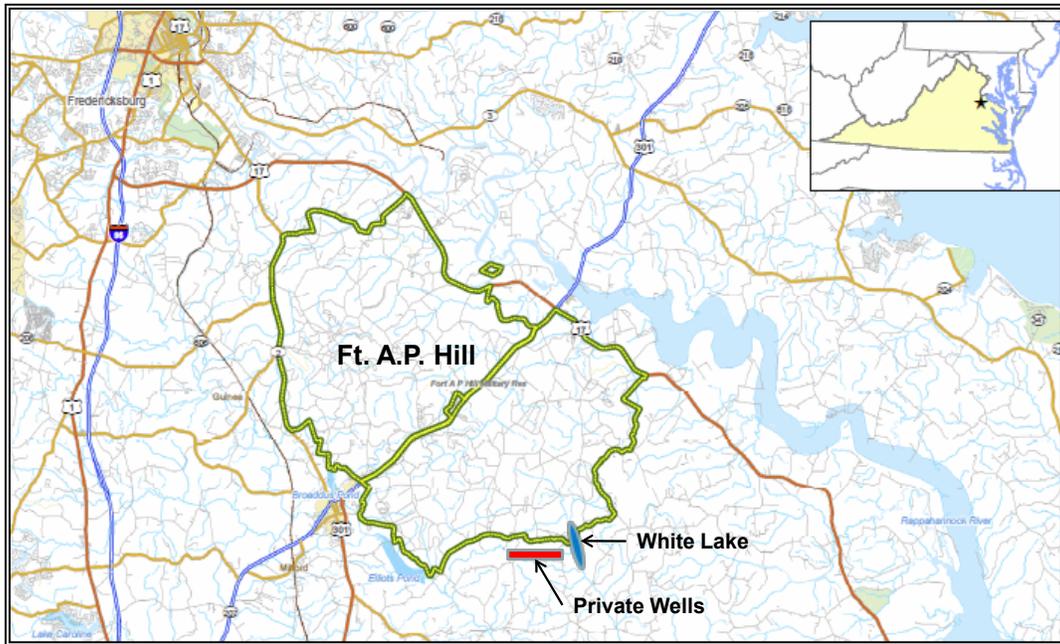


Figure 1. Vicinity map for Fort A.P. Hill, modified from EA (2006).

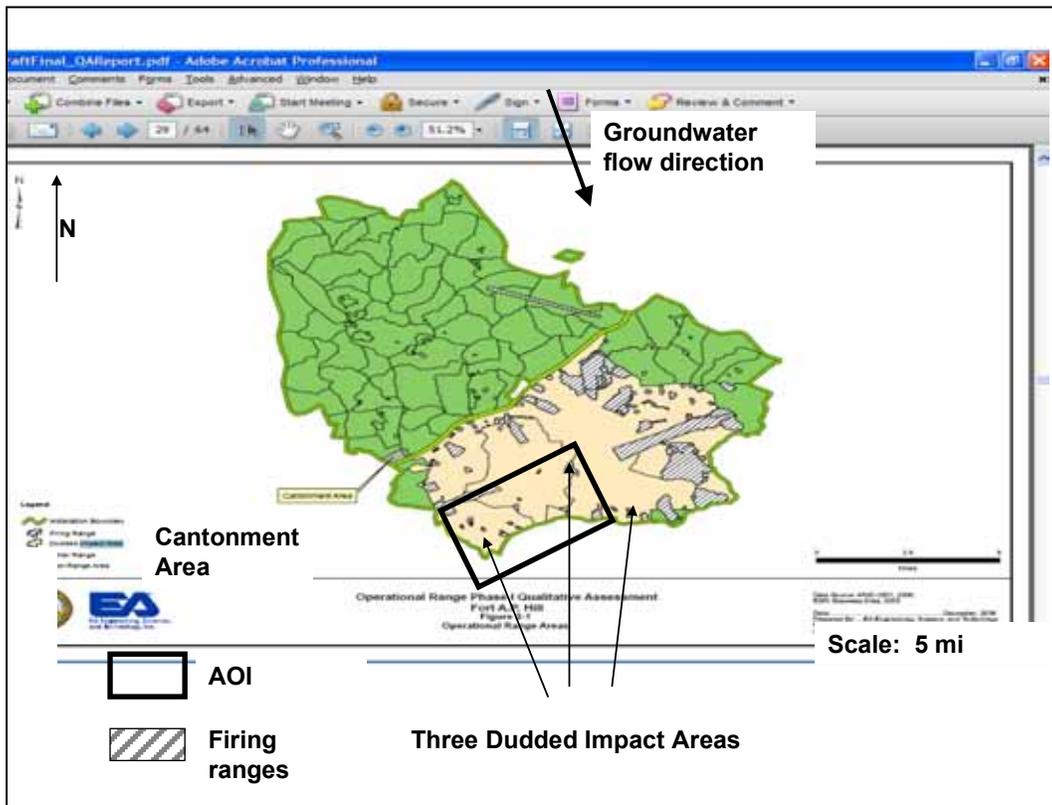


Figure 2. Fort A.P. Hill impact areas and delineated AOI, modified from EA (2006).

Both target waters are in the flow path through the AOI. General site characteristics are discussed in the POC application reports (Dortch et al. 2010, 2011b).

## Model inputs

Development of the Tier 2 model inputs for the Fort A.P. Hill AOI is described by Dortch et al. (2011b). The conditions for Test 2 in that report were used. The MC loadings are summarized in Table 1, and the other model inputs are listed in Tables 2-5 below. The loading duration was assumed to be 60 years.

**Table 1. MC loadings applied for Fort A.P. Hill AOI.**

| MC                    | Loading, g/yr |
|-----------------------|---------------|
| TNT                   | 60,729        |
| RDX                   | 15,202        |
| Lead                  | 7,127,880     |
| Copper                | 4,276,728     |
| Potassium perchlorate | 74            |

**Table 2. Tier 2 soil model input values for Fort A.P. Hill AOI.**

| Input Description  | Value                  |
|--|------------------------|
| Site Characteristics   |                        |
| AOI dimension that is parallel to the groundwater flow, m                                    | 2,285                  |
| AOI dimension that is perpendicular to the groundwater flow, m                               | 4,715                  |
| AOI surface area, m <sup>2</sup>   | 10,775,905             |
| Active soil layer thickness, m   | 0.4                    |
| Average annual temperature of soil-water matrix, °C  | 13.4                   |
| MC mass residue loading versus time, g/yr  | See Table 1            |
| Initial solid phase MC concentration in soil on a soil mass basis at time 0, mg/kg           | 0 for all constituents |
| Initial total non-solid phase MC concentration in soil on a soil mass basis at time 0, mg/kg | 0 for all constituents |
| Soil Properties  |                        |
| Volumetric soil moisture content, fraction   | 0.175                  |

Table 2. (continued).

| Input Description   | Value   |
|---|---|
| Soil dry bulk density, g/cm <sup>3</sup>  | 1.48  |
| Soil porosity, fraction   | 0.442   |
| Hydrology   |   |
| Average annual precipitation, m/yr  | 0.994   |
| Average annual rainfall, m/yr   | 0.923   |
| Average annual soil erosion rate, m/yr  | 0.000221  |
| Average annual water infiltration rate (groundwater recharge for no interflow), m/yr                | 0.201   |
| Average annual surface water runoff rate, m/yr  | 0.306   |
| Fraction of annual water infiltration flow rate and mass flux that goes to soil interflow, fraction | 0   |
| Average number of rainfall events per year  | 99  |
| Fate/Transport Parameters   |   |
| Soil-water constituent partition coefficient, L/kg  | RDX: 0.13<br>TNT: 0.31<br>Lead: 597<br>Copper: 92<br>KClO <sub>4</sub> : 4E-10 (miscible)                                       |
| Soil exchange layer thickness for rainfall ejection of pore water, m                                | 0.005   |
| Soil detachability for rainfall ejection of pore water, kg/L  | 0.4   |
| Decay/degradation half-life of liquid (water) phase constituent, yrs                                | 1.0E20 for all constituents   |
| Decay/degradation half-life of adsorbed (particulate) phase constituent, yrs                        | 1.0E20 for all constituents   |
| Initial mean diameter of solid phase constituent residue particles (assume spherical particles), μm | RDX: 12,000<br>TNT: 12,000<br>Lead: 500<br>Copper: 5,000<br>KClO <sub>4</sub> : NA  |
| Volatilization rate, m/yr   | RDX: computed, 33.7<br>TNT: computed, 26.8<br>Lead: specified, 0.<br>Copper: specified, 0.<br>KClO <sub>4</sub> : specified, 0. |

Table 2. (concluded).

| Input Description   | Value  |
|---|--|
| Switch for solid phase erosion (1 is on, and 2 is off)          | 2  |
| Chemical-Specific Properties                                    |  |
| Aqueous solubility limit, mg/L                                  | RDX: 59.8<br>TNT: 130<br>Lead: 2.24<br>Copper: 0.5<br>KClO <sub>4</sub> : 20,600         |
| Henry's law constant, atm-m <sup>3</sup> /g-mol                 | RDX: 6.31E-8<br>TNT: 4.57E-7<br>Lead: 0<br>Copper: 0<br>KClO <sub>4</sub> : 0            |
| Molecular weight (molar mass or averaged molecular mass), g/mol | RDX: 222.12<br>TNT: 227.13<br>Lead: 207.2<br>Copper: 63.55<br>KClO <sub>4</sub> : 138.55 |
| Solid phase constituent mass density, g/cm <sup>3</sup>         | RDX: 1.82<br>TNT: 1.65<br>Lead: 11.34<br>Copper: 8.94<br>KClO <sub>4</sub> : 1           |
| Model Options   |  |
| Time length of simulation, yrs                                  | 100 years  |
| Time step, yrs  | 0.01 (does not matter if use adaptive time step)   |
| Methods used for equation solution                              | Adaptive time step   |

Table 3. MEPAS vadose model input values for Fort A.P. Hill application.

| Input Description   | Value        |
|---|--------------|
| Inputs passed from soil model   |              |
| AOI dimension that is parallel to the groundwater flow, m   | 2,285        |
| AOI dimension that is perpendicular to the groundwater flow, m  | 4,715        |
| Water flow rate due to infiltration from soil (rainfall flow rate into vadose zone), m <sup>3</sup> /yr | 2,165,957    |
| MC mass flux versus time due to leaching from soil to vadose zone, g/yr                                 | Time-varying |

Table 3. (continued).

| Input Description                                  | Value  |
|--|--|
| Soil Composition                                   |  |
| Percentage of sand, %                              | 63.8   |
| Percentage of silt, %                              | 25   |
| Percentage of clay, %                              | 10   |
| Percentage of organic matter, %                    | 1.2  |
| Percentage of iron and aluminum, %                 | Unknown, set to 0  |
| Soil Characteristics                               |  |
| pH of pore water, pH units                         | 5.5  |
| Total porosity, %                                  | 44.2   |
| Field capacity, %                                  | 17.5   |
| Saturated hydraulic conductivity, cm/day           | 62.2   |
| Thickness of the vadose zone layer, m              | 6.1  |
| Longitudinal (vertical direction) dispersivity, cm | 6.1  |
| Dry bulk density, g/cm <sup>3</sup>                | 1.48   |
| Constituent Properties                             |  |
| Adsorption (partition) coefficient, ml/g           | RDX: 0.13<br>TNT: 0.31<br>Lead: 597<br>Copper: 92<br>KClO <sub>4</sub> : 4E-10   |
| Water solubility of constituent, mg/L              | RDX: 59.8<br>TNT: 130<br>Lead: 2.24<br>Copper: 0.5<br>KClO <sub>4</sub> : 20,600 |
| Half-life of constituent in groundwater, days      | 1.0E20 for all constituents  |

Table 4. Tier 2 MEPAS aquifer model input values for Fort A.P. Hill application.

| Input Description   | Value     |
|---|-----------|
| Inputs Passed from Vadose Zone Model  |           |
| AOI dimension that is parallel to the groundwater flow, m                     | 2,285     |
| AOI dimension that is perpendicular to the groundwater flow, m                | 4,715     |
| Water flow rate due to percolation (groundwater recharge), m <sup>3</sup> /yr | 2,165,957 |

Table 4. (continued).

| Input Description   | Value  |
|---|--|
| MC mass flux versus time due to percolation from the vadose zone to the aquifer, g/yr | Time-varying   |
| Composition   |  |
| Percentage of sand, %   | 63.8   |
| Percentage of silt, %   | 25   |
| Percentage of clay, %   | 10   |
| Percentage of organic matter, %   | 1.2  |
| Percentage of iron and aluminum, %  | Unknown, set to 0  |
| Sub-surface Characteristics   |  |
| Percentage of constituent flux entering the aquifer, %                                | 100  |
| pH of the pore water, pH units  | 5.5  |
| Total porosity, %   | 44.2   |
| Effective porosity, %   | 41   |
| Darcy velocity, cm/day  | 3.73   |
| Thickness of aquifer, m   | 15.2   |
| Soil dry bulk density, g/cm <sup>3</sup>  | 1.48   |
| Concentration Locations   |  |
| Longitudinal distance to well, m  | 4,000  |
| Perpendicular distance from plume center-line to well, m                              | 0  |
| Vertical distance below water table to well intake, cm                                | 0  |
| Longitudinal dispersivity, m  | 400  |
| Transverse dispersivity, m  | 132  |
| Vertical dispersivity, m  | 1  |
| Constituent Properties  |  |
| Sorption partitioning coefficient, ml/g   | RDX: 0.13<br>TNT: 0.31<br>Lead: 597<br>Copper: 92<br>KClO <sub>4</sub> : 4E-10   |
| Water solubility, mg/L  | RDX: 59.8<br>TNT: 130<br>Lead: 2.24<br>Copper: 0.5<br>KClO <sub>4</sub> : 20,800 |
| Half-life of constituent in groundwater, days   | 1.0E20 for all constituents  |

**Table 5. Tier 2 RECOVERY surface water model inputs for Fort A.P. Hill application.**

| <b>Input Description</b>  | <b>Value</b>                                |
|---|---|
| Inputs Passed from soil Model or Plus-SG Operator                                       |   |
| WFF (surface water) water flux, m <sup>3</sup> /yr                                      | 3,297,427<br>(this value is for AOI runoff) |
| WFF (surface water) mass flux, g/yr   | Time-varying                                |
| Surface Water Morphometry and Hydrology   |   |
| Total suspended solids concentration in the water column, mg/L                          | 100   |
| Weight fraction carbon in solids in water column, fraction                              | 0.01  |
| Long-term average water surface area, m <sup>2</sup>                                    | 75,000                                      |
| Long-term average of surface water mean depth, m  | 1.0   |
| Average annual water flow-through rate, m <sup>3</sup> /yr                              | 47,304,000                                  |
| Surface water residence time (computed), yr   | 0.00158                                     |
| Mixed Sediment Layer  |   |
| Contaminated sediment depth or total sediment bed depth to be modeled, m                | 1.0   |
| Depth of mixed sediment layer, m  | 0.07  |
| Mixed sediment layer surface area, m <sup>2</sup>                                       | 75,000                                      |
| Mixed sediment layer porosity, fraction   | 0.7   |
| Mixed sediment particle density or specific gravity, g/cm <sup>3</sup>                  | 2.65  |
| Mixed sediment layer weight fraction carbon in solids, fraction                         | 0.01  |
| Deep Sediment Layers  |   |
| Deep sediment porosity, fraction  | 0.5   |
| Deep sediment particle density or specific gravity, g/cm <sup>3</sup>                   | 2.65  |
| Deep sediment layer weight fraction carbon in solids, fraction                          | 0.01  |
| Mean wind speed, m/sec  | 6   |
| Enhanced diffusion between mixed sediment layer and deep sediment, cm <sup>2</sup> /sec | 0   |
| Enhanced mixing depth between mixed sediment layer and deep sediment, cm                | 0   |

Table 5. (continued).

| Input Description   | Value   |
|---|---|
| Suspended solids settling velocity, m/yr  | 36  |
| Deep sediment burial velocity (computed), m/yr  | 4.53E-3   |
| Mixed layer sediment resuspension velocity, m/yr  | 1.0E-20   |
| Constituent Properties  |   |
| Initial contaminant concentration of constituent in water, µg/L                             | 0   |
| Additional constant external loading rate of constituent, kg/yr                             | 0   |
| Initial contaminant concentration in mixed sediment, mg/kg                                  | 0   |
| Initial contaminant concentration in deep sediment, mg/kg                                   | 0   |
| Molecular diffusivity, cm <sup>2</sup> /sec   | RDX: 7.1E-6<br>TNT: 6.36E-6<br>Lead: 9.45E-6<br>Copper: 7.33E-6<br>KClO <sub>4</sub> : 6.0E-6 |
| Henry's Law Constant, atm-m <sup>3</sup> /g-mole  | RDX: 6.31E-8<br>TNT: 4.57E-7<br>Lead: 0<br>Copper: 0<br>KClO <sub>4</sub> : 0                 |
| Molecular weight, g-mole  | RDX: 222.12<br>TNT: 227.13<br>Lead: 207.2<br>Copper: 63.55<br>KClO <sub>4</sub> : 138.55      |
| Octanol-water partition coefficient, (mg/m <sup>3</sup> octanol)/ (mg/m <sup>3</sup> water) | RDX: 7.41<br>TNT: 39.8<br>Lead: NA<br>Copper: NA<br>KClO <sub>4</sub> : 6.6E-8                |
| Partition coefficient for the water column for inorganic constituents, L/kg                 | Lead: 4,000<br>Copper: 600  |
| Partition coefficient for the mixed sediment pore water for inorganic constituents, L/kg    | Lead: 4,000<br>Copper: 600  |
| Partition coefficient for the deep sediment pore water for inorganic constituents, L/kg     | Lead: 4,000<br>Copper: 600  |

Table 5. (concluded).

|   |                        |
|---|------------------------|
| Decay coefficient for dissolved contaminant in water, 1/yr                            | 0 for all constituents |
| Decay coefficient for dissolved contaminant in mixed layer, 1/yr                      | 0 for all constituents |
| Decay coefficient for dissolved contaminant in deep sediment, 1/yr                    | 0 for all constituents |
| Decay coefficient for particulate contaminant in water, 1/yr                          | 0 for all constituents |
| Decay coefficient for particulate contaminant in mixed layer, 1/yr                    | 0 for all constituents |
| Decay coefficient for particulate contaminant in deep sediment, 1/yr                  | 0 for all constituents |
| Model Control Parameters  |                        |
| Total period of simulation, yrs   | 100                    |
| Number of time steps between print intervals for output, dimensionless                | 40                     |
| Number of time steps between print intervals for sediment layer output, dimensionless | 20                     |
| Number of sediment layers to print in output, dimensionless                           | 50                     |

## Results

An initial set of results and a refined set of results are presented below for both groundwater and surface water with comparison to observed data furnished by the U.S. Army Public Health command, Army Institute of Public Health.

### Initial results

The initial application results for Fort A.P. Hill were obtained before the measured field data were available. Thus, the initial model results presented below are truly the result of a blind test of the models. The inputs for the initial results were presented in the previous section.

Computed and observed (i.e., measured) groundwater dissolved MC concentrations in parts per billion (ppb) are presented in Table 6. The observed concentrations are for two wells near White Lake, which is in the vicinity of the model well location. Observed and computed dissolved concentrations were below the measurement detection limit for all

five MC. The computed concentrations were obtained after 60 years of simulation. The model compares very favorably to the observed data for groundwater since all concentrations are below detection.

**Table 6. Groundwater dissolved MC concentrations, ppb.**

| MC                    | Computed | Measured  |
|-----------------------|----------|-----------|
| RDX                   | 3.6E-4   | ND (<0.2) |
| TNT                   | 2.7E-3   | ND (<0.2) |
| Lead                  | 0        | ND (<1)   |
| Copper                | 0        | ND (<8)   |
| Potassium perchlorate | 1.2E-3   | ND (<0.2) |

ND = non-detect

The computed and observed total concentrations of MC for White Lake surface water are shown in Table 7. The computed concentrations were obtained after 60 years of simulation. The reported measured values are the average of all reported values for the lake. All computed MC concentrations are in good agreement with measured values except for copper, which is about an order of magnitude lower than measured. The potential reasons for this are examined in the next section. The computed TNT concentration is slightly higher than ND, but no degradation was assumed for TNT, whereas TNT is known to degrade in natural environments. Computed lead concentration is about double that measured, but such agreement is remarkable given all of the uncertainty in inputs, particularly the MC loadings. The computed lead concentration does not include background lead, whereas the measured value does include background. If the average background concentration from Mill Creek of 0.55 ppb is added to the computed lead concentration, then the adjusted computed lead water concentration is 1.05 ppb, which is about 0.8 ppb too high. Computed RDX and perchlorate concentrations are below ND, as are the measurements.

**Table 7. Surface water MC total concentrations for White Lake, ppb.**

| MC                    | Computed | Measured  |
|-----------------------|----------|-----------|
| RDX                   | 0.042    | ND (<0.2) |
| TNT                   | 0.29     | ND (<0.2) |
| Lead                  | 0.5      | 0.25      |
| Copper                | 0.025    | 0.32      |
| Potassium perchlorate | 2.3E-4   | ND (<0.2) |

The computed and observed total concentrations of MC for White Lake sediments are shown in Table 7. The computed concentrations were obtained after 60 years of simulation. The reported measured values are the average of all reported values for the lake. The computed concentrations for the two explosives are less than ND, the same as the measured values. Computed perchlorate concentration was also very low, as expected, but perchlorate was not measured in the field. The computed concentration for copper is about two orders of magnitude lower than measured. The potential reasons for this are examined in the next section. Computed lead concentration is about one-sixth of that measured, but the computed lead concentration does not include background lead, and the measured value does include background lead concentrations. If the average of the background lead concentrations in sediment (at Mill Creek), which is 2.65 parts per million (ppm), is added to the computed lead concentration, then the adjusted computed value (3.55 ppm) is much closer to the measured value of 6.0 ppm. The average background concentration of copper in Mill Creek sediment is 1.7 ppm.

**Table 8. Sediment MC total concentrations for White Lake, ppm.**

| MC                    | Computed | Measured   |
|-----------------------|----------|------------|
| RDX                   | 3.8E-5   | ND (<0.15) |
| TNT                   | 3.3E-4   | ND (<0.15) |
| Lead                  | 0.9      | 6.0        |
| Copper                | 0.01     | 2.9        |
| Potassium perchlorate | 2.0E-7   | NM         |

Notes: Computed lead and copper concentrations do not include background metals; add 2.65 and 1.7 ppm for background lead and copper, respectively. NM = not measured.

### Refined results

Additional modeling for Fort A.P. Hill was conducted in an attempt to better understand why the computed copper concentrations for surface water and sediment were much lower than measured. The sediment–water partitioning or distribution coefficient,  $K_d$ , for copper was first increased to see if that would make much difference. Recommended values of  $K_d$  for heavy metals in benthic sediment, soil, and suspended sediment are reported by the U.S. Environmental Protection Agency (USEPA) (Allison and Allison 2005). The sediment partitioning coefficient values suggested for copper and lead (with correction for dissolved organic carbon) are about 1,400 and 28,000 L/kg, respectively. Modeling the lake with these values

resulted in computed sediment concentrations of 2.25 and 0.02 ppm for lead and copper, respectively. The updated, computed lead concentration is nearly the same as measured after adding background concentration. However, the updated, computed copper concentration is still several orders of magnitude less than measured. Thus,  $K_d$  values are not the primary cause in difference from observed values. Increasing  $K_d$  had very little effect on computed surface water concentrations of lead and copper.

The solubility of copper was increased from 0.5 mg/L to 18.4 mg/L for the next model run. The lower value was obtained by applying the Visual Minteq model, and the higher value was obtained by applying the Stevens Institute spreadsheet for copper solubility, as explained by Dortch et al. (2011b). The lower value seemed more reasonable, but it is possible that the higher value is more appropriate. Estimating solubility of metals is probably the most difficult and uncertain aspect of applying TREECS™.

Increasing copper solubility in the soil model from 0.5 to 18.4 mg/L had the effect of increasing the White Lake sediment concentration of copper from 0.01 ppm to 0.33 ppm. If the background copper concentration of 1.7 ppm is added to this, then the adjusted, computed concentration is 2.03 ppm, which compares favorably with the measured copper concentration of 2.9 ppm. This value is computed with the original  $K_d$  value of 600 L/kg. The higher  $K_d$  of 1400 L/kg would approximately double the computed copper concentration in sediment.

The computed surface water copper concentration after the above adjustment was 0.86 ppb compared with the measured value of 0.32 ppb. If the average background copper concentration of 0.47 ppb is added to the computed value, then the adjusted, computed value is 1.33 ppb compared to 0.32 ppb measured, or about 1 ppb too high.

## Conclusions

Tier 2 of TREECS™ provided reasonable results for groundwater where results for all five MC were predicted to be below detection after about 60 years of range use. These predictions are in agreement with recent measurements that also show concentrations for all five MC to be below detection.

Surface water and sediment concentrations of the two explosives and potassium perchlorate in White Lake were predicted to be below detection,

which is in agreement with measured values that were found to be below detection. Predicted lead concentrations in White Lake were the same order of magnitude as measured. Correction of computed lead concentrations for background lead improved the agreement with the measured sediment value.

Copper was the only MC with a predicted concentration that greatly differed from that measured. Predicted copper concentrations in sediment were two orders of magnitude lower than observed. Inaccurate specification of water solubility required as input by the soil model is considered to be a potential reason for the poor prediction. When a higher, alternative estimate of 18.4 mg/L for solubility was used rather than the initial estimate of 0.5 mg/L, copper concentrations in sediment were computed to be nearly the same as measured (after adjusting the computed value for background copper).

Water solubility of MC is one of the most sensitive inputs for Tier 2 of TREECS™. Unfortunately, solubility of metals is the most difficult input to estimate. As a result, metal solubility is also one of the most uncertain inputs of TREECS™.

### **3 Massachusetts Military Reservation Application**

#### **Background and site description**

The Massachusetts Military Reservation (MMR) is located in Barnstable County in the Cape Cod region of Massachusetts. The installation has been in use since 1911 for purposes such as Army training and maneuvers, military aircraft operations, maintenance, and support. Units or members of the National Guard are currently operating at the MMR. Demolition (Demo) Area 2 is the MMR site of interest in this study.

Demo Area 2 is located in the northern section of Camp Edwards, which is within the MMR (Figure 3). This area was used for light demolition training for roughly 10 years beginning in the late 1970s and continuing until the late 1980s. The area was used for demolition training, not for demolition of loaded munitions, so non-munitions objects were blown up rather than munitions containing explosives. Range records show that the explosives used in this area were limited to blocks of C4 and TNT demolition charges. Thus, C4, which contains RDX and plasticizers, was a prevalent explosive at this site. Some charges may not have experienced full high-order detonation, thus, resulting in unexploded explosives residue. RDX residue from these explosives has infiltrated to the groundwater beneath the demolition range.

The soils in this region are sandy and highly permeable allowing for rapid movement of groundwater at rates up to 0.6 m/day (Air Force Center for Environmental Excellence (AFCEE), 2006). The MMR is located over the recharge area of the Sagamore Lens, which is a large aquifer about 91 m thick (AFCEE 2006). Demo Area 2 is divided into four main soil regions, but the source zone area is characterized as Enfield soil type (denoted as 265B), which is silty loam down to 30 cm, a mixture of silty loam and sandy loam from 30 to 79 cm, and mostly sand at depths below 79 cm.

Figure 4 shows the groundwater contours, estimated RDX plume, and monitoring wells at Demo Area 2 as understood in 2004. Nine monitoring wells surrounded the plume during the time of sampling and two more proposed wells are also shown in the figure. The darker shade indicates

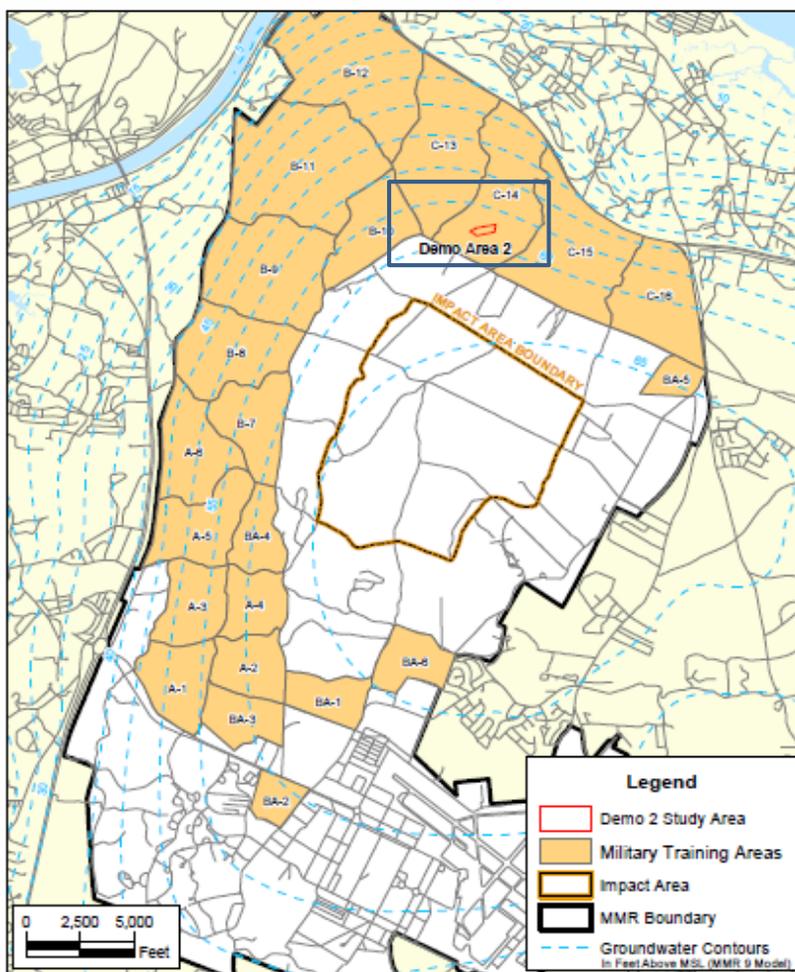


Figure 3. Site map for MMR locating Demo Area 2 (modified from AMEC Earth and Environmental (2004).

concentrations greater than 2 ppb, which was the public health advisory concentration at the time, and the lighter shade indicates concentrations above non-detection but less than or equal to 2 ppb.

Modeling of this site was performed by Dortch et al. (2007) to investigate the feasibility of using models such as the ones in TREECS™ to assess groundwater plumes of MC on military ranges. The vadose zone and aquifer model used in this earlier study are the same MEPAS models that are in TREECS™. The soil model in TREECS™ is different and newer than the MEPAS soil model that was used in the earlier study. Results of this earlier study indicated that modeling tools like TREECS™ could be useful for predicting the fate of MC on ranges. The application of TREECS™ to MMR Demo Area 2 not only provides model validation, but also allows comparison of the TREECS™ soil model to the MEPAS soil model that was used in the previous application.

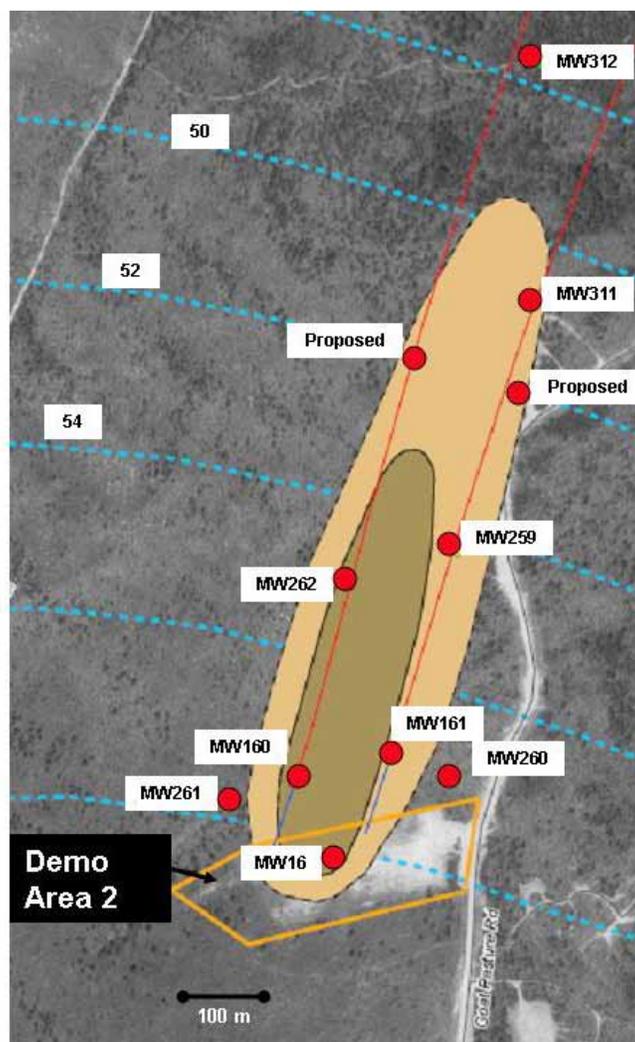


Figure 4. Locations of estimated contaminant plume (greater than non-detect and greater than 2 ppb) and monitoring wells along with groundwater contours, ft NGVD (modified from AMEC Earth and Environmental (2004)).

## Model inputs

The Tier 2 TREECS™ vadose zone and aquifer models were set up with the same inputs used in previous modeling by Dortch et al. (2007). The soil model was set up with similar inputs, but there are differences since the TREECS™ Tier 2 soil model is different from the MEPAS soil model. There was no need for using a surface water model since surface water is not a feature for Demo Area 2 of MMR. The TREECS™ Tier 2 soil model inputs for MMR are shown in Table 9. The vadose zone and aquifer model inputs are shown in Tables 10 and 11. RDX is the only modeled MC.

Table 9. Tier 2 soil model input values for the MMR AOI.

| Input Description   | Value   |
|---|---|
| Site Characteristics  |   |
| AOI dimension that is parallel to the groundwater flow, m   | 110   |
| AOI dimension that is perpendicular to the groundwater flow, m                                      | 110   |
| AOI surface, m <sup>2</sup>   | 12,100  |
| Active soil layer thickness, m  | 0.4   |
| Average annual temperature of soil-water matrix, °C   | 11.0  |
| MC mass residue loading versus time, g/yr   | 1,000   |
| Initial solid phase MC concentration in soil on a soil mass basis at time 0, mg/kg                  | 0 for all constituents                          |
| Initial total non-solid phase MC concentration in soil on a soil mass basis at time 0, mg/kg        | 0 for all constituents                          |
| Soil Properties   |   |
| Volumetric soil moisture content, fraction  | 0.155   |
| Soil dry bulk density, g/cm <sup>3</sup>  | 1.43  |
| Soil porosity, fraction   | .46   |
| Hydrology   |   |
| Average annual precipitation, m/yr  | 1.22  |
| Average annual rainfall, m/yr   | 1.22 (set to precipitation since little runoff) |
| Average annual soil erosion rate, m/yr  | 0.0   |
| Average annual water infiltration rate (groundwater recharge for no interflow), m/yr                | 0.762   |
| Average annual surface water run-off rate, m/yr   | 0.0   |
| Fraction of annual water infiltration flow rate and mass flux that goes to soil interflow, fraction | 0   |
| Average number of rainfall events per year  | 100   |
| Fate/Transport Parameters   |   |
| Soil-water constituent partition coefficient, L/kg  | RDX: 0.11                                       |
| Soil exchange layer thickness for rainfall ejection of pore water, m                                | 0.005   |
| Soil detachability for rainfall ejection of pore water, kg/L  | 0.4   |
| Decay/degradation half-life of liquid (water) phase constituent, yrs                                | 1.0E20  |

Table 9. (continued).

| Input Description  | Value   |
|--|---|
| Decay/degradation half-life of adsorbed (particulate) phase constituent, yrs                                   | 1.0E20  |
| Initial mean diameter of solid phase constituent residue particles (assume spherical particles), $\mu\text{m}$ | RDX: 12,000   |
| Volatilization rate, m/yr  | RDX: 0.0  |
| Switch for solid phase erosion (1 is on, and 2 is off)   | 2   |
| Chemical-Specific Properties   |   |
| Aqueous solubility limit, mg/L   | RDX: 29.52 (based on average annual soil temperature of 11 deg C) |
| Henry's law constant, atm-m <sup>3</sup> /g-mol  | RDX: 6.31E-8  |
| Molecular weight (molar mass or averaged molecular mass), g/mol  | RDX: 222.12   |
| Solid phase constituent mass density, g/cm <sup>3</sup>  | RDX: 1.82   |
| Model Options  |   |
| Time length of simulation, yrs   | 30  |
| Time step, yrs   | 0.01 (does not matter if use adaptive time step)                  |
| Methods used for equation solution   | Adaptive time step  |

Table 10. MEPAS vadose model input values for the MMR application.

| Input Description   | Value             |
|---|-------------------|
| Inputs Passed from Soil Model   |                   |
| AOI dimension that is parallel to the groundwater flow, m   | 110               |
| AOI dimension that is perpendicular to the groundwater flow, m  | 110               |
| Water flow rate due to infiltration from soil (rainfall flow rate into vadose zone), m <sup>3</sup> /yr | 9220              |
| MC mass flux versus time due to leaching from soil to vadose zone, g/yr                                 | Time-varying      |
| Soil Composition  |                   |
| Percentage of sand, %   | 91.83             |
| Percentage of silt, %   | 5                 |
| Percentage of clay, %   | 3                 |
| Percentage of organic matter, %   | 0.17              |
| Percentage of iron and aluminum, %  | Unknown, set to 0 |

Table 10. (continued).

| Input Description                                  | Value      |
|--|------------|
| Soil Characteristics                               |            |
| pH of pore water, pH units                         | 7          |
| Total porosity, %                                  | 38         |
| Field capacity, %                                  | 9          |
| Saturated hydraulic conductivity, cm/day           | 570        |
| Thickness of the vadose zone layer, m              | 39.6       |
| Longitudinal (vertical direction) dispersivity, cm | 3.96       |
| Dry bulk density, g/cm <sup>3</sup>                | 1.64       |
| Constituent Properties                             |            |
| Adsorption (partition) coefficient, ml/g           | RDX: 0.013 |
| Water solubility of constituent, mg/L              | RDX: 59.8  |
| Half-life of constituent in groundwater, yrs       | 100        |

Table 11. MEPAS aquifer model input values for the MMR application.

| Input Description   | Value             |
|---|-------------------|
| Inputs Passed from Vadose Zone Model  |                   |
| AOI dimension that is parallel to the groundwater flow, m                             | 110               |
| AOI dimension that is perpendicular to the groundwater flow, m                        | 110               |
| Water flow rate due to percolation (groundwater recharge), m <sup>3</sup> /yr         | 9220              |
| MC mass flux versus time due to percolation from the vadose zone to the aquifer, g/yr | Time-varying      |
| Composition   |                   |
| Percentage of sand, %   | 91.83             |
| Percentage of silt, %   | 5                 |
| Percentage of clay, %   | 3                 |
| Percentage of organic matter, %   | 0.17              |
| Percentage of iron and aluminum, %  | Unknown, set to 0 |
| Sub-surface Characteristics   |                   |
| Percentage of constituent flux entering the aquifer, %                                | 100               |
| pH of the pore water, pH units  | 7                 |
| Total porosity, %   | 38                |

Table 11. (continued).

| Input Description  | Value      |
|--|------------|
| Effective porosity, %                                    | 30         |
| Darcy velocity, cm/day                                   | 100        |
| Thickness of aquifer, m                                  | 91         |
| Soil dry bulk density, g/cm <sup>3</sup>                 | 1.64       |
| Concentration Locations                                  |            |
| Longitudinal distance to well, m                         | 198        |
| Perpendicular distance from plume center-line to well, m | 61         |
| Vertical distance below water table to well intake, cm   | 0.46       |
| Longitudinal dispersivity, m                             | 1.09       |
| Transverse dispersivity, m                               | 0.109      |
| Vertical dispersivity, m                                 | 0.00198    |
| Constituent Properties                                   |            |
| Sorption partitioning coefficient, ml/g                  | RDX: 0.013 |
| Water solubility, mg/L                                   | RDX: 59.8  |
| Half-life of constituent in groundwater, yrs             | 100        |

The loading of RDX is not well known for this site, since no use records could be found. All that is known is that C4 blocks containing RDX were used to demolish various objects that did not contain explosives. Results of the previous modeling are used here to set the loading rate of RDX, which is 1 kg/yr. This loading rate seems quite reasonable as explained by Dortch et al. (2007). This loading was applied for 10 years, which is the length of time that this site was used. The site was modeled for 30 years, covering the period of use to the time of field sampling.

## Results

### AOI soil

Computed and measured soil total concentrations of RDX within the AOI are plotted in Figure 5. The observed data were collected in 1998, which is about 20 years after the initiation of demolition activities at the site. The demolition activities lasted for about 10 years. The computed concentrations fall within about the middle of the observed concentrations, indicating relatively good performance of the soil model. The soil model treats the AOI soil layer as homogeneous, when in reality considerable variation of MC concentrations can occur as shown by the observed data. The results of the original modeling (Dortch et al. 2007) are shown in Figure 6 for comparison

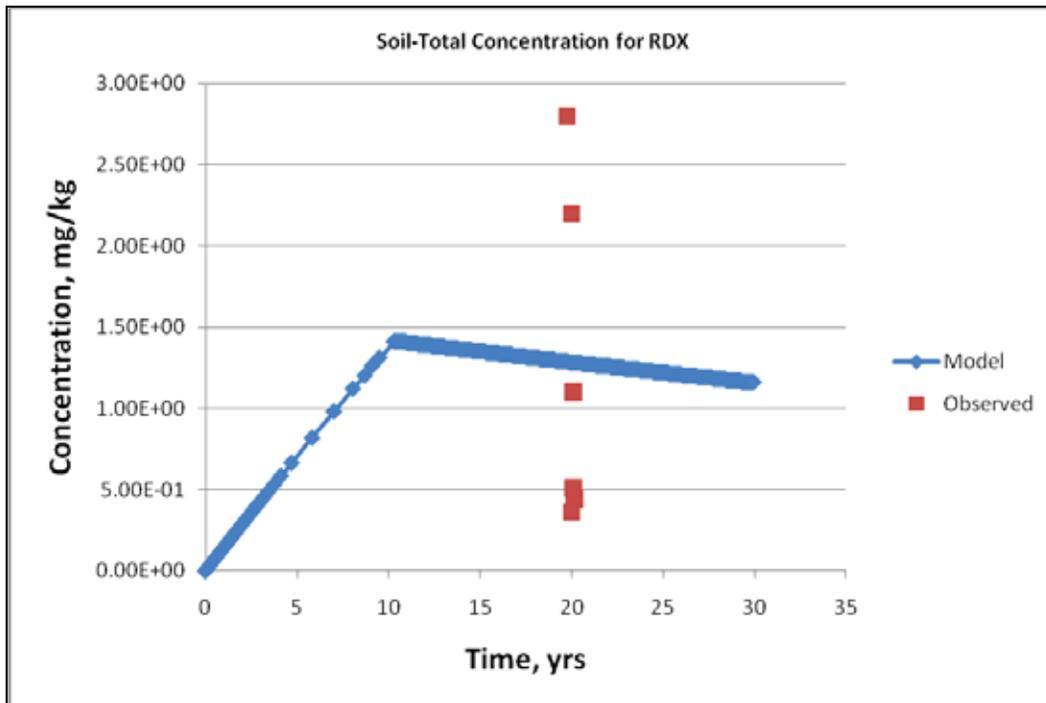


Figure 5. Computed and observed total concentrations of RDX in the soil of MMR AOI using inputs of Table 9.

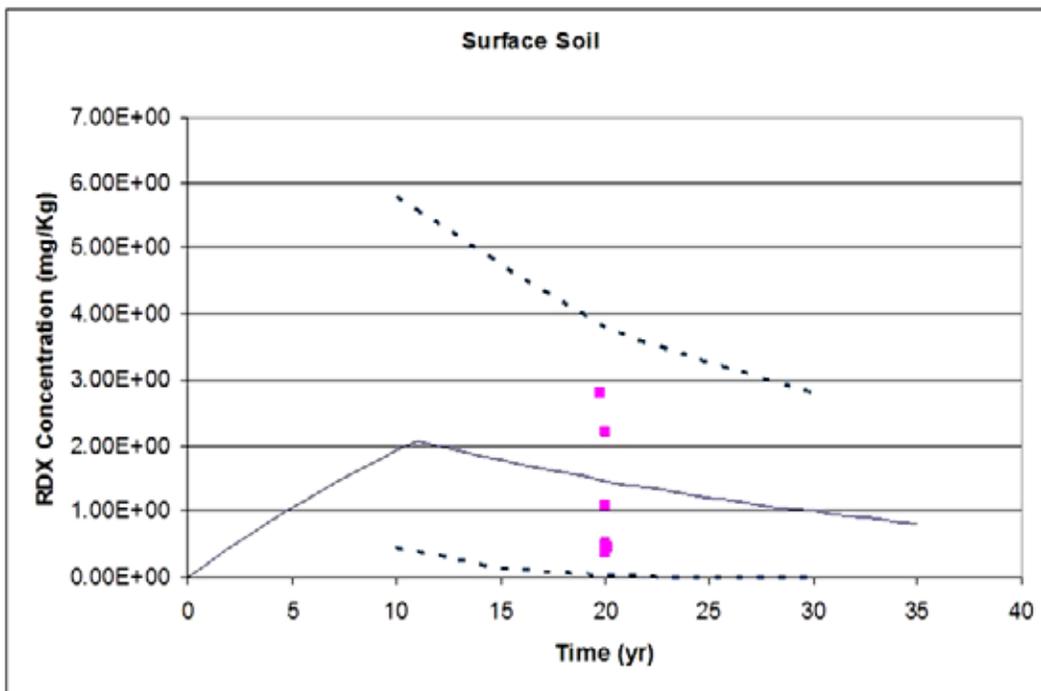


Figure 6. Computed and observed total concentrations of RDX in the soil of MMR AOI obtained in original modeling (from Dortch et al. (2007)).

to the present results. The solid line in the figure is the model mean result, the dashed lines are the 95% confidence bands of the model, and the symbols are the observed data. Comparison of Figure 5 and Figure 6 shows that the model results are quite similar.

The computed results of Figure 5 were obtained using the inputs shown in Table 9, including RDX water solubility of 29.52 mg/L, which is about half of the value of 59.8 mg/L used in the original modeling reported by Dortch et al. (2007). The lower and higher solubility values are for ambient soil water temperatures of 11 and 25 °C, respectively. The lower solubility is more appropriate for the long-term average soil water temperature of 11 °C. Thus, similar results were obtained for the two different solubility values, which is due to differences in the older and newer soil model formulations. Increasing the solubility of RDX to 59.8 mg/L in the TREECS™ Tier 2 soil model input only slightly decreased the computed soil concentrations for the declining limb of the plot in Figure 5.

The results of Figure 5 were obtained for an initial solid phase RDX mean particle residue diameter of 12,000 µm, which is the approximate mean size of explosive particle residue as determined from the literature (Dortch et al. 2011a). Solid phase MC residue particle diameter, MC solubility, and annual precipitation depths are the primary inputs affecting the computed solid phase MC dissolution rate. Of these three inputs, the value for the RDX particle diameter is the most uncertain and sensitive. Dissolution is a key mechanism required for export (or loss) of MC from the AOI soil. Solid phase loading is the only source of MC within the AOI. Thus, computed soil concentrations of RDX are highly sensitive to input values for the solid phase particle diameter and loading rate. The loading rate of RDX that occurred at Demo Area 2 is highly uncertain as discussed by Dortch et al. (2007). The value of 1 kg/yr used in the above results was determined from the original modeling and deemed reasonable based upon the demolition charges used. Results fairly similar to those above (Figure 5) can be obtained using half the particle diameter (6,000 µm) and a 50% higher loading rate (1.5 kg/yr), as shown in Figure 7.

### **Groundwater**

Computed groundwater concentrations for monitoring well (MW) 161 are compared to observed concentrations in Figure 8. The results from the original modeling (Dortch et al. 2007) are provided in Figure 9 for comparison. The peak groundwater concentrations at MW161 in the

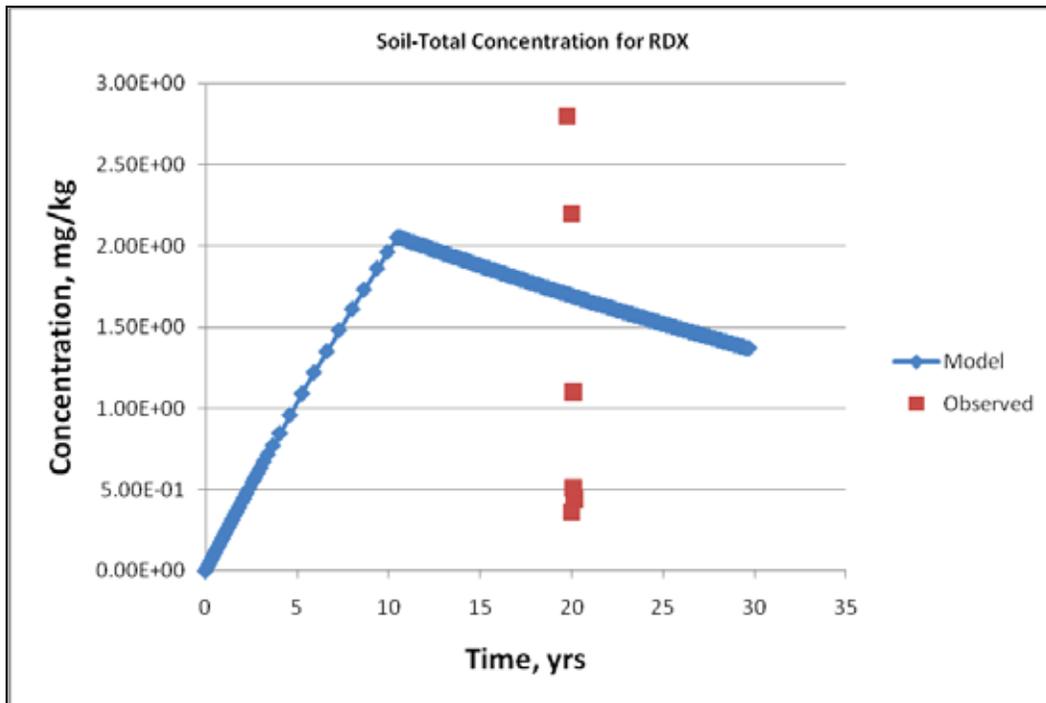


Figure 7. Computed and observed total concentrations of RDX in the soil of MMR AOI using inputs of Table 9 except for particle diameter of 6,000  $\mu\text{m}$  and loading rate of 1.5 kg/yr.

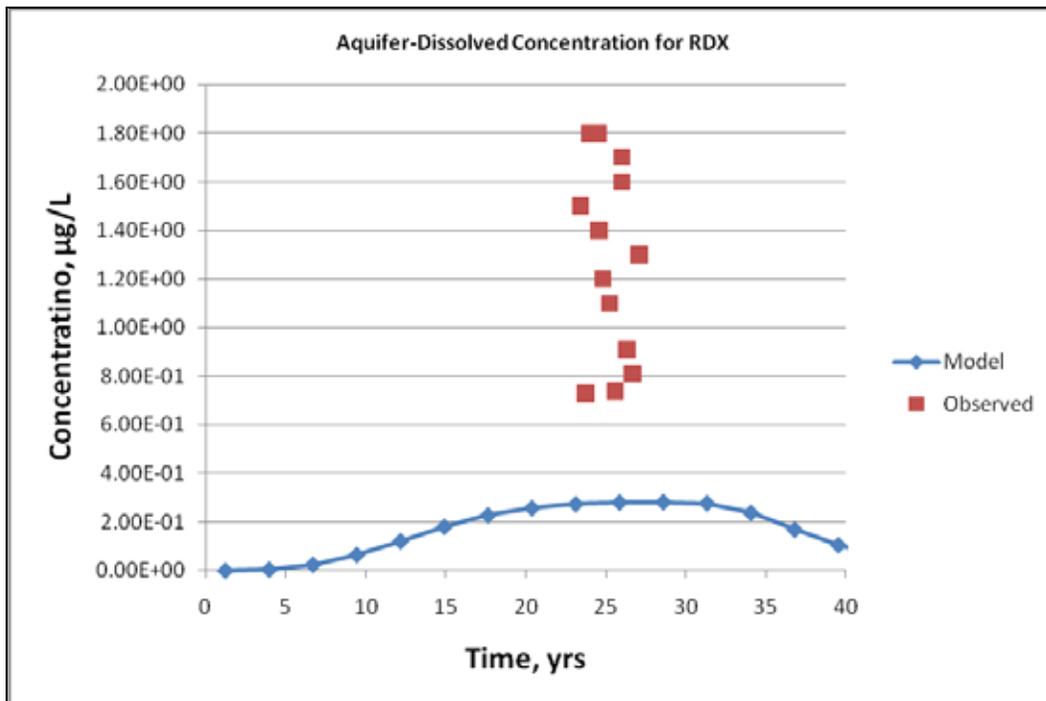


Figure 8. Computed and observed dissolved concentrations of RDX in MMR groundwater at MW161 using inputs of Tables 9 through 11.

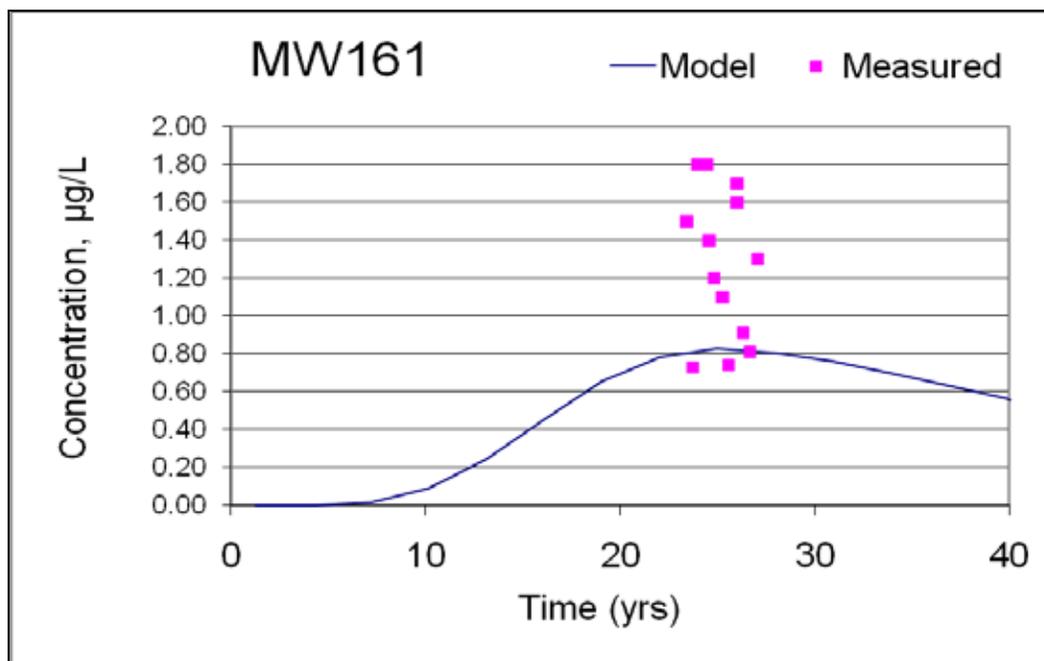


Figure 9. Computed and observed dissolved concentrations of RDX in MMR groundwater at MW161 obtained in original modeling (modified from Dortch et al. (2007)).

present results are about half of those in the previous modeling due to differences in the leaching fluxes as affected by differences in the dissolution rates computed by the new and old soil models.

The computed results in Figure 8 were obtained with the inputs shown in Tables 9 through 11. Increasing the RDX solubility from 29.5 to 59.8 mg/L (value used in original modeling) in the Tier 2 soil model input approximately doubled the peak groundwater concentration from 0.27 to 0.6 ppb, thus yielding results that agree more closely with the previous modeling results in Figure 9. Alternatively, using the proper solubility in soil-water of 29.52 mg/L but with half the particle diameter (i.e., 6,000  $\mu\text{m}$ ) and 50% higher loading of 1.5 kg/yr produces results very similar to those in Figure 9. Computed and observed values are shown in Figure 10.

Results can also be very sensitive to the location of the well and the dispersivities used in the aquifer model. For example, if the perpendicular (lateral) distance of the well from the groundwater plume centerline is reduced 5 m from 61 to 56 m (see Table 11), the computed results are very similar to those shown in Figure 10. The location of the plume centerline was estimated (AMEC Earth and Environmental 2004) based on monitoring well data, so it is not precisely known. Results are also sensitive to variations in dispersivity. The dispersivity values used in this modeling are based on MMR field tracer tests and other modeling (AFCEE 2006).

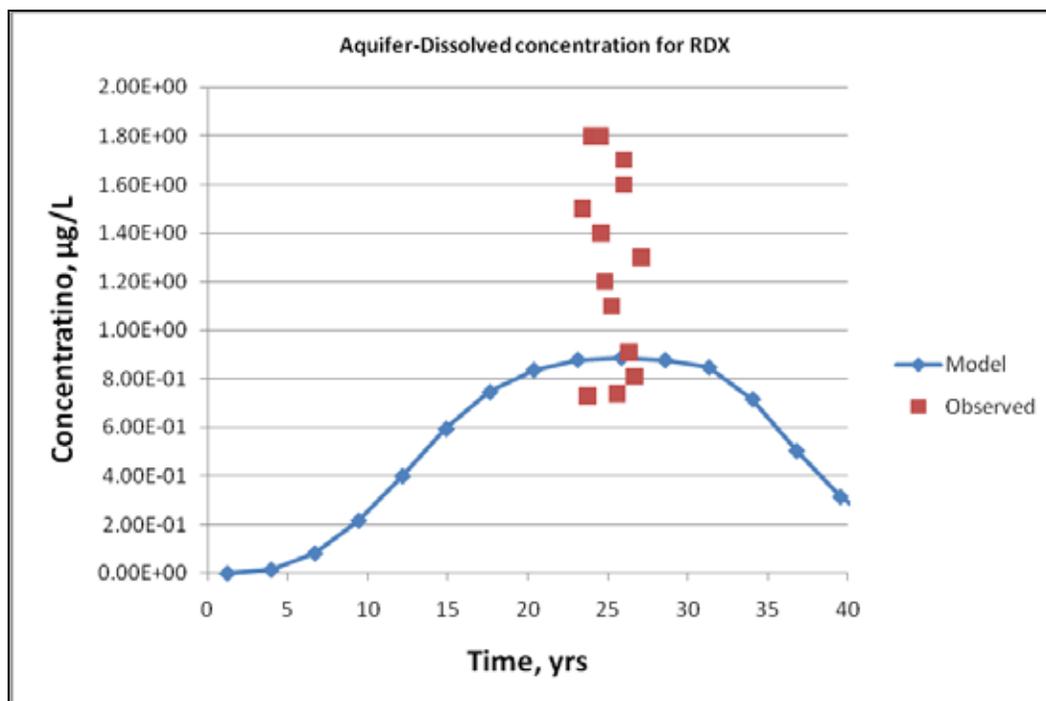


Figure 10. Computed and observed dissolved concentrations of RDX in MMR groundwater at MW161 using inputs of Tables 9 through 11, except for a particle diameter of 6,000  $\mu\text{m}$  and a loading rate of 1.5 kg/yr.

The observed data can be more accurately matched with the model by making relatively minor and reasonable adjustments to the uncertain inputs of particle diameter, loading rate, and location of the monitoring well. As an example, a loading rate of 1.5 kg/yr, particle diameter of 6,000  $\mu\text{m}$ , and a perpendicular distance of 59 m from the plume centerline to MW161 (rather than 61 m) resulted in the results shown in Figure 11. These results are for the same input conditions as the results in Figure 10 except for moving the location of the well 2 m closer to the plume centerline. The computed AOI soil concentrations for this test are the same as those shown in Figure 7.

## Conclusions

It was possible to fairly accurately predict the observed RDX soil concentrations within the AOI, as well as match reasonably well the soil concentrations computed during the original modeling, using previously determined site characteristics and inputs from the original modeling as well as the default value for residue particle diameter of 12,000  $\mu\text{m}$ . Computed soil concentrations are sensitive to MC residue loading rate and particle diameter. Both of these inputs have considerable uncertainty, but reasonable variations in these two inputs produce results within the range of those measured at the site.

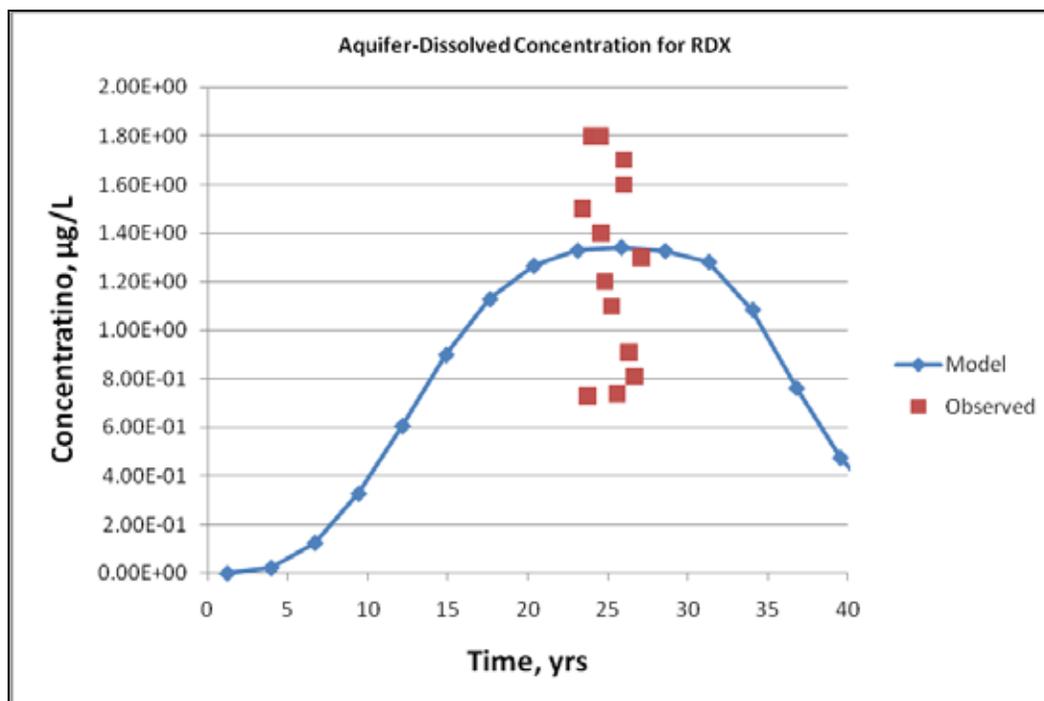


Figure 11. Computed and observed dissolved concentrations of RDX in MMR groundwater at MW161 using inputs of Tables 9 through 11, except for a particle diameter of 6,000  $\mu\text{m}$ , loading rate of 1.5 kg/yr, and perpendicular distance from the plume of 59 m.

Using previously determined site characteristics, original modeling inputs, and the default value for residue particle diameter resulted in computed groundwater concentrations of RDX that were about one-fourth of those measured for MW161. Model results were rather sensitive to input values for RDX residue loading rate and particle diameter, as well as perpendicular distance of the monitoring well from the RDX plume centerline, all of which are uncertain inputs. The model can be more accurately matched with the observed data by making relatively minor and reasonable adjustments to these three inputs. Overall, the results of this application support successful validation of the TREECS™ soil, vadose, and aquifer models.

## 4 West Point Application

### Site description

The site description information presented here was obtained from the U.S. Army Aberdeen Test Center (ATC) (2004a). The U.S. Military Academy (USMA) is located at West Point in southeastern New York on the west side of the Hudson River, approximately 45 miles north of New York City. The academic, administrative, and housing areas are located on the main post. The training area consists of approximately 14,000 acres and serves primarily as the summer training facility for the cadets. The area surrounding the USMA is dominated by residential, agricultural, and recreational land uses (see map in Figure 12).



Figure 12. Site map of USMA (modified from ATC (2004a)).

The climate of the area is temperate with cold winters and moderately warm summers. The average annual precipitation is about 1.14 m/yr. Average seasonal snowfall is 37.5 in., which has a water equivalency of about 0.14 m. Surface water on the military reservation generally flows to the south and drains into Popolopen Creek, which discharges into the Hudson River. Shallow soil, glacial geology, and abundant rainfall produce a regionally high water table, resulting in numerous swamps, lakes, and ponds (see Figure 13).

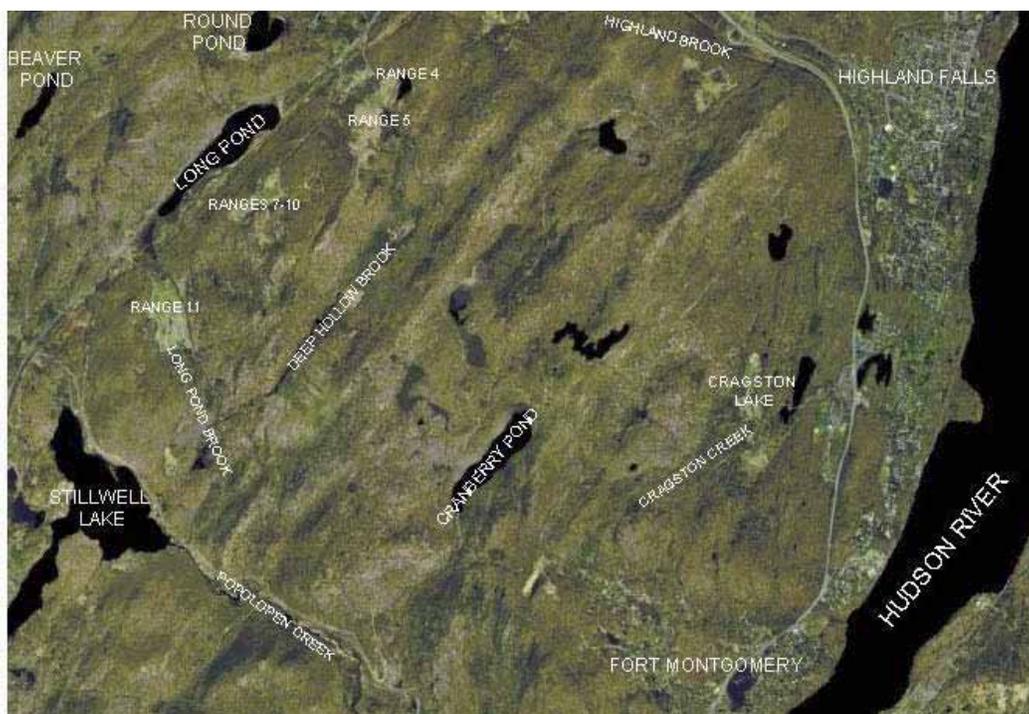


Figure 13. Satellite image of USMA range and training complex (RTC) (from ATC (2004a)).

USMA is located in the Hudson Highlands where underlying rocks consist of granite, gneiss, and diorite. Overlying the bedrock are glacially deposited till and alluvium. The unstratified till was deposited from glacial ice and consists of large boulders and lesser amounts of clay, sand, and gravel. The stratified alluvium consists primarily of sand and gravel that were deposited in glacial streams and lakes. Overlying the deposits are recent-age stream deposits that consist of clay, silt, and sand. The deposits range from approximately 0.3 to 30 m in thickness.

The dominant soil type at the installation is Hollis-Rock Outcrop, which is characterized by well-drained, sloping to moderately steep, medium-texture soils that overlie crystalline bedrock. The Hollis soils are gravel-sand loams, which have a fairly high permeability. The Udorthents soil is found on many of the training ranges at USMA. Udorthents soil consists of excavated earthy material that is generally brought from other locations and leveled. These soils are excessively drained to moderately well drained. Soil characteristics vary greatly from one area to another.

The groundwater at USMA exists as unconfined within the alluvial deposits and within a confined bedrock aquifer. Depth to groundwater varies significantly, with depths ranging from less than 1 m to 30 m. The

aquifer systems have low well yields and limited extent, so they are incapable of municipal supply.

The range and training complex (RTC) of the USMA is largely undeveloped and primarily wooded. The RTC is used each year from June through August by approximately 2500 cadets for training. The RTC is located in the Hudson-Wappinger watershed and is drained by many small tributaries, which discharge into the Hudson River. Long Pond is a prominent water body in close proximity to the ranges, as shown in Figure 14.

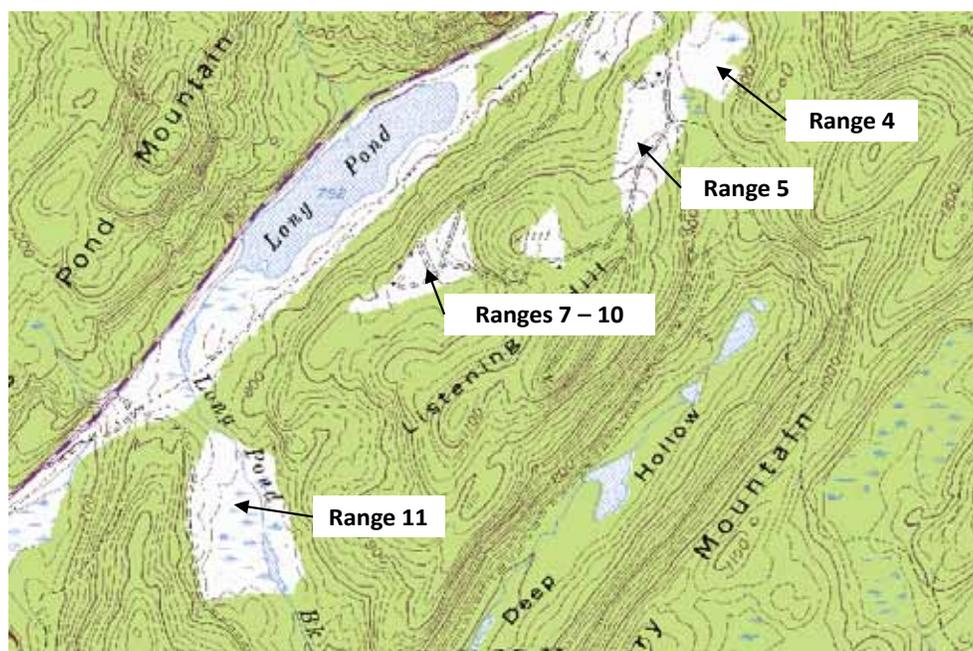


Figure 14. RTC site map, Hudson-Wappinger watershed (modified from ATC (2004a)).

## Study scope

The West Point application actually consisted of three TREECS™ applications with the following file names: WP78, WP78\_2, and WPPb. All three applications focused on soil and surface water media. Groundwater was not considered since the upper aquifer is close to the ground surface, unconfined, and has a shallow depth. Additionally, a relatively high runoff rate is suspected since the ground slope is rather steep, and there is considerable bedrock close to the surface.

The WP78 application consisted of Ranges 7 and 8 as the AOI, with RDX as the MC of interest and Long Pond as the target receiving water. The WP78\_2 application also focused on Ranges 7 and 8 as the AOI, with RDX as the MC of interest, but the target receiving water was the drainage ditch

adjacent and down-gradient of the range impact area. The WPPb application consisted of Ranges 7–10 as the AOI, with lead as the MC of interest and Long Pond as the target receiving water. The MC residue for the first two applications was a result of unexploded HE contained within the projectiles of medium-caliber munitions, such as AT-4 rockets and M203 grenade launchers (ATC 2004b). Lead (Pb), the MC residue of the third application, was a result of small arms firing with the 9-mm round being the predominant ammunition.

Each of the three applications is discussed separately in the following sections, which include additional site characteristics pertaining to the application.

## **WP78 application**

### **Site characteristics**

Web Soil Survey (WSS), which was developed for World Wide Web applications (<http://websoilsurvey.nrcs.usda.gov/app/WebSoilSurvey.aspx>) by the Natural Resources Conservation Service of the U.S. Department of Agriculture, was used to obtain additional site characterization data for the AOI of Ranges 7 and 8. The WSS image of the AOI (impact area of Ranges 7 and 8) is shown in Figure 15. A photograph of the AOI is shown in Figure 16. The AOI soils are 73% Hollis and 27% rock outcrop. The AOI area is 11 acres, with a slope that varies between 15 and 25% (with an assumed average of 20%). The approximate average depth of bedrock below the surface soil is 0.38 m. The Hollis soil is a gravelly loam of about 15% clay, 37% silt, and 48% sand for the soil (non-rock) portion, and it has a soil erodibility factor of approximately 0.2.

The primary munitions used at Ranges 7 and 8 that contain RDX are DODIC (Department of Defense Identification Code) B568 and B546, which both include 40-mm HE projectiles.

### **RDX loadings**

As of 2004, Ranges 7 and 8 had been operational for about 56 years (ATC 2004a). Firing records for these two ranges were available for 2006 and 2009 and were used to estimate annual average RDX residue loading as follows. The most dominant medium-caliber DODICs used on Ranges 7 and 8 that contained RDX were B546 and B568, both of which are 40-mm

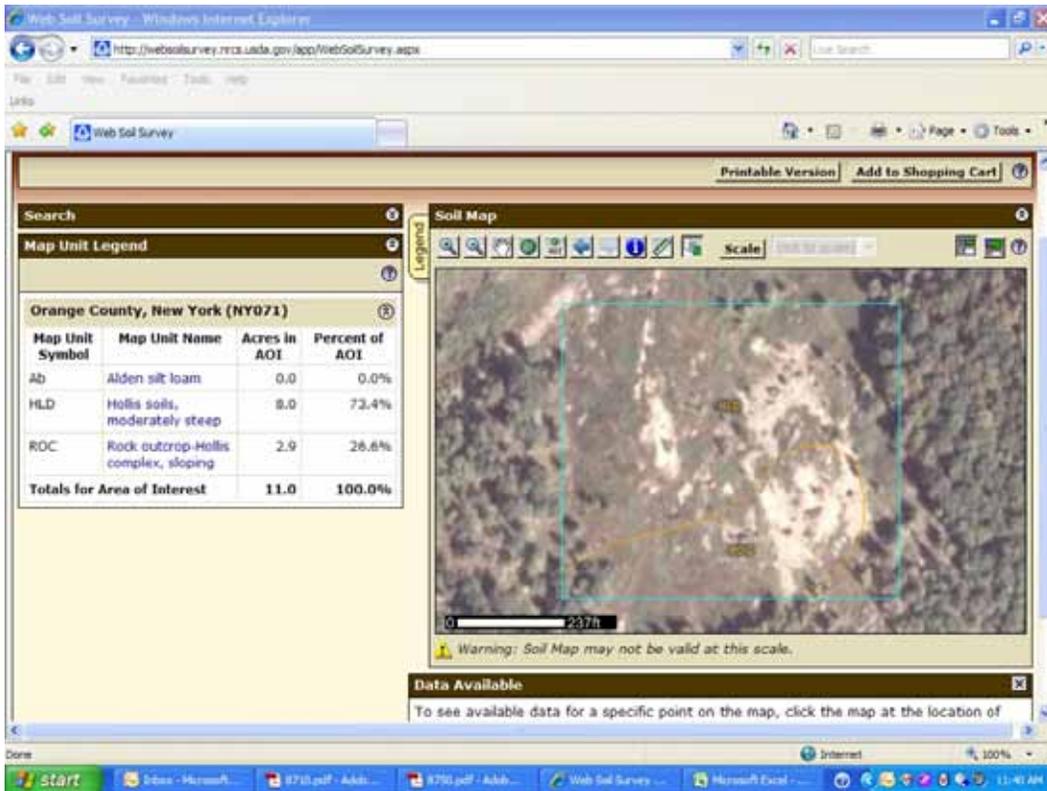


Figure 15. Screen capture of WSS interface and image with Ranges 7 and 8 AOI box prescribed.



Figure 16. Photograph of impact area of Ranges 7 and 8 (from ATC (2004b)).

munitions. The total numbers of items fired for these two munitions for 2006 and 2009 were provided in the RTC training ammunition usage report. The number of duds each year for each munitions type was also provided. The number of items fired and the number of duds for each of these two munitions and for each year are shown in Table 12. Based on the Munition Items Disposition Action System (MIDAS) database, the B546 and B568 munitions contain 44.7 and 22.2 g of RDX, respectively. As shown in one of the TREES help dialogs, which was based on information reported by Concurrent Technologies Corporation (2004), the low order rates for anti-tank rockets, grenade-launched munitions, and 40-mm munitions are all about one-third of the dud rate. This resulted in low order rates that varied between 0.2 and 0.5%, as shown in Table 12. The low order yield of RDX was assumed to be 50%. With this information, the RDX residues for 2006 and 2009 were computed, and the results for the two years were averaged to yield an average RDX residue loading rate of 279 g/yr as shown in Table 12.

Table 12. Ranges 7 and 8 munitions usage and computed RDX residue loading rates.

| Year | DODIC | Numbers fired | RDX mass per item, g | Number of duds | Fraction of low order | RDX residue loading rate, g/yr |
|------|-------|---------------|----------------------|----------------|-----------------------|--------------------------------|
| 2006 | B546  | 5,482         | 44.7                 | 60             | 0.00365               | 447                            |
|      | B568  | 474           | 22.2                 | 7              | 0.00492               | 26                             |
|      |       |               |                      |                | Total                 | 473                            |
| 2009 | B568  | 3,998         | 22.15                | 23             | 0.00192               | 85                             |
|      |       |               |                      |                |                       |                                |
|      |       |               |                      |                | Annual average        | 279                            |

The TREECS™ munitions database is based on a subset of MIDAS data; thus, it does not contain all of the munitions that are within MIDAS. As such, it is referred to as the MIDAS extraction database. Neither of the two above munitions is presently within the MIDAS extraction database. Thus, a similar 40-mm munition (B542) containing RDX was selected within the *Site Conditions/Operational Inputs* screen of TREECS™ to represent the two munitions used at these ranges. The approach was to adjust the number of B542 items fired per year on the *Operational Inputs* screen to force the MC loading rate computed by the module to match the MC residue loading rate estimated (Table 12). With 3,250 B542 rounds fired per year, a low order rate of 0.5%, a low order yield of 50%, and an assumed high order yield of 99.99997%, the TREECS™ MC residue loading module computed an RDX residue loading rate of 279 g/yr to match the value in Table 12.

## Model inputs

*Soil model.* AOI soil characteristics were based on the Hollis soil features presented in the previous section. Daily precipitation and minimum and maximum daily average air temperatures were obtained from a meteorological station at West Point. These data were used within the TREECS™ Hydro-Geo-Characteristics Toolkit (HGCT) with a Soil Conservation Service (SCS) curve number of 87 to compute local hydrology. The computed hydrology required by the TREECS™ Tier 2 soil model included: average annual precipitation = 1.14 m; average annual rainfall = 1.0 m; average annual soil erosion = 0.0023 m; average annual infiltration = 0.12 m; average annual surface runoff = 0.66 m; average annual number of rainfall events = 144; and average annual soil-water matrix temperature = 10.87 °C. Soil interflow was assumed to be negligible. The soil erosion was computed within HGCT using the universal soil loss equation (USLE).

Based on the Hollis soil features, a loam texture was selected within the HGCT (42% sand, 38% silt, and 20% clay), resulting in the following soil properties: porosity = 46.6 %; volumetric moisture content = 23.5%; dry bulk density = 1.42 g/cm<sup>3</sup>; saturated hydraulic conductivity = 32 cm/day; and soil erodibility factor = 0.2. Other inputs needed for the USLE included: a regional rainfall factor of 125; a land slope of 0.2 and LS factor of 5.9; a crop management factor of 0.1; and conservation practice factor of 1.0, which is the default value for ranges. The sediment delivery ratio correction to the USLE result was not used. The USLE within the HGCT computed an erosion rate of 0.0023 m/yr as stated previously.

The soil  $K_d$  for RDX was estimated to be 0.25 L/kg based on 45.5% sand, 37% silt, 15% clay, and 2.5% organic matter. The half life of RDX in soil for degradation was assumed to be 10 years, and the calculated volatilization rate was 18.7 m/yr. The RDX solid phase residue particle size was set to 12,000 µm. The computed RDX solubility for the soil-water matrix temperature was 29.32 mg/L. The FRAMES constituent database within TREECS™ was used to obtain values for Henry's constant, molecular weight, and solid phase density. Solid phase erosion was turned off, since it is suspected that most of the eroded particles are deposited in the local drainage ditches before reaching Long Pond. All of the soil model inputs are shown in Table 13.

Table 13. Tier 2 soil model input values for the West Point AOI.

| Input Description   | Value                  |
|---|------------------------|
| Site Characteristics  |                        |
| AOI dimension that is parallel to the groundwater flow, m   | 220                    |
| AOI dimension that is perpendicular to the groundwater flow, m                                      | 220                    |
| AOI surface area, m <sup>2</sup>  | 48,400                 |
| Active soil layer thickness, m  | 0.4                    |
| Average annual temperature of soil-water matrix, °C   | 10.87                  |
| MC mass residue loading versus time, g/yr   | 279                    |
| Initial solid phase MC concentration in soil on a soil mass basis at time 0, mg/kg                  | 0 for all constituents |
| Initial total non-solid phase MC concentration in soil on a soil mass basis at time 0, mg/kg        | 0 for all constituents |
| Soil Properties   |                        |
| Volumetric soil moisture content, fraction  | 0.235                  |
| Soil dry bulk density, g/cm <sup>3</sup>  | 1.42                   |
| Soil porosity, fraction   | .466                   |
| Hydrology   |                        |
| Average annual precipitation, m/yr  | 1.14                   |
| Average annual rainfall, m/yr   | 1.0                    |
| Average annual soil erosion rate, m/yr  | 0.0023                 |
| Average annual water infiltration rate (groundwater recharge for no interflow), m/yr                | 0.12                   |
| Average annual surface water runoff rate, m/yr  | 0.66                   |
| Fraction of annual water infiltration flow rate and mass flux that goes to soil interflow, fraction | 0                      |
| Average number of rainfall events per year  | 144                    |
| Fate/Transport Parameters   |                        |
| Soil-water constituent partition coefficient, L/kg  | RDX: 0.25              |
| Soil exchange layer thickness for rainfall ejection of pore water, m                                | 0.005                  |
| Soil detachability for rainfall ejection of pore water, kg/L  | 0.4                    |
| Decay/degradation half-life of liquid (water) phase constituent, yrs                                | 10                     |
| Decay/degradation half-life of adsorbed (particulate) phase constituent, yrs                        | 10                     |

Table 13. (continued).

| Input Description  | Value  |
|--|--|
| Initial mean diameter of solid phase constituent residue particles (assume spherical particles), $\mu\text{m}$ | RDX: 12,000  |
| Volatilization rate, m/yr  | RDX: 18.7  |
| Switch for solid phase erosion (1 is on, and 2 is off)   | 2  |
| Chemical-Specific Properties   |  |
| Aqueous solubility limit, mg/L   | RDX: 29.32 (based on average annual soil temperature of 10.87 deg C) |
| Henry's law constant, $\text{atm}\cdot\text{m}^3/\text{g}\cdot\text{mol}$                                      | RDX: 6.23E-8   |
| Molecular weight (molar mass or averaged molecular mass), g/mol  | RDX: 222.12  |
| Solid phase constituent mass density, $\text{g}/\text{cm}^3$   | RDX: 1.8   |
| Model Options  |  |
| Time length of simulation, yrs   | 60   |
| Time step, yrs   | 0.01 (does not matter if use adaptive time step)                     |
| Methods used for equation solution   | Adaptive time step   |

*Surface water model.* The RECOVERY model was selected in TREECS™ to represent Long Pond. No images were readily available to bring into the TREECS™ geographical information system (GIS), thus Google Earth™ provided an alternative method for spatial analysis. Hydrology of Long Pond was determined from Google Earth™ images as follows. The approximate watershed drainage area for Long Pond was determined by examining site images at various angles and tilt to judge terrain features, and then using the polygon ruler tool in Google Earth™ to construct and measure the watershed area. The drainage area of Long Pond was determined to be approximately 0.65 square mile. This area and the estimated annual runoff depth of 0.66 m were used to compute the average annual flow through the pond of 1.11E6 m<sup>3</sup>/yr. The water surface area was determined from Google Earth™ to be 158,500 m<sup>2</sup>, and the pond depth was assumed to be 1 m. These dimensions and flow result in a pond water residence time of 0.143 year.

The total suspended solids (TSS) value in the pond was set to 3 mg/L based on data reported by ATC (2004a) for Ranges 7 through 10 runoff water quality; thus, it was assumed that the TSS in the pond was the same as for the ranges that run off into this pond. The fraction of organic carbon of the TSS in the water column was assumed to be 0.02, which is a fairly typical

value. The depth of the mixed sediment layer was assumed to be 0.1 m with a porosity of 0.85, a specific gravity of 2.65, and a fraction of organic carbon in solids ( $f_{oc}$ ) of 0.02. The same specific gravity and  $f_{oc}$  were used for the deep sediment layers, but the porosity was reduced to 0.5 to account for consolidation. A regional average wind speed of 5 m/sec was used for volatilization. Pond sediment resuspension was assumed negligible; the TSS settling rate was set to 36 m/yr; and the sediment burial rate was computed to be 2.72E-4 m/yr.

Initial RDX concentrations in the pond were set to zero. Chemical-specific properties of RDX used in the RECOVERY model were provided by the FRAMES constituent database within TREECS™. The model user-interface-computed values for  $K_d$  and volatilization rate were 0.086 L/kg and 0.43 yr<sup>-1</sup>, respectively. No RDX degradation for water and sediment was assumed. The model simulation period was set to 60 years. The RECOVERY model inputs are summarized in Table 14.

**Table 14. Tier 2 RECOVERY surface water model input values for Long Pond near West Point ranges.**

| Input Description  | Value                                    |
|--|--|
| Inputs Passed from Soil Model or Plus-SG Operator                        |  |
| WFF (surface water) water flux, m <sup>3</sup> /yr                       | 31,944<br>(this value is for AOI runoff) |
| WFF (surface water) mass flux, g/yr                                      | Time-varying                             |
| Surface Water Morphometry and Hydrology                                  |  |
| Total suspended solids concentration in the water column, mg/L           | 3  |
| Weight fraction carbon in solids in water column, fraction               | 0.02                                     |
| Long-term average water surface area, m <sup>2</sup>                     | 158,500                                  |
| Long-term average of surface water mean depth, m                         | 1.0                                      |
| Average annual water flow-through rate, m <sup>3</sup> /yr               | 1.11E6                                   |
| Surface water residence time (computed), yr                              | 0.143                                    |
| Mixed Sediment Layer   |  |
| Contaminated sediment depth or total sediment bed depth to be modeled, m | 0.5                                      |
| Depth of mixed sediment layer, m   | 0.1                                      |
| Mixed sediment layer surface area, m <sup>2</sup>                        | 158,000                                  |
| Mixed sediment layer porosity, fraction                                  | 0.85                                     |
| Mixed sediment particle density or specific gravity, g/cm <sup>3</sup>   | 2.65                                     |

Table 14. (continued).

| Input Description  | Value                  |
|--|------------------------|
| Mixed sediment layer weight fraction carbon in solids, fraction                            | 0.02                   |
| Deep Sediment Layers   |                        |
| Deep sediment porosity, fraction   | 0.5                    |
| Deep sediment particle density or specific gravity, g/cm <sup>3</sup>                      | 2.65                   |
| Deep sediment layer weight fraction carbon in solids, fraction                             | 0.02                   |
| Mean wind speed, m/sec   | 5                      |
| Enhanced diffusion between mixed sediment layer and deep sediment, cm <sup>2</sup> /sec    | 0                      |
| Enhanced mixing depth between mixed sediment layer and deep sediment, cm                   | 0                      |
| Suspended solids settling velocity, m/yr   | 36                     |
| Deep sediment burial velocity (computed), m/yr   | 2.72E-4                |
| Mixed layer sediment resuspension velocity, m/yr   | 1.0E-20                |
| Constituent Properties   |                        |
| Initial contaminant concentration of constituent in water, µg/L                            | 0                      |
| Additional constant external loading rate of constituent, kg/yr                            | 0                      |
| Initial contaminant concentration in mixed sediment, mg/kg                                 | 0                      |
| Initial contaminant concentration in deep sediment, mg/kg                                  | 0                      |
| Molecular diffusivity, cm <sup>2</sup> /sec  | RDX: 5.9E-6            |
| Henry's Law Constant, atm-m <sup>3</sup> /g-mole   | RDX: 6.23E-8           |
| Molecular weight, g-mole   | RDX: 222.12            |
| Octanol-water partition coefficient, (mg/m <sup>3</sup> octanol)/(mg/m <sup>3</sup> water) | RDX: 7.0               |
| Decay coefficient for dissolved contaminant in water, 1/yr                                 | 0 for all constituents |
| Decay coefficient for dissolved contaminant in mixed layer, 1/yr                           | 0 for all constituents |
| Decay coefficient for dissolved contaminant in deep sediment, 1/yr                         | 0 for all constituents |
| Decay coefficient for particulate contaminant in water, 1/yr                               | 0 for all constituents |
| Decay coefficient for particulate contaminant in mixed layer, 1/yr                         | 0 for all constituents |

Table 14. (concluded).

| Input Description   | Value                  |
|---|------------------------|
| Decay coefficient for particulate contaminant in deep sediment, 1/yr                  | 0 for all constituents |
| Model Control Parameters  |                        |
| Total period of simulation, yrs   | 60                     |
| Number of time steps between print intervals for output, dimensionless                | 20                     |
| Number of time steps between print intervals for sediment layer output, dimensionless | 20                     |
| Number of sediment layers to print in output, dimensionless                           | 20                     |

## Results

RDX concentrations in Long Pond were measured in 2003, 55 years after Ranges 7 and 8 became operational. The measured concentrations in the water column were fairly consistent over the pond, varying between 0.019 and 0.026  $\mu\text{g}/\text{L}$  for all samples except for one located near the influent ditch from the ranges, which measured 0.31  $\mu\text{g}/\text{L}$  (ATC 2004b). The average concentration of the water column RDX concentrations, excluding the one sample near the influent ditch, is 0.023  $\mu\text{g}/\text{L}$  (or ppb). All of the measured sediment concentrations of RDX were below the detection limit (ATC 2004b).

The computed water column total concentration of RDX in Long Pond after 55 years of range use was 0.035  $\mu\text{g}/\text{L}$ , which agrees well with the measured average concentration of 0.023  $\mu\text{g}/\text{L}$ . The computed sediment total concentration of RDX in Long Pond after 55 years was 0.077  $\mu\text{g}/\text{kg}$ , which is below any perceivable detection limit since detection limits for RDX in sediment are about 1  $\mu\text{g}/\text{kg}$  at best.<sup>1</sup> Thus, the predicted water and sediment concentrations for RDX in Long Pond are in good agreement with the observed data.

## WP78\_2 application

The site conditions for this application are the same as those discussed above for the WP78 application. The only difference in this application from the previous one is that the target surface water is the ditch down-

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<sup>1</sup> Personal communication: 2011. Dr. Anthony Bednar, Chemistry Branch, Environmental Laboratory, U.S. Army Research and Development Center, Vicksburg, MS.

slope of the ranges that collects most of the runoff. As a result, the site characteristics and input descriptions below are restricted to describing the receiving ditch.

### **Site characteristics**

The receiving ditch was estimated with Google Earth™ to be roughly 300 m long. Its width and depth were assumed to be 1 m and 0.1 m, respectively. The procedures described previously for estimating the drainage area via Google Earth™ were used to estimate the drainage area feeding the ditch, which is 0.05 square mile. With this area and a runoff depth of 0.66 m/yr, the annual average flow through the ditch is 85,500 m<sup>3</sup>/yr.

### **Model inputs**

The soil model inputs were the same as those described previously for the WP78 application with one exception. The solid phase particle erosion was turned on since it is suspected that this process occurs, and the ditch traps this material.

The RECOVERY model was used to represent the receiving ditch. Most of the inputs were similar to those described for Long Pond with the primary exception being the size of the water body and the flow through the water body. The water surface area was changed to 300 m<sup>2</sup>, the depth was changed to 0.1 m, and the flow-through rate was changed to 85,500 m<sup>3</sup>/yr. This resulted in a water residence time of 1.17E-5 years, or about 6 minutes. A higher TSS settling rate of 360 m/yr was used since it is suspected that much of the sediment erosion is coarser material that settles at a faster rate within the ditch. All of the other inputs were the same as before.

### **Results**

The water total concentrations of RDX sampled in 2003 within the ditch just below Ranges 7 and 8 averaged 0.77 µg/L (ATC 2004b). The model-computed surface water total concentration of RDX for the ditch reached 1.13 µg/L after 55 years of simulation. This is considered an extremely good agreement considering the uncertainty in the inputs. The measured sediment total concentrations of RDX in the ditch in 2003 averaged about 0.12 mg/kg (ATC 2004b). The model-computed sediment total concentration of RDX after 55 years was 0.0025 mg/kg, which is almost two orders of magnitude lower than measured. It is noted that the average measured

sediment concentration of RDX is based on two values of 0.055 mg/kg and 0.2 mg/kg measured at station SED-R7-10-009. All of the other sediment measurements in the ditch upstream and downstream of this station were below the detection limit.

It is hypothesized that particulate RDX was eroded into the ditch, deposited, and accumulated at or near this station. The entire drainage ditch was treated as a single fully mixed cell in the model, whereas the observed data indicate that the RDX in sediment was concentrated in one relatively short reach of the ditch. It is likely that solid phase RDX particles were eroded and deposited at this location and did not migrate any farther. The simplistic representation of the entire ditch by a single model cell precluded the model depicting this localized concentration.

## **WPPB application**

The site conditions for this application are the same as those discussed above for the WP78 application. The primary difference in this application from the previous ones is that the MC of interest is lead, stemming from firing of small arms (9-mm rounds). The target surface water is Long Pond. The site characteristics are the same as those described for the WP78 application. The only differences in model inputs were associated with the loading rate and the chemical-specific properties and transport parameters for lead. This application could have been included as part of the WP78 application by simply adding an additional MC, appropriate range usage information, and model inputs for the additional MC.

### **Model inputs**

Lead in the study area predominantly results from firing 9-mm rounds. Approximately 109,000 rounds are fired each year on Ranges 7 – 9, which results in about 1513 lb (696,902 g) of lead deposited on the ranges each year (ATC 2004a). For the TREECS™ application, the DODIC A363 was selected to represent the 9-mm rounds, and the number of rounds fired each year was adjusted to 107,500 so that the total lead residue reached 696,645 g per year, which closely matches the amount reported by ATC (2004a).

The only changes to the soil model inputs shown in Table 13 were that the properties and fate/transport parameters had to be changed to those suitable for lead. The soil-water  $K_d$  was set to 597 L/kg. The degradation

half lives for lead in soil were set to a large number (1.0E20 yrs) to represent no degradation. The solid phase particle diameter was set to 500  $\mu\text{m}$ , which is representative of lead particles from bullets (Dortch et al. 2011b). Solid phase erosion was turned off since the target water body was Long Pond, and it is suspected that most lead particles settle out before reaching the pond. Volatilization for lead was set to zero. The water solubility of lead was set to 3 mg/L, which is approximately the value determined for the Fort A.P. Hill proof-of-concept application (Dortch et al. 2011b). Lead molecular weight of 207 g/mol and solid phase density of 11.35 g/cm<sup>3</sup> were provided by the TREECS™ FRAMES constituent database.

The only changes to the RECOVERY model inputs shown in Table 14 were that the properties and fate/transport parameters had to be changed to those suitable for lead. The molecular diffusivity of lead in water was set to 9.45E-6 cm<sup>2</sup>/sec. The molecular weight of 207 was provided by the constituent database. The  $K_d$  values for suspended sediment and benthic sediment were set to 500,000 and 40,000 L/kg, respectively, based on USEPA guidance (Allison and Allison 2005). All degradation rates were set to zero.

## Results

Only one sample was collected and analyzed for lead in Long Pond, sample R7-10-001 (ATC 2004a), which was collected during 2003. The measurement for lead concentration in water was below the detection limit of 1.0 mg/L, and the measured lead concentration (total) in sediment was 30.3 mg/kg. The model-computed concentrations (total) of lead in water and sediment for Long Pond after 55 years were 3  $\mu\text{g/L}$  and 30.1 mg/kg, respectively. The computed value for the water column is in agreement with the observed value being below detection. The computed value for sediment agrees extremely well with the observed value. However, variations in uncertain inputs of lead solubility, solid phase particle size, and lead  $K_d$  values can cause substantial differences in computed sediment concentrations as indicated by the sensitivity results discussed below.

Each sensitivity test was conducted using the inputs described above, but with one input change for each sensitivity run as described. All results are for sediment total concentration after 55 years of simulation. Increasing the water solubility of lead in soil from 3 to 6 mg/L resulted in increasing the Long Pond sediment concentration of lead from 30.1 to 56.9 mg/kg. Increasing the lead  $K_d$  value for soil from 597 to 5,000 L/kg resulted in a

sediment concentration of 28.4 mg/kg rather than 30.1 mg/kg. Increasing the solid phase lead particle diameter from 500 to 5,000  $\mu\text{m}$  resulted in decreasing the sediment concentration of lead from 30.1 to 3.1 mg/kg. Reducing the suspended and benthic sediment  $K_d$  for lead from 500,000 and 40,000 L/kg to 4,000 L/kg for both resulted in decreasing the sediment concentration of lead from 30.1 to 8.3 mg/kg. If only the suspended sediment  $K_d$  for lead is reduced from 500,000 to 40,000 L/kg, and 40,000 L/kg is used for benthic sediment, then the computed sediment concentration of lead is 17.3 rather than 30.1 mg/kg. Computed sediment concentrations are fairly sensitive to all of the above inputs except for the soil  $K_d$  value. It is interesting how sensitive results are to the suspended sediment  $K_d$  for lead.

## Conclusions

Good agreement was obtained for predicted versus observed water concentrations of RDX in Long Pond after 55 years of range use. The computed concentration was 0.035  $\mu\text{g/L}$  compared to 0.023  $\mu\text{g/L}$  observed. Both computed and observed sediment concentrations of RDX were below detection levels.

There was also good agreement for predicted versus observed water concentrations of RDX in the drainage ditch below Ranges 7 and 8, where the observed values averaged 0.77  $\mu\text{g/L}$ , and the predicted value was 1.13  $\mu\text{g/L}$  after 55 years of range use. The agreement between predicted and observed sediment concentrations of RDX in the ditch were not as good, where the observed concentration averaged about 0.12 mg/kg just below the ranges and the predicted concentration was 0.0025 mg/kg. However, all of the other sediment measurements in the ditch upstream and downstream of this sampling station were below the detection limit, indicating heterogeneous concentrations that the model could not characterize.

Excellent agreement was obtained for predicted and observed lead concentrations in Long Pond. The observed concentration of lead in Long Pond sediment was 30.3 mg/kg compared with the predicted value of 30.1 mg/kg. The computed value for the water column was in agreement with the observed, with both being below detection. Model sensitivity testing indicated that lead solubility, particle size, and distribution coefficients for sediment-water sorption are particularly sensitive for affecting computed sediment concentrations.

## 5 Fort Jackson Application

### Site description

This site description information was obtained from the report by ATC (2005). Fort Jackson, located in central South Carolina, occupies approximately 52,000 acres east of Columbia, South Carolina. This area is located in the upper Atlantic Coastal Plain geologic province of South Carolina and is characterized as rolling, sandy hills of low elevation. The installation is predominantly covered with pine forests, except in the low-lying areas and floodplains where more deciduous trees and marsh vegetation are present.

Fort Jackson is the U.S. Army's premier basic training facility where approximately 40,000 soldiers complete basic training annually. Fort Jackson was established in 1917 as an infantry training center. After World War I, Fort Jackson was demobilized as a full-time training site, and the post was state-controlled as a training area for troops of the South Carolina National Guard. The installation was returned to Federal control in 1940 for U.S. Army infantry training for World War II (WWII). During WWII, the fort was expanded to approximately its present size. The Fort has been an active U.S. Army Basic Training Center since 1973.

There is a training complex within the Gills Creek watershed that consists of 14 active small arms firing ranges. Ranges 1 through 13 are located consecutively along Train Fire Road, and Range 20 is located approximately 1 mile from Ranges 1–13, but is within the same watershed boundary. These ranges are used primarily for soldier basic training that involves M16A2 rifles and M855 5.56-mm ball rounds. Minor amounts of training are performed on Range 6 with 9-mm pistols and shotguns. Comprehensive firing data were not available for range use prior to the year 2000. The soils of the SAFRs are loamy sand with approximately 83% sand, 11% silt, and 6% clay.

Groundwater is generally plentiful at Fort Jackson. The Tuscaloosa Formation, of Upper Cretaceous age, underlies Fort Jackson and is the primary source of groundwater in the area. The Tuscaloosa Formation is at the surface over most of Fort Jackson. The formation consists of fine to coarse sand and clay, causing groundwater to occur under both unconfined and confined conditions. Groundwater is unconfined in the upper part of

the zone of saturation. At a depth of about 99–251 ft, permeable sand zones are frequently overlain by less permeable clay zones, and groundwater exists under confined conditions. The regional aquifer functions as an unconfined, surficial aquifer before dipping below other aquifers and confining units moving east toward the coast. Shallow groundwater is assumed to discharge as base flow into the network of small creeks on the installation.

Primary surface water features in the study area include Gills, Mack, Rowell, and Bynum Creeks. These creeks can potentially be affected by stormwater runoff, and are likely the discharge point for shallow groundwater base flow from the small arms range area. Gills Creek is particularly important in that this creek flows off the installation. Under a USEPA national watershed analysis program, Gills Creek has been monitored at two locations several miles downstream of Fort Jackson. Metals are not listed as a concern based on the results from this sampling.

Considerable erosion from the small arms ranges has been observed in past years. As a result, Fort Jackson entered into a Memorandum of Agreement (MOA) with the Natural Resources Conservation Service (NRCS) in 1994 for support in rehabilitating and controlling soil erosion throughout the training area. Under the MOA, Fort Jackson and the NRCS have developed and are implementing range land rehabilitation, range land management, and stormwater management projects to control soil erosion on and around the small arms ranges.

Runoff from Ranges 1–3, part of Range 4, and all of Range 20 drains into the Mach Creek sub-watershed. Runoff from part of Range 4 and from Ranges 5–9 drains into the Rowell Creek sub-watershed. Runoff from Ranges 10–13 drains into the Bynum Creek sub-watershed. All three sub-watershed creeks discharge into Gills Creek and are part of the Gills Creek watershed, as shown in Figure 17. Much of Gills Creek is flat and marshy. Gills Creek discharges into Boyden Arbor Pond prior to leaving the installation. This low energy area should reduce sediment loads by settling. Thus, Gills Creek and Boyden Arbor Pond are likely acting as filters for suspended sediment loads that may be washing off the small arms range area.

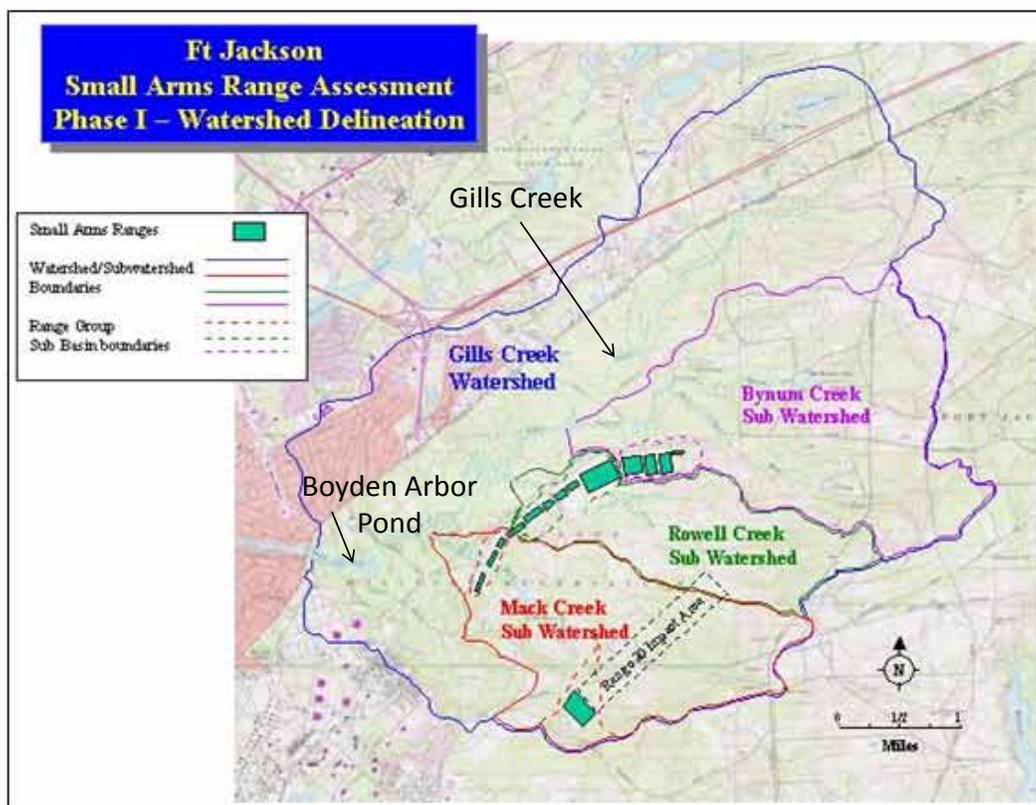


Figure 17. Small arms ranges and their sub-watersheds within Gills Creek watershed (modified from ATC (2005)).

## Scope

The Fort Jackson application focused on the fate of heavy metals residue on the SAFRs, which consisted of Ranges 1–13 and 20. All of these ranges drain into Gills Creek, which flows into Boyden Arbor Pond and tends to act as a filter for MC reaching Gills Creek. Thus, the target receiving water was Boyden Arbor Pond. Groundwater was not considered in this application since the MCs of interest were metals, which do not migrate easily into groundwater due to high partitioning to soils. The AOI consisted of the 14 SAFRs. The MCs of interest included lead, antimony, copper, and zinc, all of which are found in 5.56-mm rounds.

## Model inputs

*MC loading.* The primary munitions used on the SAFRs are the 5.56-mm ball M855 rounds (ATC 2005). DODIC A059 was selected within the TREECS™ Operational Inputs screen to represent the M855 round. This round contains 0.02076 g of antimony (Sb), 1.30106 g of copper (Cu), 2.0555 g of lead (Pb), and 0.18915 g of zinc (Zn). Approximately

9,300,000 5.56-mm rounds are fired per year at these 14 ranges. With this firing rate and the known quantity of metals in each round, the TREECS™ loading module computed the following MC residue loading rates: Pb = 19,116,150 g/yr; Sb = 193,068 g/yr; Cu = 12,099,858 g/yr; and Zn = 1,759,095 g/yr. It was assumed that the most substantial loadings of metals started around 1940 and continued until today. However, a comprehensive data collection effort, including metals sampling/analysis in Boyden Arbor Pond, was conducted in 2001 (Bricka 2002); thus, MC loadings and model runs were set for 60 years.

*Soil model.* The AOI was delineated with the aid of WSS and is shown in Figure 18. The AOI dimensions are approximately 3200 m long by 250 m wide on average with a surface area of 200 acres (809,371 m<sup>2</sup>) as computed by WSS. WSS also provided soil organic matter content of 1.3% for the AOI.

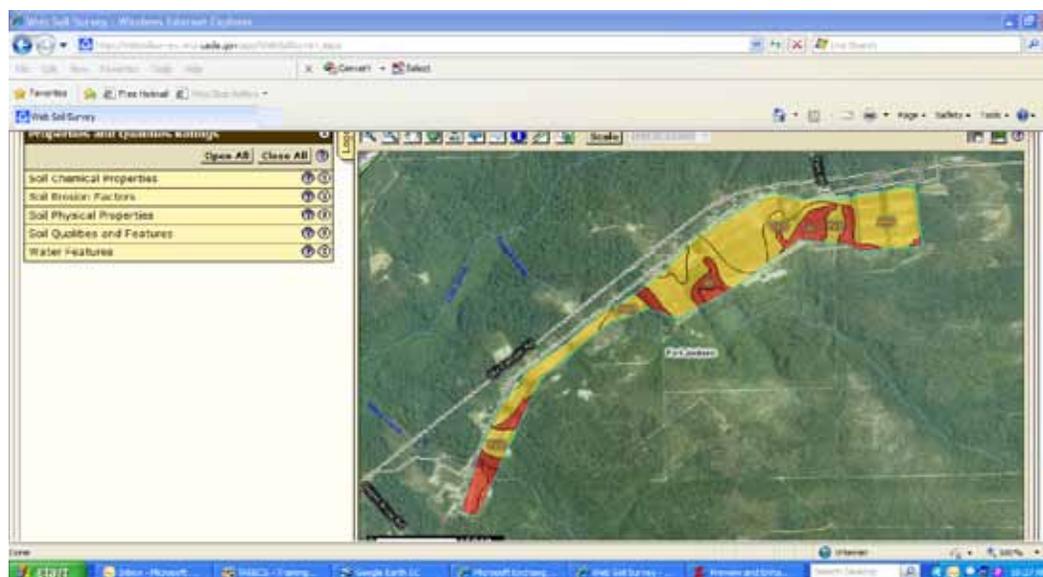


Figure 18. Fort Jackson SAFRs AOI delineated within WSS (colors represent different soil types).

For loamy sand, the HGCT provides a porosity of 43.7%, a dry bulk density of 1.49, a volumetric moisture content of 12%, and a saturated hydraulic conductivity of 164 cm/day. From WSS, the soil erodibility factor and the average slope of the ranges were estimated to be 0.15 and 0.07, respectively. The regional rainfall factor is about 250. The LS factor is 1.64, and the crop management factor was estimated to be about 0.45. The conservation practice factor is set to 1 by default for ranges. The area of the three sub-watersheds that the SAFRs reside in is approximately 9.7 square miles. With these inputs, the USLE within HGCT computed a soil erosion rate of 6.52E-4 m/yr.

Daily precipitation and maximum and minimum air temperatures were obtained from a meteorological station in Columbia, SC. The two air temperatures were averaged to get daily mean. WSS showed the hydrologic soil group to be between B and C. The SCS curve number was estimated to be 86. These data were used within HGCT to compute hydrology for the site and the annual average air temperature of 19.5 °C.

Shallow-water well sampling (approximately 4 to 14 ft below ground surface) for lead on Range 2 revealed that considerable lead leaches into shallow groundwater in the sandy soils (ATC 2005). However, two of the three shallow groundwater wells showed low lead concentrations in shallow groundwater due to interstitial layers of clay in the subsurface soils. Clay tends to adsorb metals, thus limiting their migration. It is hypothesized by ATC (2005) that much of the shallow groundwater discharges into the local creeks. The unknown issue is whether or not the shallow water discharge to surface water is carrying metals or not. If the discharge is transporting metals, then interflow in the soil model should be activated. If not, then it should not be activated. The level of interflow transport of metals is dependent on the amount of clay along the interflow path. Therefore, interflow was varied for sensitivity.

Some of the more important modeling inputs for metals are  $K_d$  for soil, sediment, and TSS. USEPA recommended mean  $K_d$  values (Allison and Allison 2005) for the four MC metals of interest are shown in Table 15, including the  $K_d$  for partitioning of the metals to dissolved organic carbon (DOC). The TREECS™ models do not explicitly account for sorption to and transport with DOC. However,  $K_d$  can be adjusted ( $K'_d$ ) to account for the effects of DOC, which is referred to as DOC-facilitated transport. The adjusted partitioning distribution coefficient is computed as follows

$$K'_d = \frac{K_d}{1 + 10^{-6} KDOC_d DOC} \quad (1)$$

where  $DOC$  is in units of mg/L,  $10^{-6}$  is the conversion from mg to kg, and  $KDOC_d$  (L/kg) is the distribution coefficient for partition to DOC. After converting from log units, Equation 1 was used to modify the  $K_d$  values in Table 15 using an assumed but reasonable DOC value of 5 mg/L, resulting in the adjusted  $K_d$  values shown in Table 16.

Table 15. Log of partitioning distribution coefficients for metals obtained from Allison and Allison (2005).

| Metal    | Soil log $K_d$ (L/kg) | Sediment log $K_d$ (L/kg) | TSS log $K_d$ (L/kg) | DOC log $K_d$ (L/kg) |
|----------|-----------------------|---------------------------|----------------------|----------------------|
| Copper   | 2.5                   | 3.5                       | 4.7                  | 5.4                  |
| Lead     | 3.7                   | 4.6                       | 5.7                  | 4.9                  |
| Antimony | 2.3                   | 3.6                       | 4.8                  | 2                    |
| Zinc     | 2.7                   | 4.1                       | 5                    | 5.1                  |

Table 16. Partitioning distribution coefficients for metals following DOC adjustment.

| Metal    | Soil $K_d$ (L/kg) | Sediment $K_d$ (L/kg) | TSS $K_d$ (L/kg) |
|----------|-------------------|-----------------------|------------------|
| Copper   | 140               | 1,402                 | 22,216           |
| Lead     | 3,587             | 28,494                | 358,718          |
| Antimony | 199               | 3,979                 | 63,064           |
| Zinc     | 308               | 7,726                 | 61,370           |

The TREECS™ Tier 2 soil model has a tool for estimating MC  $K_d$  values for soil. For metals, this tool requires input of soil texture (percents of sand, silt, and clay), percent of soil organic matter, percent of soil iron and aluminum, and soil pH. Since the tool-estimated metal  $K_d$  is based on ambient conditions, this tool was used to estimate the metal  $K_d$  values for soil rather than using the values in Table 16. For loamy sand, the soil texture is 83% sand, 11% silt, and 6% clay. The organic matter content of the range soils was set to 1.3%; thus, the sand content was reduced to 81.7%, so the total contents summed to 100% as required by the estimation tool. The amounts of iron and aluminum were not known, so those inputs were set to zero. The soil pH was set to 5.1 based on data reported by ATC (2005). These inputs resulted in estimated  $K_d$  values of 234, 2, and 41.9 L/kg for Pb, Sb, and Cu, respectively. These values were used for the soil model. The estimator did not contain data for Zn, so the  $K_d$  value for Zn was set to 84, which is double the value estimated for Cu. The doubling of the value for Zn is based on the fact that the Zn  $K_d$  is about double the one for Cu in Table 16.

Metals do not degrade, so the half-life values were set to very large numbers (1.0E20 yrs). The solid phase residue initial particle diameter was set to 500  $\mu\text{m}$  for all four metals based on guidance for lead. Solid

phase particle erosion was turned on for all four metals, since it is believed that much of the eroded material is transported to Gills Creek and trapped in the creek or Boyden Arbor Pond. Metals do not volatilize, so those rates were set to zero as well as the values for Henry's constant. The spherical particle shape was assumed for dissolution.

Estimating water solubility for the metals is most difficult, and computed fates are sensitive to this input. The Pb and Cu solubility were set to 2.24 and 0.5 mg/L, respectively, based upon previous analysis for Fort A.P. Hill (Dortch et al. 2011b). Some investigation was required to establish solubility for Sb and Zn. Antimony trioxide ( $\text{Sb}_2\text{O}_3$ ) is the most stable and oxidized form of weathered Sb. The solubility of  $\text{Sb}_2\text{O}_3$  is 0.017 mg/L (World Health Organization (WHO) 2003). One of the more common forms of zinc that has weathered in the presence of water is zinc hydroxide. The solubility of zinc associated with zinc hydroxide in water at room temperature and pH of 7 is about 100 mg/L (Dyer et al. 1998). The solubility of zinc is greater at lower pH, but it is suspected that the presence of lead in the soil will result in pH near 7.

Molecular weight and solid phase density of the metals were provided by the TREECS™ Army Range Constituent Database, which was selected for the application. The soil model inputs for the Fort Jackson application are summarized in Table 17.

Table 17. Tier 2 soil model input values for the Fort Jackson AOI.

| Input Description  | Value  |
|--|--|
| Site Characteristics   |  |
| AOI dimension that is parallel to the groundwater flow, m                          | 3,200  |
| AOI dimension that is perpendicular to the groundwater flow, m                     | 250  |
| AOI surface area, m <sup>2</sup>   | 809,371  |
| Active soil layer thickness, m   | 0.4  |
| Average annual temperature of soil-water matrix, °C                                | 19.5   |
| MC mass residue loading versus time, g/yr, for 60 yrs                              | Lead: 19,116,150<br>Antimony: 193,068<br>Copper: 12,099,858<br>Zinc: 1,759,095 |
| Initial solid phase MC concentration in soil on a soil mass basis at time 0, mg/kg | 0 for all constituents   |

Table 17. (continued).

| Input Description   | Value  |
|---|--|
| Initial total non-solid phase MC concentration in soil on a soil mass basis at time 0, mg/kg        | 0 for all constituents                                   |
| Soil Properties   |  |
| Volumetric soil moisture content, fraction  | 0.12   |
| Soil dry bulk density, g/cm <sup>3</sup>  | 1.49   |
| Soil porosity, fraction   | .437   |
| Hydrology   |  |
| Average annual precipitation, m/yr  | 1.21   |
| Average annual rainfall, m/yr   | 1.20   |
| Average annual soil erosion rate, m/yr  | 6.52E-4  |
| Average annual water infiltration rate (groundwater recharge for no interflow), m/yr                | 0.13   |
| Average annual surface water runoff rate, m/yr  | 0.57   |
| Fraction of annual water infiltration flow rate and mass flux that goes to soil interflow, fraction | 0  |
| Average number of rainfall events per year, yr <sup>-1</sup>  | 107  |
| Fate/Transport Parameters   |  |
| Soil-water constituent partition coefficient, L/kg  | Lead: 234<br>Antimony: 2<br>Copper: 41.9<br>Zinc: 84     |
| Soil exchange layer thickness for rainfall ejection of pore water, m                                | 0.005  |
| Soil detachability for rainfall ejection of pore water, kg/L  | 0.4  |
| Decay/degradation half-life of liquid (water) phase constituent, yrs                                | 1.0E20 for all MC  |
| Decay/degradation half-life of adsorbed (particulate) phase constituent, yrs                        | 1.0E20 for all MC  |
| Initial mean diameter of solid phase constituent residue particles (assume spherical particles), μm | 500 for all MC   |
| Volatilization rate, m/yr   | 0 for all MC   |
| Switch for solid phase erosion (1 is on, and 2 is off)  | 1 for all MC   |
| Chemical-Specific Properties  |  |
| Aqueous solubility limit, mg/L  | Lead: 2.24<br>Antimony: 0.02<br>Copper: 0.5<br>Zinc: 100 |
| Henry's law constant, atm-m <sup>3</sup> /g-mol   | 0 for all MC   |

Table 17. (concluded).

| Input Description   | Value  |
|---|--|
| Molecular weight (molar mass or averaged molecular mass), g/mol | Lead: 207.19<br>Antimony: 121.75<br>Copper: 63.55<br>Zinc: 65.39 |
| Solid phase constituent mass density, g/cm <sup>3</sup>         | Lead: 11.34<br>Antimony: 6.68<br>Copper: 8.90<br>Zinc: 7.14      |
| Model Options   |  |
| Time length of simulation, yrs                                  | 60   |
| Time step, yrs  | 0.01 (does not matter if use adaptive time step)                 |
| Methods used for equation solution                              | Adaptive time step   |

*Surface water model:* Characteristics of Boyden Arbor Pond were used as inputs for the RECOVERY surface water and sediment model. The observed data indicate that the upstream portion of the pond may trap most of the entering metals, so only the upper portion was modeled. The upper and lower pond appear to be separated by a narrow channel. The surface area of the upper pond was estimated to be 25,000 m<sup>2</sup> using Google Earth™. The mean depth was assumed to be 1.0 m. The total average annual flow-through rate of 11,810,346 m<sup>3</sup>/yr was estimated from the product of the average annual runoff of 0.24 m/yr and the area of the Gills Creek watershed of 19 square miles (49,209,774 m<sup>2</sup>) (ATC 2005). The runoff was estimated with the HGCT using a SCS curve number of 62 for forested land in good condition with a hydrologic soil group between B and C. The residence time of the upper pond for this flow is 0.0021 year (or about three-fourths of a day). The measured value of pond TSS was 28 mg/L (Bricka 2002).

Properties of the mixed and deep sediments and settling/resuspension rates were fixed at typical values used in other applications as shown in Table 18. All initial concentrations and external loadings (other than loadings from the ranges) were set to zero. Database values for molecular diffusivities in water were used. Sediment–water partition distribution coefficients were set to the values shown in Table 16 for TSS and benthic sediment as adjusted for  $K_{oc}$ . All degradation rates were set to zero as well as values for Henry’s constant. All inputs for the RECOVERY model are summarized in Table 18.

**Table 18. Tier 2 RECOVERY surface water model input values for Boyden Arbor Pond near Fort Jackson ranges.**

| Input Description   | Value                                     |
|---|---|
| Inputs Passed from Soil Model or Plus-SG Operator                                       |   |
| WFF (surface water) water flux, m <sup>3</sup> /yr                                      | 461,343<br>(this value is for AOI runoff) |
| WFF (surface water) mass flux, g/yr   | Time-varying                              |
| Surface Water Morphometry and Hydrology   |   |
| Total suspended solids concentration in the water column, mg/L                          | 28  |
| Weight fraction carbon in solids in water column, fraction                              | 0.02                                      |
| Long-term average water surface area, m <sup>2</sup>                                    | 25,000                                    |
| Long-term average of surface water mean depth, m  | 1.0                                       |
| Average annual water flow-through rate, m <sup>3</sup> /yr                              | 11,810,346                                |
| Surface water residence time (computed), yr   | 0.0021                                    |
| Mixed Sediment Layer  |   |
| Contaminated sediment depth or total sediment bed depth to be modeled, m                | 0.5                                       |
| Depth of mixed sediment layer, m  | 0.1                                       |
| Mixed sediment layer surface area, m <sup>2</sup>                                       | 25,000                                    |
| Mixed sediment layer porosity, fraction   | 0.85                                      |
| Mixed sediment particle density or specific gravity, g/cm <sup>3</sup>                  | 2.65                                      |
| Mixed sediment layer weight fraction carbon in solids, fraction                         | 0.02                                      |
| Deep Sediment Layers  |   |
| Deep sediment porosity, fraction  | 0.5                                       |
| Deep sediment particle density or specific gravity, g/cm <sup>3</sup>                   | 2.65                                      |
| Deep sediment layer weight fraction carbon in solids, fraction                          | 0.02                                      |
| Mean wind speed, m/sec  | 5   |
| Enhanced diffusion between mixed sediment layer and deep sediment, cm <sup>2</sup> /sec | 0   |
| Enhanced mixing depth between mixed sediment layer and deep sediment, cm                | 0   |
| Suspended solids settling velocity, m/yr  | 36  |
| Deep sediment burial velocity (computed), m/yr  | 2.54E-3                                   |

Table 18. (continued).

| Input Description  | Value  |
|--|--|
| Mixed layer sediment resuspension velocity, m/yr   | 1.0E-20  |
| Constituent Properties   |  |
| Initial contaminant concentration of constituent in water, $\mu\text{g/L}$   | 0 for all MC   |
| Additional constant external loading rate of constituent, kg/yr  | 0 for all MC   |
| Initial contaminant concentration in mixed sediment, mg/kg   | 0 for all MC   |
| Initial contaminant concentration in deep sediment, mg/kg  | 0 for all MC   |
| Molecular diffusivity, $\text{cm}^2/\text{sec}$  | Lead: 9.45E-6<br>Antimony: 8.25E-6<br>Copper: 7.33E-6<br>Zinc: 7.15E-6 |
| Henry's Law Constant, $\text{atm}\cdot\text{m}^3/\text{g}\cdot\text{mole}$   | 0 for all MC   |
| Molecular weight, g-mole   | Lead: 207.19<br>Antimony: 121.75<br>Copper: 63.54<br>Zinc: 65.39       |
| Octanol-water partition coefficient, $(\text{mg}/\text{m}^3 \text{ octanol})/(\text{mg}/\text{m}^3 \text{ water})$ | 0 for all MC   |
| Sediment – water distribution coefficient for TSS, L/kg  | Lead: 358,718<br>Antimony: 63,064<br>Copper: 22,216<br>Zinc: 61,370    |
| Sediment – water distribution coefficient for benthic mixed layer sediment, L/kg                                   | Lead: 28,494<br>Antimony: 3,979<br>Copper: 1,402<br>Zinc: 7,726        |
| Sediment – water distribution coefficient for benthic deep sediment, L/kg  | Lead: 28,494<br>Antimony: 3,979<br>Copper: 1,402<br>Zinc: 7,726        |
| Decay coefficient for dissolved contaminant in water, 1/yr   | 0 for all MC   |
| Decay coefficient for dissolved contaminant in mixed layer, 1/yr   | 0 for all MC   |
| Decay coefficient for dissolved contaminant in deep sediment, 1/yr   | 0 for all MC   |
| Decay coefficient for particulate contaminant in water, 1/yr   | 0 for all MC   |

Table 18. (concluded).

| Input Description   | Value        |
|---|--------------|
| Decay coefficient for particulate contaminant in mixed layer, 1/yr                    | 0 for all MC |
| Decay coefficient for particulate contaminant in deep sediment, 1/yr                  | 0 for all MC |
| Model Control Parameters  |              |
| Total period of simulation, yrs   | 60           |
| Number of time steps between print intervals for output, dimensionless                | 20           |
| Number of time steps between print intervals for sediment layer output, dimensionless | 20           |
| Number of sediment layers to print in output, dimensionless                           | 20           |

## Results

RECOVERY model results for water and mixed sediment layer MC concentrations at the end of 60 years of simulation were compared with measured data from the upper portion of Boyden Arbor Pond (Location 16) as reported by Bricka (2002). The computed total concentrations for water and sediment are shown along with the measured total concentrations in Table 19. The detection limits (DL) are also shown in Table 19.

Table 19. Computed and observed sediment and water concentrations for Boyden Arbor Pond near Fort Jackson ranges including measurement detection limits.

| MC                         | Computed for sediment, mg/kg | Measured in sediment, mg/kg | Sediment DL, mg/kg | Computed for water, µg/L | Measured in water, µg/L | Water DL, µg/L |
|----------------------------|------------------------------|-----------------------------|--------------------|--------------------------|-------------------------|----------------|
| Lead                       | 2280                         | 257                         | 5.52               | 148                      | BDL                     | 68.1           |
| Antimony                   | 14                           | 32                          | 19.93              | 1.48                     | BDL                     | 246            |
| Copper                     | 468                          | 92                          | 22.16              | 99                       | BDL                     | 274            |
| Zinc                       | 313                          | 95                          | 0.24               | 30                       | 123                     | 3              |
| BDL: Below detection limit |                              |                             |                    |                          |                         |                |

For three of the four MC, the computed sediment concentrations are higher than the observed. Computed sediment concentration of lead is about 10 times greater than observed, and computed sediment concentrations of copper and zinc are about three to four times greater than observed. Only the computed sediment concentration of antimony is less than observed by about a factor of 2.

The computed water concentrations of antimony and copper are below detection, which is the case of the observed values. The computed water concentration for lead is above the detection limit, while the observed is below detection. The computed water concentration of zinc is about one fourth of the observed value, but it is suspected that there were background water concentrations of zinc that are not accounted for in the model results.

Another model run was made where the sediment–water partitioning distribution coefficient  $K_d$  of each MC for water column TSS was set to the same value as used for the benthic sediment mixed layer and deep sediments. This resulted in lower mixed layer sediment concentrations for each MC. The sediment concentrations for lead, antimony, copper, and zinc were 1214, 3, 88, and 105 mg/kg, respectively. These changes resulted in very close agreement between computed and observed (measured) sediment concentrations of copper and zinc. Computed lead concentration is closer to observed, but it is still five to six times greater. The computed concentration of antimony is about one tenth of observed. The computed water total concentrations for lead, antimony, copper, and zinc were 153, 1.53, 101, and 31 µg/L, respectively, which are fairly close to the previously computed values as shown in Table 19. Assuming the water column  $K_d$  is the same as the sediment values seems reasonable.

An additional run was made in which the sediment–water  $K_d$  values for lead and copper were set to those used in the Fort A.P. Hill application, which were 4,000 and 600 L/kg for lead and copper, respectively. These values were used for TSS, mixed layer, and deep sediments. These changes resulted in computed mixed layer sediment concentrations of 326 and 44 mg/kg for lead and copper, compared with observed concentrations of 257 and 92 for lead and copper, respectively. The agreement for lead is much better, but computed copper is about half of the observed value. The water concentrations associated with this run were 156 and 101 µg/L for lead and copper, which are similar to the other computed values associated with higher  $K_d$  values.

Estimating accurate  $K_d$  values for metals in sediments/water is difficult given metal complexation and presence of various clays and minerals. It is important to consider uncertainty of this input in predictive applications.

It is noted that the observed field data indicate that some metal mass exported from the ranges is deposited within Gills Creek upstream of

Boyden Arbor Pond. The model assumes that all of the exported mass reaches the pond. Potential background concentrations of metals were not included in the model. It is also noted that the representation of munitions use and subsequent loadings is a crude estimate of what actually occurred over the 60-year period. In addition to uncertainty in  $K_d$ , it is emphasized that the estimation of metal solubility and solid phase particle size can be quite uncertain, yet important, for predicting metal dissolution and fate. Given these problems and uncertainties, it is encouraging that the computed metal concentrations for the pond agree relatively well with the observed data.

A sensitivity test was conducted to assess the effect of turning off solid phase MC particle erosion. The second set of conditions was used, i.e.,  $K_d$  values for surface water were set to the same values used for sediment; however, the solid phase MC particle erosion was turned off (unchecked) in the soil model UI. This run resulted in computed sediment concentrations after 60 years for lead, antimony, copper, and zinc of 114, 0.037, 6.15, and 99.5 mg/kg, respectively. These values should be compared with the values 1214, 3, 88, and 105 mg/kg from the prior run with the same conditions except for solid phase MC particle erosion turned on. This input change had a profound impact on lead, antimony, and copper, all of which have relatively low values for solubility; computed sediment concentrations were reduced by a factor of about 10 to 100. The impact on zinc, which has a much higher solubility, is fairly minor (99.5 versus 105). In reality, there is probably less solid phase MC particle erosion for lead than occurs in the model since lead has such a high solid phase density. Turning on this feature may be reasonable for the other three metals, but lead should probably be assessed with this erosion feature turned on and off.

Another sensitivity run was made with soil interflow. Soil interflow was set to 100% in the soil model UI, which means all of the soil infiltration becomes interflow that is diverted to the surface water body. The resulting mixed layer sediment concentrations of the pond were computed to be 1,253, 3.2, 93, and 163 mg/kg for lead, antimony, copper, and zinc, respectively. With the exception of zinc, these concentrations are similar to the values computed previously (initial predictions with water column TSS partitioning set the same as benthic sediments). The concentration for zinc is about 60 % greater than the previously computed value due to the higher solubility of zinc, which accelerates dissolution and promotes water-phase export.

## Conclusions

USEPA recommended values for metal sorption partitioning coefficients ( $K_d$ ) for water-sediment media provided reasonable predictions of sediment and water concentrations of metals in Boyden Arbor Pond on Gills Creek downstream of the firing ranges at Fort Jackson following about 60 years of range use. However, it was necessary to use uniform  $K_d$  values for each MC among the three media (water column TSS, mixed layer sediment, and deep sediment). There was very close agreement (within 10 % error) between computed and observed (measured) sediment concentrations of copper and zinc. Computed lead concentration in sediment was five to six times greater than observed. Computed antimony concentration in sediment was about one tenth of that observed after 60 years of range use.

The computed water concentrations of antimony and copper were below detection, which was also the case with the observed values. The computed water concentration for lead was above the detection limit, while the observed concentration was below detection. The computed water concentration of zinc was about one fourth of the observed value, but it is suspected that there are background water concentrations of zinc that were not accounted for in the model results.

Model results for all four metals were sensitive to inputs for their respective  $K_d$  values for the pond water column TSS and sediments. Additionally, results for lead, antimony, and copper were sensitive to turning off/on solid phase MC particle erosion. Results could be sensitive to other inputs in the surface water model that were not tested.

## 6 Summary

TREECS™ Tier 2 was applied to four Army installations to validate the ability of the models to represent results observed in the field. This report describes these applications and compares model computed (predicted) results against measured (observed) field data.

For Fort A.P. Hill, reasonable results for groundwater were predicted where results for all five MC were below detection after about 60 years of range use. These predictions are in agreement with recent measurements that also show concentrations for all five MC to be below detection. Surface water and sediment concentrations of RDX, TNT, and potassium perchlorate in White Lake were predicted to be below detection, which is in agreement with measured values that were found to be below detection. Predicted lead concentrations in White Lake were the same order of magnitude as measured. Predicted copper concentrations in White Lake sediment were two orders of magnitude lower than observed, but increasing the solubility from 0.5 to 18.4 mg/L resulted in concentrations that were nearly the same as measured (after adjusting the computed value for background copper). Other than this adjustment for copper, all model results for Fort A.P. Hill were blind predictions, since this modeling was done prior to receiving the data.

RDX soil concentrations within the AOI of demolition area 2 of MMR were fairly accurately predicted compared with the observed soil concentrations by using previously determined site characteristics and inputs from the original modeling as well as the default value for RDX residue particle diameter of 12,000  $\mu\text{m}$ . Computed soil concentrations are sensitive to MC residue loading rate and particle diameter. Both of these inputs have considerable uncertainty, but reasonable variations in these two inputs produced results within the range of those measured at the site.

Using previously determined site characteristics, original modeling inputs, and the default value for residue particle diameter resulted in computed groundwater concentrations of RDX at MMR that were about one fourth of those measured for the target monitoring well (MW161). Model results are rather sensitive to input values for RDX residue loading rate and particle diameter, as well as perpendicular distance of the monitoring well

from the RDX plume centerline, all of which are uncertain inputs. The model can be more accurately matched with the observed data by making relatively minor and reasonable adjustments to these three inputs. Overall, the results of the MMR application support successful validation of the TREECS™ soil, vadose, and aquifer models.

Good agreement was obtained for predicted versus observed water concentrations of RDX in Long Pond downstream of the West Point training complex after 55 years of range use. The computed concentration was 0.035 µg/L compared to 0.023 µg/L observed. Both computed and observed sediment concentrations of RDX were below detection levels. There was also good agreement for predicted versus observed water concentrations of RDX in the drainage ditch below Ranges 7 and 8 at West Point, where the observed values averaged 0.77 µg/L, and the predicted value was 1.13 µg/L after 55 years of range use. The agreement between predicted and observed sediment concentrations of RDX in the ditch were not close, where the observed concentration averaged about 0.12 mg/kg just below the ranges and the predicted concentration was 0.0025 mg/kg. However, all of the other sediment measurements in the ditch upstream and downstream of this sampling station were below the detection limit, indicating heterogeneous concentrations along the ditch that the model could not characterize.

Excellent agreement was obtained for predicted and observed lead concentrations in Long Pond of West Point. The observed concentration of lead in Long Pond sediment was 30.3 mg/kg compared with the predicted value of 30.1 mg/kg. The computed value for the water column was in agreement with the observed, with both being below detection. Testing indicated that lead solubility, particle size, and distribution coefficients for sediment-water sorption (partitioning) are particularly sensitive for affecting computed sediment concentrations.

The concentrations of four metals were computed for Boyden Arbor Pond on Gills Creek downstream of the firing ranges at Fort Jackson following about 60 years of range use. Reasonably good agreement between computed and observed sediment concentrations was obtained when using the USEPA-recommended values for metal sorption partitioning coefficients ( $K_d$ ) for water-sediment media. However, it was necessary to use uniform  $K_d$  values for each MC among the three media of water column TSS, mixed layer sediment, and deep sediment. There was very close agreement

(within 10% error) between computed and observed sediment concentrations of copper and zinc. Computed lead concentration in sediment was five to six times greater than observed. Computed antimony concentration in sediment was about one tenth of that observed after 60 years of range use.

Water concentrations of antimony and copper were computed to be below detection, which was the case of the observed values. The computed water concentration for lead was above the detection limit, while the observed value was below detection. The computed water concentration of zinc was about one fourth of the observed value, but it is suspected that there are background water concentrations of zinc that were not accounted for in the model results.

In all applications, the inputs that were always the most difficult to estimate included metal solubility and metal sediment-water partitioning,  $K_d$ . Model results are usually quite sensitive to these inputs. The metal  $K_d$  for AOI soils is not as difficult to estimate, since there is a utility within the soil model for estimating this for some metals.

The applications of TREECS™ Tier 2 to these four Army installations resulted in relatively good agreement between computed results and observed data. The results of these applications help validate TREECS™ and build confidence in its use for predicting export and fate of MC associated with munitions usage on firing and training ranges.

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# REPORT DOCUMENTATION PAGE

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| <b>14. ABSTRACT</b><br><br>The Training Range Environmental Evaluation and Characterization System (TREECS™) is being developed for the Army with varying levels of capability to forecast the fate of and risk from munitions constituents (MC), such as high explosives (HE), within and transported from firing/training ranges to surface water and groundwater. The overall objective is to provide environmental specialists with tools to assess the potential for migration of MC into surface water and groundwater systems and to assess range management strategies to protect human and environmental health.<br><br>TREECS™ includes two tiers of analysis. Tier 1 consists of screening-level methods that assume highly conservative, steady-state MC loading and fate. Tier 1 requires minimal data input requirements and can be easily and quickly applied to assess the potential for migration into surface water and groundwater. Tier 2 provides time-varying analyses, since it does not make the highly conservative assumptions of steady-state (time-invariant) conditions with no MC loss or degradation as used for Tier 1. The Tier 2 soil model solves mass balance equations for both solid and non-solid phase MC with dissolution. Additionally, MC residue loadings to the range soil can vary from year to year based on munitions use. Thus, media concentrations computed with Tier 2 should be closer to reality.<br><br>As with any model, validation applications are needed to gain confidence in using the model. Validation applications involve comparing model-predicted results against data measured from the modeled site so that the model can be evaluated in terms of representing real-world conditions. Tier 2 of TREECS™ was applied to four sites at four different Army installations for validation purposes. This report describes the results of those applications with comparisons of computed and observed MC concentrations in surface water and groundwater. |                                    |                                       |  |  |  |
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