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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 and risk of 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 the range manager with tools to assess range management strategies to meet environmental compliance goals. Tier 1 will consist of screening-level methods that require minimal data input requirements and can be easily and quickly applied by range managers or their local environmental staff to assess whether or not there is potential for MC compliance concern, such as predicted surface water and/or groundwater MC concentrations exceeding protective health benchmarks at receptor locations.

This report describes the Army's existing and perceived future requirements for TREECS Tier 1 tools and provides recommendations and a plan for technology developments to meet those needs. The information provided in this report is sufficient to serve as design and specifications for development of models and software that will comprise Tier 1 of TREECS. The details of the model formulations provided herein can also serve as documentation for the Tier 1 TREECS models.

The highly conservative assumptions of steady-state (time-invariant) conditions and no MC degradation are used. Thus, MC loadings to the range are constant over time, and fluxes to and concentrations within receiving water media reach a constant MC concentration for comparison to protective ecological and human health benchmarks. Tier 1 will include an analytical range soil model with its computed leaching flux linked to a semi-analytical-numerical aquifer model and with its computed runoff-erosion flux linked to a numerical surface water model. Tier 1 will also include an MC loading module, a hydro-geo-chemical toolkit for estimating input parameters, constituent databases for chemical-specific properties, and a database of ecological and human protective health benchmarks. All components will be packaged within a user-friendly PC client-based application with an emphasis on ease of use.

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Preface

This study was funded by the U.S. Army's Environmental Quality Technology and Installations (EQI) Research Program. This report was prepared by Drs. Mark Dortch and Billy Johnson and Mr. Jeffrey Gerald of the Water Quality and Contaminant Modeling Branch (WQCMB), Environmental Processes and Effects Division (EPED), Environmental Laboratory (EL) of the U.S. Army Engineer Research and Development Center (ERDC). The study was conducted under the general direction of Dr. Beth Fleming, Director of the EL; Dr. Richard Price, Chief, EPED, and Dr. Mansour Zakikhani, acting Chief, WQCMB. Dr. John Cullinane was Director of the EQI Program.

Dr. James R. Houston was Director of ERDC. COL Gary E. Johnston was Commander and Executive Director.

Unit Conversion Factors

Multiply	By	To Obtain
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	453.59	grams
slugs	14.59390	kilograms
square feet	0.09290304	square meters

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), within and transported from firing/training ranges to surface water and groundwater. The overall objective is to provide the range manager with tools to assess range management strategies to meet environmental compliance goals. TREECS will be accessible from the World Wide Web and will initially have two tiers for assessments. Tier 1 will be screening-level methods that require minimal data input requirements and can be easily and quickly applied by range managers or their local environmental staff to assess whether or not there is potential for MC compliance concern, such as surface water and/or groundwater MC concentrations exceeding protective health benchmarks at receptor locations. Assumptions, such as steady-state conditions, will be made to provide conservative or worst case estimates for potential compliance concerns 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.

Tier 2 assessment methods will require more detailed site data, and will require more knowledge and skill to apply, but can be applied by local environmental staff that have a cursory understanding of multi-media fate and transport modeling. The Tier 2 approach will allow time-varying analyses. A time-varying analysis should provide more accurate predictions with generally lower concentrations due to mediating effects of transport phasing and dampening. Tiers 1 and 2 will focus on contaminant stressors and human and ecological health end point metrics.

Scope

This report describes the Army’s existing and perceived future requirements for a Tier 1 screening-level tool and provides recommendations and a plan for technology developments to meet those needs. The information provided in this report is sufficient to serve as design and specifications for development of models and software that will comprise Tier 1 of TREECS.

The details of the model formulations provided herein can also serve as documentation for the Tier 1 TREECS models.

Requirements

In accordance with Department of Defense (DoD) Directive 4715.11, “Environmental and Explosives Safety Management on Operational Ranges Within the United States” (10 May 2004) and Department of Defense Instruction (DODI) 4715.14, “Operational Range Assessments” (30 November 2005), the Army is currently conducting operational range assessments at all Army installations, including Army Reserve and Army National Guard installations, located within the United States and its territories. The Army is assessing approximately 425 operational range complexes with over 11,000 individual ranges, and 15 million acres. Ranges being assessed include small arms ranges, medium- and large-caliber ranges, impact areas, maneuver and training areas, drop zones, open burn/open detonation ranges, landing zones, testing ranges, and other miscellaneous ranges. Munitions typically used on these ranges include small caliber, medium and large caliber, and smokes and pyrotechnics. These munitions may be practice rounds, dummy rounds, or high explosive rounds. The Army’s Operational Range Assessment Program (ORAP) is being conducted in two phases: a Qualitative Assessment (Phase I) and a Quantitative Assessment (Phase II).

The assessment strategy for Phase I is similar to a Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) Preliminary Assessment (PA). Sampling is not performed during Phase I, although existing sampling information is used if available. The purpose of the Phase I assessment is to use existing, available data and site reconnaissance to determine whether or not a potential exists for a release or a substantial threat of a release of Munitions Constituents of Concern (MCOC) to an off-range area that may pose an unacceptable risk to human health or the environment. MCOC are defined as those munitions constituents that have the potential to migrate from a source area, to an off-range receptor (human or ecological), in sufficient quantity, to cause an unacceptable risk to human health or the environment. Conceptual Site Models (CSMs) are developed to depict the relationship between potential source areas, potential migration pathways, and off-range receptors (both human and ecological). A draft report with conclusions is prepared, where conclusions place the range into one of three categories: unlikely, inconclusive, or referred. Ranges categorized as “unlikely” require no further action, and the range is placed into a 5-year review cycle. Ranges categorized as “inconclusive” will require a follow-up Phase II assessment. Ranges categorized as “referred” are those with compelling evidence (i.e. sampling data) to indicate the presence of an off-range release, which could pose an unacceptable risk to human health or the environment. Operational range areas categorized as “referred” will be referred to an appropriate cleanup program for further action.

During Phase II, sampling will be performed on the appropriate environmental media as recommended by the Phase I assessment. Phase II assessments will place ranges into either the “unlikely” category or “referred” category. The strategy for conducting Phase II assessments is based on application of the EPA’s systematic planning or Data Quality Objective (DQO) process. Application of the DQO process will ensure that sampling efforts are focused on the appropriate media and that the appropriate data are collected to determine if there is an off-range migration that may pose an unacceptable risk to human health or the environment. The challenge of Phase II assessments is knowing or estimating where and when to sample.

The Army is scheduled to complete all ORAP Phase I assessments by the end of FY 09. Phase II assessments will commence in FY 10, subsequent to the completion of all Phase I assessments. Given this timetable and the more comprehensive needs and challenges of the Phase II assessments, ERDC, in consultation with the Army Environmental Command (AEC), decided that the Tier 1 tools of TREECS should help support needs within the Phase II ORAP. Additionally, the Tier 1 tools should help address the question of “how much can a range be used (i.e., how much annual loading of MC) before there is a problem with off-site migration to potential receptors at concentrations of concern?” Source soil on ranges will not be sampled during Phase II ORAP for several reasons:

1. To accurately characterize the amount of MCOC present and mobile within the large area and mass of soil present on the ranges with today's technologies is not practicable.
2. The focus of the ORAP program is on off-range risk. There is no exposure to on-range soils.
3. On-range soil sampling is hazardous, and likely to interfere with training exercises.

The lack of source soil concentrations makes answering the above question more difficult since soil concentrations must be estimated based on range use in order to estimate off-site migration. Thus, soil concentrations must be estimated using a soil fate/transport model with mass loading inputs estimated based on range use.

In general, the Tier 1 tools should provide the following information to address needs of the Army:

1. Given range use, estimate the MC mass loading rate, mass (M) per time (T), M/T.
2. Given the mass loading rate of MC, estimate the soil concentration on the range area of interest and the mass fluxes (M/T) off the range to other media (e.g., surface water and groundwater).
3. Given the mass fluxes to other media, estimate the media concentrations at points of interest off-range.
4. Given the media concentrations at points of interest off-range, determine if protective health benchmark concentrations are exceeded.

Information from the last two steps above can help in determining where to sample and the potential for range use to lead to an environmental compliance concern. Furthermore, the range use strategies could be adjusted or managed in the first step in an effort to promote range sustainment while satisfying compliance goals or requirements.

2 Approach

The challenge is to develop Tier 1 tools or models that can provide the information in steps 1-4 (cited above in the Requirements Section) in a manner that minimizes data input and maximizes ease of use such that special training is not required for application. Assumptions are required in order to reduce and constrain the problem set to something that can be easily and quickly modeled and evaluated with limited data and effort, while providing a conservative estimate. The assumptions that will be made for the Tier 1 modeling tools are summarized in this chapter. Descriptions of the models follow.

Basic assumptions

The range area of concern will be treated as a single fully mixed comparetment, thus, soil concentrations are assumed to be uniform throughout the soil horizon within the area. As an example, the primary impact zone of a range will be treated as a single homogenous area. A range is not homogeneous in reality, rather some range areas are a somewhat heterogeneous mixture of point sources on the soil surface. Treating a heterogeneous range as homogeneous is not a fatal assumption because the total MC source mass loading is the driving variable for export flux, not MC concentration. Although the soil concentration of MC depends on heterogeneities and even the size of the source area for a homogeneous site, the fluxes or export rate of mass from the source area to other media does not depend on the area of the source zone or the source concentration as will be shown in Chapter 3. Of course, a large range with source mass clusters that differ substantially could be treated as multiple sources with each assessed individually.

Loading of MC into the area of concern will be estimated from the numbers and types of munitions used on an annual basis and assumed low order detonation percentages of each. Initially, the Tier I tools will address only impact areas and will not include firing points. However, firing points could potentially be added later. Additionally, the user will have the option to specify a *known* loading rate of MC that may have been estimated from other activities, such as small arms use. The homogenous area assumption relates to step 1 and part of step 2 in the Requirements section above.

The steady-state assumption will be used to further constrain the problem. This assumption requires that the loading of MC into the area of concern be constant over time, which will allow soil concentration and export fluxes that are constant over time. This assumption greatly reduces input requirements and output information, and gives a result that will indicate whether or not exposure concentrations will ever reach a value of concern. Time-varying MC loadings and response can be quite complicated. For example, if a loading of MC occurs for a 10-year period and then ceases, it may take another 10 years after the loading ceases for groundwater concentration to peak, and the time of the peak varies with the distance of the well from the source area and environmental factors. These variations can complicate the analysis and interpretation of results. However, with a steady-state analysis, time is removed as a variable, and all concentrations reach constant values with respect to time at all locations, although steady-state concentrations will differ among locations.

The steady-state assumption is a highly conservative approach that yields worst-case results, since it assumes that loading continues and concentrations persist indefinitely over time. Thus, such an analysis indicates whether or not there is likely to ever be an exposure concern. If a Tier 1 analysis indicates that there should not be an exposure concern, further analysis and sampling may not be warranted.

Assuming steady-state conditions also removes the importance of some input parameters from the analysis, thus eliminating the need for the user to estimate and specify those parameters in the application. For example, the corrosion and/or dissolution rates are in balance with MC loading and do not affect media concentrations under steady-state conditions, whereas under time-varying loadings and conditions, the dissolution rate is very important (Dortch et al. 2007). Thus, for the steady-state assumption, solid phase MC (including explosives residue) will be assumed to be converted to aqueous phase instantly upon loading into the range area. This assumption may prove overly conservative for metals fate since their corrosion and subsequent dissolution can take many years (potentially hundreds and even thousands) to reach steady-state. Thus, assessments for metals may be better done with Tier 2 than Tier 1.

A steady-state analysis negates the need for knowing initial soil MC concentrations, thus initial conditions are not required. To support highly conservative estimates, it will be assumed that there is no decay or degradation of MC in any of the media. Three of the primary model inputs will be soil infiltration rate q_w (length L per time T), surface runoff rate Q (L/T), and soil layer erosion rate E (L/T), all of which will be constant over time, thus, annual average values. A utility will be provided within TREECS for estimating q_w, Q, and E based on annual average rainfall and soil and landscape characteristics as explained later in this report. Runoff and erosion export result in MC mass removal that is proportional to total MC mass dissolved in water and adsorbed to soil, respectively. Infiltration export is only dependent on the portion of constituent dissolved in water.

It will be assumed that all of the runoff and eroded soil and associated MC mass will travel to the receiving surface water if the surface water route is being considered in the application. Thus, there will be no losses between the range and receiving surface water. The receiving surface water can be a stream, pond, lake, wetland, or any type of surface water. This assumption provides a conservative, worst-case scenario while greatly reducing model complexity and data input requirements. More detailed modeling assumptions are addressed within the next chapter on Model Formulations.

Conceptual model description

For land-based firing ranges, four media can contain MC: soil, vadose zone, groundwater or aquifer, and surface water (including surface water sediments). Air concentrations are a limited, short-duration, local issue and are not considered for range sustainment. A conceptual site model for range MC is shown in Figure 1. MC residue loading first enters the range soil. MC can move from soil to surface water via runoff and erosion and from soil to the vadose zone via infiltration or leaching. MC can then percolate through the vadose zone into a receiving aquifer. Aquifer and surface water concentrations of MC depend on the locations within each receiving water relative to the point of MC influx. Receiving water concentrations can be estimated and compared with benchmarks for compliance. There can also be pathways from groundwater to surface water and vice versa; however, these pathways are not considered in this report, but they may be considered later within the Tier 1 approach.

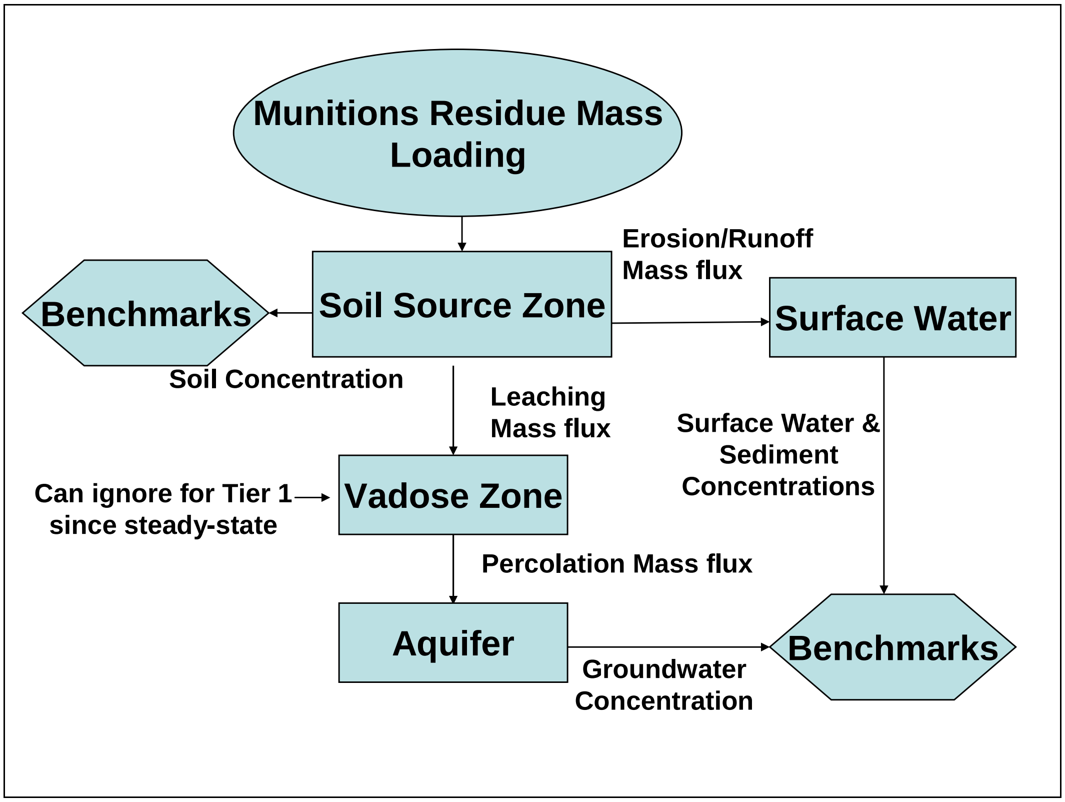


Figure 1. Tier 1 conceptual model schematic.

With the steady-state assumption and no degradation, it turns out that the vadose zone is not important for an analysis. MC mass simply passes through the vadose zone unaltered. There can be sorption of MC within the vadose zone, but at steady-state, the mass flux from the vadose into the aquifer must equal the leaching flux from soil. Thus, a vadose zone model is not required. However, models for soil, aquifer, and surface water are required and are described in the next chapter.

The soil model will compute steady-state soil concentrations and mass export fluxes for erosion, runoff, and infiltration/leaching. The aquifer model will use the leached mass influx rate and the receptor location to compute the groundwater concentration at the receptor location. Similarly, the surface water model will use the runoff and eroded mass influx rate to compute the surface water concentration. The location of the receptor will not be required for the surface water model since the concentration will be computed for a reach of water at or near the point of influx. A limited number of model input parameters must be specified by the user to apply the three models. These parameters will be discussed later in Chapter 4 of this report.

3 Model Formulations

The formulations for the soil, aquifer, and surface water models are described below.

Soil model

Consider a layer of surface soil that has a constituent concentration that is fully mixed over the surface soil layer depth Z_b (m), and over a given area, A (m^2). Thus, a continuously stirred tank reactor (CSTR) model is assumed. The constituent is assumed to be fully dissolved into the aqueous phase from the solid phase and partitioned in equilibrium between water dissolved and adsorbed to soil particles. It is also assumed that the Henry's constant is very low; thus, there is little or no constituent mass in the vapor phase and no degradation. The constituent mass balance for the soil layer with a constant source loading (L, g/yr), runoff flux (F_r, g/yr), erosion flux (F_e, g/yr), and leaching flux (F_l, g/yr), but with no decay is stated as

$$\frac{dM}{dt} = L - F_r - F_e - F_l \tag{1}$$

where M is the mass of constituent (g), and t is time (yr). The total (particulate and dissolved) constituent concentration on a total volume basis, C_{tt} (g/m^3) is

$$C_{tt} = \frac{M}{V} = \frac{M}{A\,Z_b} \tag{2}$$

where V is the volume (m^3). Note that the surficial soil layer Z_b is assumed to be constant. Thus, it is assumed that an active soil layer of the same thickness is reestablished although there is soil loss with erosion. Since the soil mass balance will be assumed to be at steady state, all fluxes should be long-term annual averages.

The erosion flux is computed from

$$F_e = E\,A C_{tt} \tag{3}$$

where E is the annual average erosion rate (m/yr). It can be shown that F_e includes the flux of chemical adsorbed to eroded soil particles and pore water chemical that is within the eroded soil layer.

The leaching flux is computed from

$$F_l = q_w \, A F_{dp} C_{tt} \tag{4}$$

where q_w is the annual average Darcy water infiltration rate (m/yr), and F_{dp} is a factor to convert from total concentration on a total volume basis to dissolved concentration on a water volume basis and can be computed from

$$F_{dp} = \frac{1}{\theta_w + \rho_b K_d} \tag{5}$$

where:

θ_w = soil volumetric moisture content or ratio of water volume to total volume; θ_w can't be greater than soil porosity (fraction)
ρ_b = soil dry bulk density, g/ml
K_d = distribution coefficient for partitioning constituent between soil particles and water, ml/g or L/kg.

Rain induced pore water ejection and runoff is used to estimate runoff flux F_r. Chemical can be transferred from soil pore water to overland runoff due to rainfall impacting the soil surface, even when there is no erosion. The event-based runoff mass removal rate of pore water Re_{dQ} (g/sec) due to rain induced ejection can be computed from

$$\mathrm{Re}_{dQ} = e_r A \bar{C}_e \tag{6}$$

where e_r (m/sec) is the rate of soil pore water ejection during a rainfall event, and $\bar{C}_e$ is the rainfall event time-averaged soil pore water chemical concentration (g/m^3) in the soil exchange layer adjacent to the overland water. The soil water ejection rate is defined (Gao et al. 2004) as

$$e_r = \frac{aI\varphi}{\rho_b} \tag{7}$$

where I is the rainfall intensity (m/sec), a is the soil detachability (kg/L), and N is the saturated water content, which is the soil porosity. The instantaneous soil pore water chemical concentration in the exchange layer during a rainfall event can be approximated (Gao et al. 2004) by

$$C_e \approx C_o \exp(-\beta t) \tag{8}$$

where C_o is the soil pore water concentration below the exchange layer and is equal to $F_{dp}C_{tt}$, t is time (sec), and

$$\beta = \frac{e_r F_{dp}}{d_e} \tag{9}$$

where d_e is the soil exchange layer thickness (m); β has units of sec^{-1}. The event time average of Equation 8 is

$$\bar{C}_e = \frac{C_o \int_o^T e^{-\beta t} dt}{T} = \frac{C_o}{T\beta}\left(1 - e^{-\beta T}\right) \tag{10}$$

where T is the time averaging interval, which is the event duration (sec). Substituting the definition of C_o and Equations 7, 9, and 10 into Equation 6 results in

$$Re_{dQ} = \frac{Ad_e}{T}\left(1 - e^{-\beta T}\right)C_{tt} \tag{11}$$

The goal is to be able to apply Equation 11 to develop an annual average rainfall extraction of pore water with runoff. To do this, an average or typical rainfall intensity $\bar{I}$ and associated duration $\bar{T}$ are required for use in Equations 7, 9, and 11, resulting in an average event runoff flux, $\overline{Re}_{dQ}$. Multiplying $\overline{Re}_{dQ}$ by $\bar{T}$ results in the average event pore water mass removed with runoff. The number of such events occurring within a year, N (events/yr), can be multiplied times $\overline{Re}_{dQ}\bar{T}$ to obtain the pore water mass removed with runoff per year or the annual runoff export F_r. The above statements are expressed in mathematical form as

$$F_r = Ad_e\left(1 - e^{-\bar{\beta}\bar{T}}\right)C_{tt}N \tag{12}$$

The values used for $\overline{I}$, $\overline{T}$, and N should satisfy the following relation,

$$P = \overline{I}\,\overline{T}\,N \tag{13}$$

where P is the annual average precipitation P (m/yr). $\overline{T}$ and $\overline{I}$ drop out of Equation 12 when $\overline{\beta}$ is multiplied by $\overline{T}$ since $\overline{\beta}$ has rainfall intensity in it, which is a function of $\overline{T}$, P, and N (see Equation 13). Thus, the average event intensity and duration do not affect the annual export; rather it is the annual rainfall and number of storm events that are important for computing annual runoff export. A reasonable approach is to count the number of days per year that rainfall occurs or exceeds a threshold (e.g., 0.1 inch) to approximate N. Equation 12 can be rewritten as shown below given the above discussion,

$$F_r = Ad_e\left(1 - e^{-\kappa}\right)C_{tt}N \tag{14}$$

where,

$$\kappa = \frac{a\varphi F_{dp}P}{\rho_b d_e N} \tag{15}$$

The result computed by Equations 14 and 15 is fairly sensitive to all input parameters. However, the only two parameters that are not easily determined are d_e and a, so typical values found in the literature like those reported by Gao et al. (2004) must be used. It is expected that both of these parameters are affected by soil texture, land use and cover, and possibly soil chemistry.

Substituting relations from Equations 2–4 and 14 into Equation 1 yields

$$AZ_b\frac{dC_{tt}}{dt} = L - EAC_{tt} - q_w AF_{dp}C_{tt} - Ad_e\left(1 - e^{-\kappa}\right)C_{tt}N \tag{16}$$

Rearranging and cancelling terms results in

$$\frac{dC_{tt}}{dt} = \frac{L}{AZ_b} - \frac{\left(E + q_w F_{dp} + d_e N\left[1 - e^{-\kappa}\right]\right)C_{tt}}{Z_b} \tag{17}$$

Assuming steady-state, Equation 17 simplifies to

$$C_{tt} = \frac{L}{A\left[E + q_w F_{dp} + d_e N\left(1 - e^{-\kappa}\right)\right]} \tag{18}$$

Substituting Equation 18 for C_{tt} into the equations for erosion, leaching, rain induced pore water runoff fluxes results in the steady-state fluxes

$$F_e = \frac{EL}{\left[E + q_w F_{dp} + d_e N\left(1 - e^{-\kappa}\right)\right]} \tag{19}$$

$$F_l = \frac{q_w F_{dp} L}{\left[E + q_w F_{dp} + d_e N\left(1 - e^{-\kappa}\right)\right]} \tag{20}$$

$$F_r = \frac{d_e NL\left(1 - e^{-\kappa}\right)}{\left[E + q_w F_{dp} + d_e N\left(1 - e^{-\kappa}\right)\right]} \tag{21}$$

It should be noted that the fluxes in Equations 12 – 14 do not depend on the soil concentration or the area of the site of interest, rather they depend primarily on the loading, L, and the respective removal rates E, q_w, and d_eN. Of course, the soil concentration does depend on the site area, A.

The runoff, erosion, and infiltration rates can be estimated based on soil and watershed characteristics as discussed in Appendix B. The loading can be estimated from munitions use. The soil parameters can be estimated from soil classification, and K_d can be estimated from either the constituent octanol to water partitioning coefficient or organic carbon to water partitioning coefficient, all as discussed in Appendix B. Values for a and d_e are more difficult to estimate as previously mentioned, but typical values are on the order of 0.4 kg/L and 0.005 m, respectively.

The constituent dissolved concentration (g/m^3) on a water volume basis in the pore water C_o cannot exceed the solubility of the constituent C_s (g/m^3). If the value of C_o computed from $F_{dp}C_{tt}$ exceeds C_s, the leaching flux becomes,

$$F_l = q_w A C_s \tag{22}$$

The rainfall induced pore water runoff is calculated from Equations 14 and 15, but with $F_{dp} = C_s / C_{tt}$. In this case, the soil concentration and export fluxes can no longer reach steady-state, but continue to increase with time. Note that the flux does depend on the site area for this case. For these situations, it is probably prudent to proceed to a Tier 2 analysis.

Aquifer model

The Multimedia Environmental Pollutant Assessment System (MEPAS) (Buck et al. 1995) consists of various models of reduced form for computing multimedia fate and transport, human exposure concentrations, and human receptor doses and health risks. One of the MEPAS models is a time-varying aquifer fate/transport model. The MEPAS aquifer model, version 5.0 (http://mepas.pnl.gov/mepas/maqu/index.html) will be used within Tier 1 of TREECS to compute groundwater concentrations. An overview of the model formulation is provided below, but details can be found at the above Web site.

A schematic of a typical site with export to groundwater is shown in Figure 2. The purpose of the aquifer model is to compute the MC plume. Cartesian coordinates for the plume calculation are shown in Figure 3 along with locations for the withdrawal well. The range source zone area is the black box in the top of Figures 2 and 3. The well is located x distance downstream from the origin or the Y axis, y distance laterally from the plume centerline (X axis), and z distance vertically from the water table surface. The model computes groundwater concentrations at the well location (x, y, z).

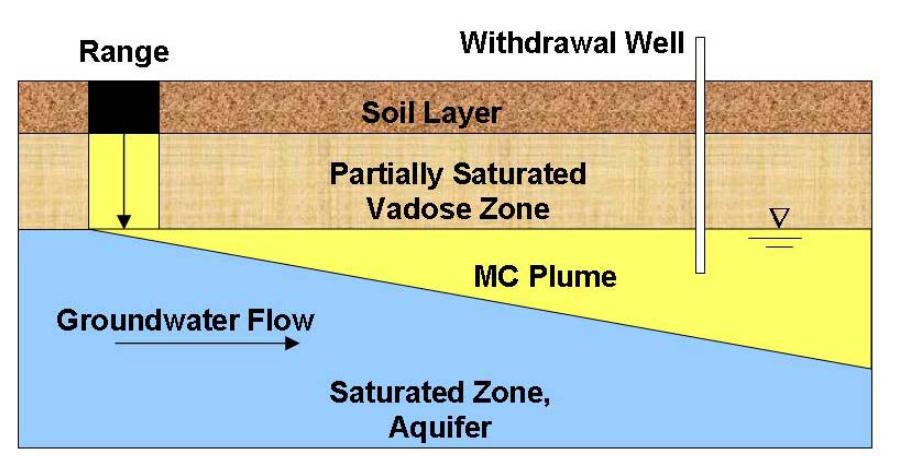


Figure 2. Site schematic with export to groundwater.

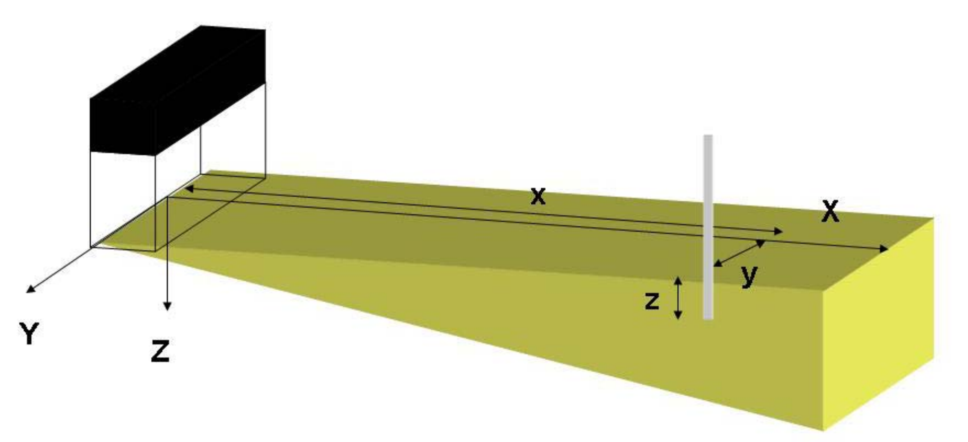


Figure 3. Plume coordinates and well location.

The MEPAS aquifer model solves the one-dimensional advective, three-dimensional dispersive mass transport equation for solute movement through a porous medium with a unidirectional, constant or steady-state, uniform flow velocity and with first-order degradation/decay and equilibrium sorption partitioning. Other assumptions include the following:

- The groundwater environment is initially free of contamination.
- All transport media properties are homogeneous and isotropic.
- The aquifer is of finite, constant thickness and of infinite lateral extent.
- Drawdown effects of withdrawal wells and other transient stresses on the aquifer are not considered by the semi-analytical solutions.
- Flow velocities are provided by the user.
- Density differences between a contaminant plume and the natural groundwater are negligible.

The governing equation for groundwater transport becomes

$$\frac{\partial C}{\partial t}+\left(\frac{u}{R_{f1}}\right)\left(\frac{\partial C}{\partial x}\right)=\left(\frac{D_x}{R_{f1}}\right)\left(\frac{\partial^2 C}{\partial x^2}\right)+\left(\frac{D_y}{R_{f1}}\right)\left(\frac{\partial^2 C}{\partial y^2}\right)+\left(\frac{D_z}{R_{f1}}\right)\left(\frac{\partial^2 C}{\partial z^2}\right)-\lambda C \tag{23}$$

where

$$R_{f1}=1+\frac{\beta_d}{n_e}K_d \tag{24}$$

and

$$D = \alpha u + D_{mol} \tag{25}$$

Other variables are defined as:

C = dissolved concentration (mg/L)
u = pore-water velocity (cm/sec)
R_{f1} = retardation factor (dimensionless)
t = time (sec)
β_d = dry bulk density (g/cm^3)
K_d = equilibrium (partition or distribution) coefficient (mL g-1)
D = dispersion coefficients in the x-, y-, and z-directions (cm^2/sec)
α = dispersivity in the x-, y-, and z-directions (cm)
λ = degradation / decay rate (sec-1)
n_e = effective porosity (fraction)
D_{mol} = molecular diffusivity (cm^2/sec).

The estimation of parameters used in Equations 23–25 are discussed in the next chapter. Although Equation 23 is time-varying, and the steady-state assumption is made for Tier 1, the MEPAS aquifer model can still be used by applying constant influx boundary conditions and running the model long enough to reach steady-state concentrations. In this manner, it is possible to use the MEPAS aquifer model without modifications for steady-state conditions. Additionally, for Tier 1, the degradation/decay rate is assumed to be zero, which can be easily specified with other input values. The aquifer model automatically runs long enough to reach steady-state or peak concentrations.

A combination of analytical and numerical methods are used to solve Equation 23 for a variety of boundary conditions, including a source influx specified over an area, such as a firing range impact zone. The solution scheme also accounts for boundary effects of aquifers of limited vertical thickness such as perched aquifers or aquifer water tables that are close to bedrock.

Surface Water Model

A wide variety of surface water types may be encountered, such as streams, lakes, ponds, estuaries, and wetlands. The goal is to select a model type that can be used for any type of surface water. Two model types were considered for the Tier 1 modeling, the time-varying, one-dimensional, longitudinal, Contaminant Model for Streams (CMS) described by Fant and Dortch (2007), and the RECOVERY model (Ruiz and Gerald 2001), which is a time-varying contaminant model for standing surface water. Given the assumption that the receiving water receptor point of interest is located within the vicinity of the MC influx and the need to describe a variety of surface water types, the hope was to be able to use the more generic RECOVERY model rather than CMS, which was developed explicitly for streams with long reaches between influx and receptor. However, it was necessary to conduct testing to determine whether RECOVERY would be satisfactory. This testing and the results are described in Appendix A. Results indicated that RECOVERY would be satisfactory for the intended use within Tier 1, and it can be used for both streams and standing surface water. Appendix A also gives guidance on selecting the appropriate reach length to use in stream applications.

RECOVERY is the surface water model that will be used in Tier 1 and is described briefly below. Although RECOVERY is a time-varying model, there is nothing that precludes using it for a steady-state analysis as long as the model is supplied constant mass influx and is run long enough to reach steady-state conditions. Testing with the model showed that 100 years is more than adequate to reach steady-state for most expected conditions.

RECOVERY simulates the long-term, time-varying concentration of contaminants in surface water and bottom sediments for both dissolved and particulate contaminants. A schematic of how the water-sediment system is handled in RECOVERY is shown in Figure 4. The water column is treated as a fully mixed volume, or a CSTR. The bottom sediments are divided into two types, a surficial mixed sediment layer at the sediment-water interface, and deep sediments below the surficial mixed layer. This treatment results in three mass balance equations with three unknowns, which apply to the water column, mixed sediment layer, and deep sediment layers. Two coupled ordinary differential equations are solved for the contaminant concentration in surface water (C_w) and in the mixed sediment layer (C_m). A partial differential equation is solved for sediment concentrations (C_s) in all of the deep sediment layers. Each mass balance equation accounts for mass fate processes, such as sorption, degradation, etc., which are shown in Figure 5. Equilibrium, reversible, sorption partitioning is assumed. Loading boundary conditions can include inflowing contaminant mass and external loadings of contaminant mass. The deep sediment extends below the depth of contamination into clean sediment so that a zero concentration gradient boundary condition can be applied. The equations and solution schemes are not repeated here, but they are well documented by Ruiz and Gerald (2001).

The area and depth of the water body must be specified in RECOVERY, and either the volumetric water flow rate, which is assumed constant over time, or the average water residence time must also be specified, where residence time is water body volume (depth times area) divided by the flow rate. The long-term average sediment settling, resuspension, and burial rates (L/T) are required. The user can input any two of the three rates, and the model computes the third rate assuming a steady-state sediment mass balance for the mixed layer. There are other required inputs, such as chemical and sediment properties, that are discussed in the next chapter.

Although RECOVERY was the model that best suited the Tier 1 analysis needs, it is envisioned that both RECOVERY and CMS will be available within Tier 2 where the user can select RECOVERY for standing surface water or CMS for flowing streams and rivers.

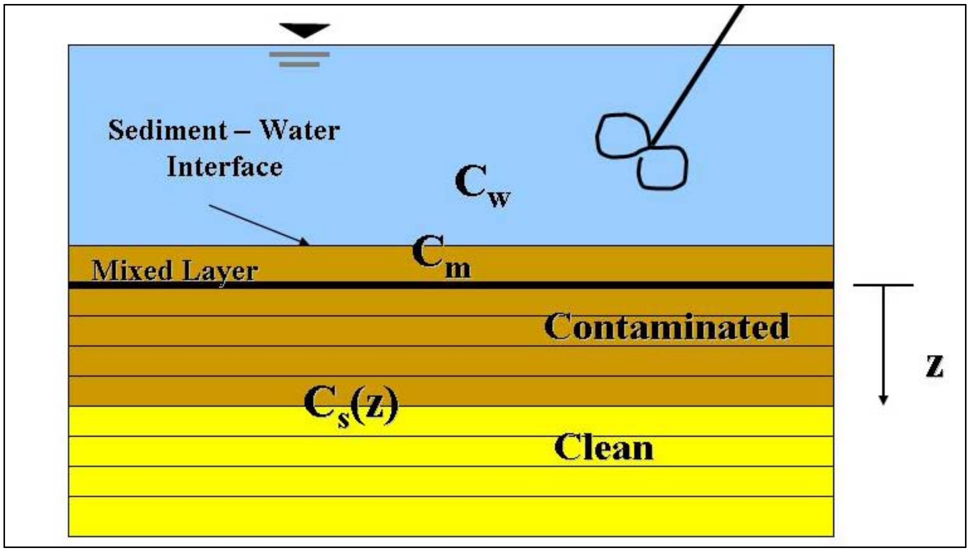


Figure 4. Schematic of the RECOVERY model.

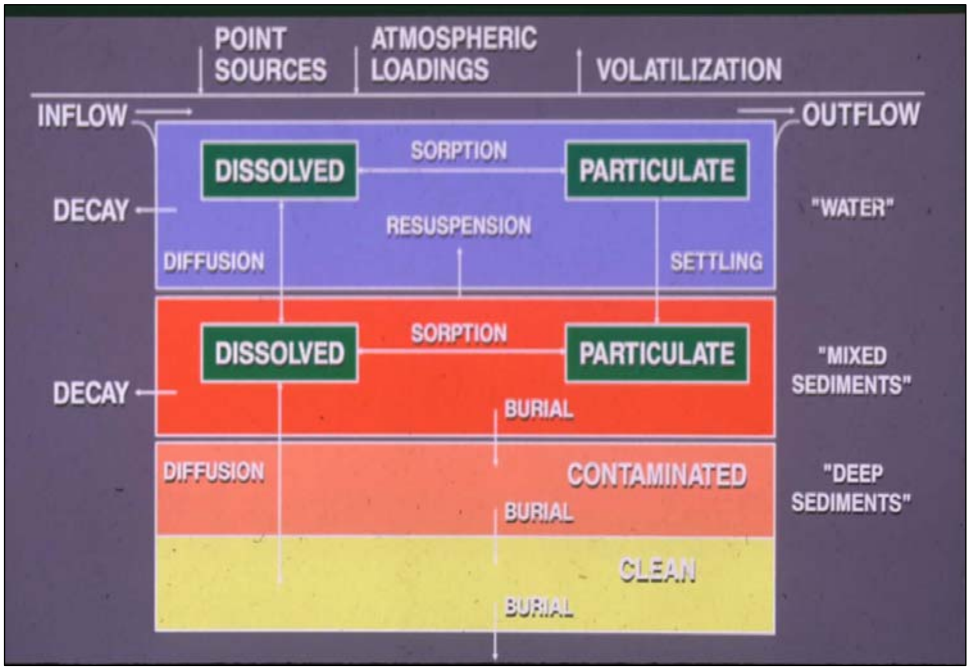


Figure 5. Fate processes within the RECOVERY model.

4 Model Implementations

This chapter discusses the input requirements for each model and how those are addressed for Tier 1 analyses. Various sensitivity tests were performed to evaluate the importance of inputs so that the input requirements could be minimized. Results of those tests are also discussed within this chapter.

Soil model

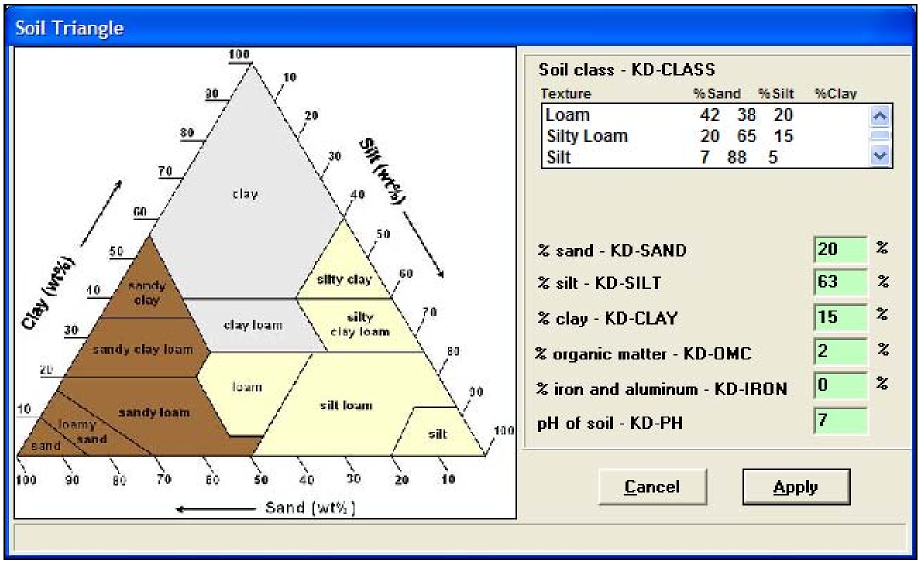
The soil model described in the previous chapter has the following input requirements:

- Volumetric soil moisture content (θ_w)
- Soil dry bulk density (ρ_b)
- Soil porosity (N)
- Partitioning distribution coefficient (K_d)
- Annual average MC residue loading rate (L)
- Loading site surface area (A)
- MC constituent solubility (C_s)
- Annual average water infiltration rate (q_w)
- Annual average soil erosion rate (E)
- Annual average rainfall (P)
- Annual average number of rainfall events per year (N)
- Soil exchange layer thickness for rainfall ejection of pore water (d_e)
- Soil detachability for rainfall ejection of pore water (a)

These variables fall into three general categories including: site-specific characteristics, which include soil properties and hydrologic variables; chemical-specific parameters, such as C_s; and operations-specific inputs, which are A and L. K_d is a mixture of site-specific and chemical-specific parameters.

Site-specific soil properties θ_w and ρ_b can be estimated based upon soil texture, such as silty loam, sandy clay loam, etc. There are tables for estimating field capacity and ρ_b given soil texture (see Appendix B). Field capacity can be used as an estimate for θ_w in partially saturated soils since the water content tends to fluctuate above and below the field capacity over the period of a year. *A* hydro-geo-chemical toolkit (HGCT) will be provided within TREECS for estimating site-specific soil properties as described within Appendix B.

There is a utility (see Figure 6) within the MEPAS models, including the Aquifer model, for selecting soil texture to obtain percentages of sand, silt, and clay. These percentages along with percent organic matter, percent iron and aluminum, pH, and the organic carbon to water partitioning coefficient (K_{oc}), or the octonol-water partitioning coefficient (K_{ow}), can be used to estimate K_d (Streile et al. 1996). This utility will be provided within the HGCT as described in Appendix B.



Soil class - KD-CLASS

Texture	%Sand	%Silt	%Clay
Loam	42	38	20
Silty Loam	20	65	15
Silt	7	88	5

% sand - KD-SAND 20 %
% silt - KD-SILT 63 %
% clay - KD-CLAY 15 %
% organic matter - KD-OMC 2 %
% iron and aluminum - KD-IRON 0 %
pH of soil - KD-PH 7

Figure 6. MEPAS utility for soil classification used in K_d estimation.

Constituent chemical-specific properties will be provided within TREECS using the DoD range constituent database (Zakikhani et al. 2002), and modifications to it (Dortch et al. 2005). The DoD range database includes K_{ow}, C_s, and other chemical-specific properties. The Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) constituent database (http://mepas.pnl.gov/FRAMESV1/mmede.stm) and the Risk Assessment Information System (RAIS) constituent database (http://rais.ornl.gov/index.shtml) will also be available in TREECS for specifying constituent chemical-specific properties.

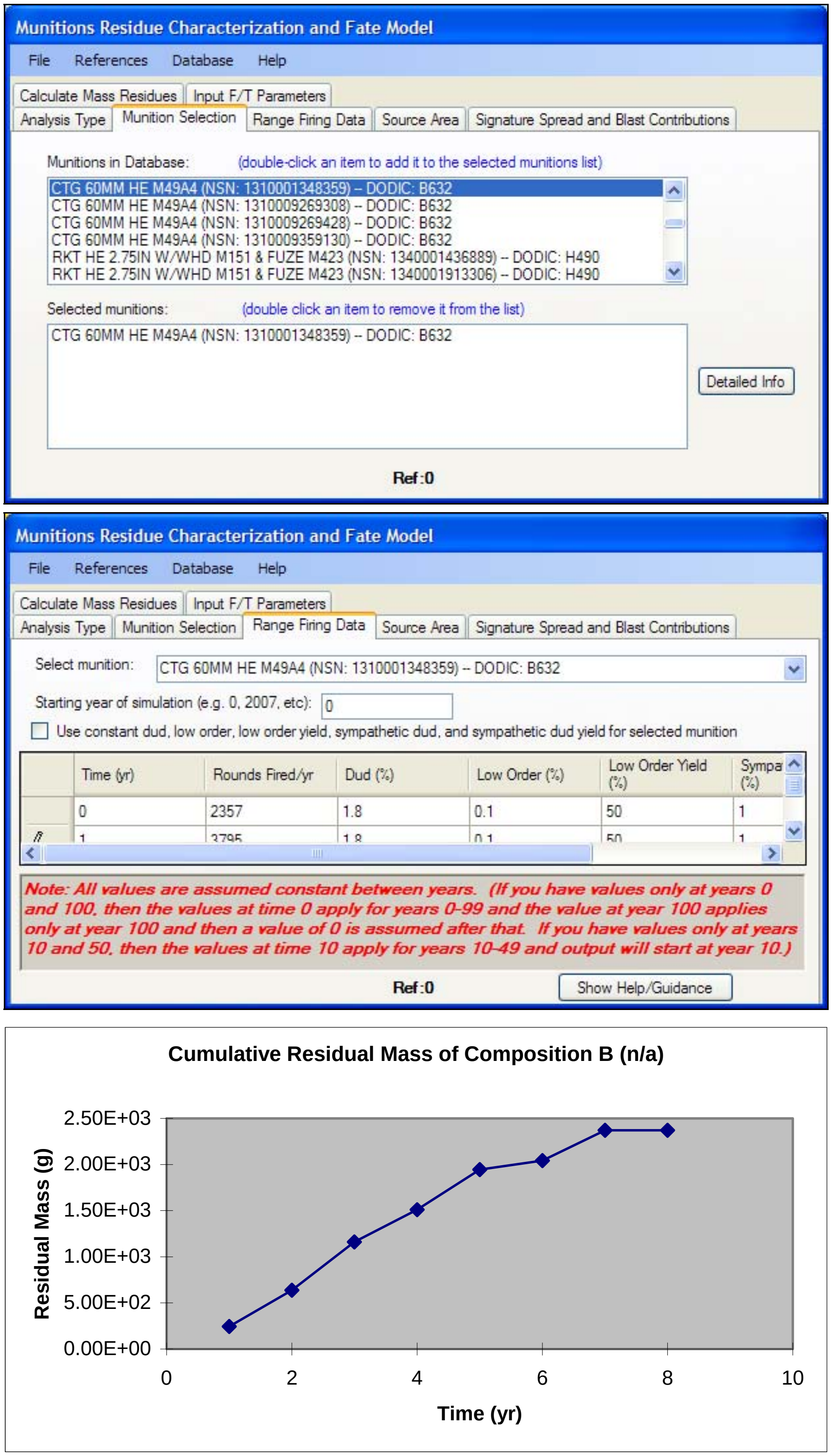
The site-specific, hydrology-related variables P, N, q_w and E can be estimated as described in Appendix B. The operations-specific variables A and L depend on the range use, such as area of the impact zone and numbers and types of munitions fired. A utility (see Figure 7) will be included in

TREECS for estimating L given the number and types (National Stock Number, NSN, of Department of Defense Identification Code, DODIC) of munitions used (Gerald et al. 2007). The MC loading utility uses the Munitions Items Disposition Action System (MIDAS) database (https://midas.dac.army.mil/) to obtain quantities of MC within each munitions type.

Aquifer model

Sensitivity tests were first conducted on the MEPAS Aquifer model described in Chapter 3 to determine which inputs are important under steady-state conditions. The sensitivity analysis was performed using version 1.7 of FRAMES (http://mepas.pnl.gov/FRAMESV1/documents/PNNL11748-frames doc.pdf). The general concepts of FRAMES are described by Whelan et al. (1997). Those parameters that are sensitive to variations will generally require the user to supply those in the model user interface. Those parameters that are not sensitive can either be ignored as input or can be estimated based on other inputs describing the site, thus simplifying the input requirements of the user.

The sensitivity analysis was begun by first creating a spreadsheet of all the input parameters in the MEPAS Aquifer model. Input parameters are listed in Table 1. Next, model test cases were created with assumed and specified values for the input parameters. No decay (i.e., a very long half-life, or WZ-GHALF = 1.o E20) of the constituent was assumed to allow highly conservative concentrations to be reached in the aquifer. The modeled constituent was RDX (Chemical Abstracts Service Registry Number, or CASRN, 121824). Also, it was assumed that 100 percent of the constituent flux that leached through the soil reached the aquifer (i.e., WZ-FRAC = 100). The literature and the FRAMES constituent database were canvassed in order to determine a typical range of values for the other input parameters. Since the application of TREECS is intended to cover all MC constituents of potential concern, the range of parameter values were obtained across many constituents where applicable. From the range of values obtained, the low, high, and typical or expected values were determined for each parameter, and a FRAMES/MEPAS aquifer test case was created for each. These test cases were run individually to steady state for each high and low input value and compared to the base test case with the expected input values, and the difference in the aquifer constituent concentration was noted. Results of this manual sensitivity testing are summarized in Table 2, including those input parameters that were found to be sensitive for steady-state conditions.



Munitions in Database: (double-click an item to add it to the selected munitions list)

CTG 60MM HE M49A4 (NSN: 1310001348359) -- DODIC: B632
CTG 60MM HE M49A4 (NSN: 1310009269308) -- DODIC: B632
CTG 60MM HE M49A4 (NSN: 1310009269428) -- DODIC: B632
CTG 60MM HE M49A4 (NSN: 1310009359130) -- DODIC: B632
RKT HE 2.75IN W/WHD M151 & FUZE M423 (NSN: 1340001436889) -- DODIC: H490
RKT HE 2.75IN W/WHD M151 & FUZE M423 (NSN: 1340001913306) -- DODIC: H490

Selected munitions: (double click an item to remove it from the list)

CTG 60MM HE M49A4 (NSN: 1310001348359) -- DODIC: B632

Select munition: CTG 60MM HE M49A4 (NSN: 1310001348359) -- DODIC: B632

Starting year of simulation (e.g. 0, 2007, etc): 0

☐ Use constant dud, low order, low order yield, sympathetic dud, and sympathetic dud yield for selected munition

Time (yr)	Rounds Fired/yr	Dud (%)	Low Order (%)	Low Order Yield (%)	Sympa (%)
0	2357	1.8	0.1	50	1
1	3795	1.8	0.1	50	1

Note: All values are assumed constant between years. (If you have values only at years 0 and 100, then the values at time 0 apply for years 0-99 and the value at year 100 applies only at year 100 and then a value of 0 is assumed after that. If you have values only at years 10 and 50, then the values at time 10 apply for years 10-49 and output will start at year 10.)

Figure 7. Screens from utility for estimating MC residue loading given munitions use.

Finally, a FRAMES test case was created where the MEPAS Sensitivity/ Uncertainty (S/U) Monte Carlo simulation module was used to perform 500 realizations in order to determine whether there are any statistically significant parameters whose variations affect the constituent concentration in the saturated zone. The distributions of the input parameters were all set as normal distributions with the exception of the dry bulk density, which was set to a log normal distribution. The groundwater half-life parameter was excluded from the S/U module and assumed to be fixed at a very high value in order to achieve no decay and therefore provide a conservative estimate of groundwater contaminant concentration.

Table 1. MEPAS aquifer model input parameters.

Parameter Name	Units	Description
WZ-SAND	%	Percentage of sand
WZ-SILT	%	Percentage of silt
WZ-CLAY	%	Percentage of clay
WZ-OMC	%	Percentage of organic matter
WZ-IRON	%	Percentage of iron and aluminum
WZ-FRAC	%	Percentage of constituent flux entering the aquifer
WZ-PH	Dimensionless	pH of the pore water
WZ-TOTPOR	% or fraction	Total porosity
WZ-EFFPOR	% or fraction	Effective porosity
WZ-PVELOC	cm/day	Darcy velocity
WZ-THICK	m	Thickness of aquifer
WZ-BULKD	g/cm^3	Soil dry bulk density
WZ-DIST	m	Longitudinal distance to well
WZ-YDIST	m	Perpendicular distance from plume center-line to well
WZ-AQDEPTH	m	Vertical distance below water table to well intake
WZ-LDISP	m	Longitudinal dispersivity
WZ-TDISP	m	Transverse dispersivity
WZ-VDISP	m	Vertical dispersivity
WA-SUBKD	ml/g	Sorption partitioning coefficient
WZ-RSOL	mg/L	Water solubility
WZ-GHALF	years	Half-life of constituent in groundwater

Table 2. Important MEPAS aquifer model input parameters determined from manual sensitivity analysis.

Parameter Name	Description
WZ-PVELOC	Darcy velocity
WZ-DIST	Longitudinal distance to well
WZ-AQDEPTH	Vertical distance below water table to well intake
WZ-YDIST	Perpendicular distance from plume center-line to well
WZ-THICK	Thickness of aquifer
WZ-LDISP	Longitudinal dispersivity
WZ-TDISP	Transverse dispersivity
WZ-VDISP	Vertical dispersivity

Results of the S/U analysis indicated that variance of certain input parameters could have more significance than others on the constituent concentration in the aquifer. Table 3 lists parameters that the S/U analysis determined as being sensitive. For the values shown in the last column of Table 3, the lower numbers indicate greater significance. The primary parameters that showed significance were the same as those of the manual analysis (Table 2) with the exception of the addition of the sorption partitioning coefficient. Both the depth from water table to well and aquifer thickness were found to be moderately sensitive ($Pr\ (>t) = 0.14$ to 0.15).

Table 3. S/U module analysis results for significant MEPAS Aquifer model input parameters.

Parameter Name	Description	Significance Rating (Pr(>|t|))*
WZ-PVELOC	Darcy velocity	1.01E-11
WZ-DIST	Longitudinal distance to well	0.0805
WZ-AQDEPTH	Vertical distance below water table to well intake	0.150
WZ-THICK	Thickness of aquifer	0.145
WZ-YDIST	Perpendicular distance from plume center-line to well	0.000825
WZ-VDISP	Vertical dispersivity	1.11E-08
WZ-TDISP	Transverse dispersivity	0.000800
WZ-LDISP	Longitudinal dispersivity	0.018960
WA-SUBKD	Adsorption coefficient	0.063495

* Lower values indicate greater significance of the variation of the parameter on the output

The simulation period is an input that requires special consideration when performing the S/U analysis on the MEPAS Aquifer model. The S/U module searches the model output looking for the maximum concentration, which should occur after reaching steady state. However, not all sensitivity runs may have reached steady state, potentially and erroneously indicating sensitivity. By default, the model will only run a simulation for up to 10,000 years maximum. The simulation run length can be set to greater than 10,000 years by the user, but then the run is limited to only 40 time-steps. Obviously, this limitation can have serious drawbacks in certain circumstances. Thus, there are some questions regarding the S/U results of Table 3, such as the sorption partitioning coefficient, which should not be important at steady state.

Based upon the S/U analysis, the Darcy velocity was the most sensitive parameter, which is expected because of its impact on the dispersion of the constituent. Thus, the Darcy velocity will have to be input by the user, but the HGCT within TREECS can be used for estimating Darcy velocity (see Appendix B).

Vertical, transverse, and longitudinal dispersivity were sensitive as well, but the TREECS aquifer model can estimate these. The model will be applied within Tier 1 of TREECS such that these three dispersivity parameters are internally calculated and set, freeing the user of having to input them, but the user will still have the option of inputting each.

The perpendicular distance from plume center-line to well and the depth from water table to well intake were sensitive, but a worst-case value of zero will be assumed for these parameters in order to ensure a maximum (conservative) groundwater concentration estimate. The longitudinal distance to the well was also a sensitive parameter, thus, the TREECS aquifer model will require that the user supply the longitudinal distance to the well(s).

The sorption partitioning coefficient was indicated as sensitive, but as noted above, this is probably due to not reaching steady state in the S/U analysis. A low value for a default partitioning coefficient will be set internally such that steady state can be achieved in a relatively short period of time.

Finally, the aquifer model is moderately sensitive to the thickness of the aquifer, so information for this parameter must be supplied by the user. A default value of 30 m will be provided.

Two additional input parameters, length (L_f) and width (W_f) of the source flux zone, were discovered following the above analysis. These two inputs are normally provided to the aquifer model from an upstream model, such as vadose zone model or a known source of infiltrating flow and contaminant mass. Thus, these two inputs were not varied during the sensitivity analysis. However, these two parameters can affect aquifer concentrations when the receptor well is close to the source of contamination, such as less than 10 times the source width. W_f is defined as the site source dimension that is perpendicular to the groundwater flow. L_f is the site source dimension that is parallel to the groundwater flow. The downstream longitudinal distance of the well (WZ-DIST) is measured from the site center, or at $L_f/2$. As a rule of thumb, the well should not be closer than 1.5 L_f from the site center to properly apply the MEPAS aquifer model. The user will be required to enter L_f and W_f. Infiltrating water flux (m^3/yr) from soil to aquifer is also required, but this information will be available from the soil model application.

The methods for supplying all inputs required for the Tier 1 MEPAS aquifer model are summarized in Table 4. The list has been reduced to only five input parameters that must be provided by the user along with five optional inputs.

Time-varying models, such as the MEPAS aquifer model, can be used for steady-state analyses if they are run for a long time (e.g., hundreds of years) with a constant loading to reach steady state. It is possible that under some unusual conditions, such as a very low Darcy velocity, steady state will not have been reached with the default maximum simulation time of 10,000 years. The model is designed to run long enough to reach a peak in aquifer concentration as long as that peak occurs within 10,000 years. Times-to-peak that exceed 10,000 years are probably not of concern for range management anyway.

Surface Water Model

Sensitivity tests were conducted on the RECOVERY surface water model described in Chapter 3 to determine which inputs are important under steady-state conditions. The sensitivity analysis was performed using version 1.7 of FRAMES, as was done with the MEPAS aquifer model. Those parameters that are sensitive to variations will generally require the user to supply those in the model user interface. Those parameters that are not sensitive can either be ignored as input or can be estimated based on other inputs describing the site, simplifying the input requirements of the user.

Table 4. Methods for setting Tier 1 MEPAS aquifer model inputs.

Parameter Name	Units	Description	Method of Obtaining Input
WZ-SAND	%	Percentage of sand	Assumed to be 32 although it won't affect Tier 1 results
WZ-SILT	%	Percentage of silt	Assumed to be 33 although it won't affect Tier 1 results
WZ-CLAY	%	Percentage of clay	Assumed to be 33 although it won't affect Tier 1 results
WZ-OMC	%	Percentage of organic matter	Assumed to be 2 although it won't affect Tier 1 results
WZ-IRON	%	Percentage of iron and aluminum	Assumed to be 0.0 although it won't affect Tier 1 results
WZ-FRAC	%	Percentage of constituent flux entering the aquifer	Assumed to be 100
WZ-PH	Dimensionless	pH of pore water	Assumed to be 7.0 although it won't affect Tier 1 results
WZ-TOTPOR	% or fraction	Total porosity	Assumed to be 50% although it won't affect Tier 1 results
WZ-EFFPOR	% or fraction	Effective porosity	Assumed to be 45% although it won't affect Tier 1 results
WZ-PVELOC	cm/day	Darcy velocity	Specified by user or estimated by HGCT
WZ-THICK	m	Thickness of aquifer	Specified by user with a default value of 30 m
WZ-BULKD	g/cm^3	Soil dry bulk density	Set to 1.33 although it won't affect Tier 1 results
WZ-DIST	m	Longitudinal distance to well measured from center of source zone	Specified by user
L_f	m	Site source zone dimension parallel to groundwater flow	Specified by user
W_f	m	Site source zone dimension perpendicular to groundwater flow	Specified by user
WZ-YDIST	m	Perpendicular distance from plume center-line to well	Default set to 0.0
WZ-AQDEPTH	m	Vertical distance below water table to well intake	Default set to 0.0
WZ-LDISP	m	Longitudinal dispersivity	Calculated by MUI

Parameter Name	Units	Description	Method of Obtaining Input
WZ-TDISP	m	Transverse dispersivity	Calculated by MUI
WZ-VDISP	m	Vertical dispersivity	Calculated by MUI
WA-SUBKD	ml/g	Sorption partitioning coefficient	Set to 1.0 although it won't affect Tier 1 results
WZ-RSOL	mg/L	Water solubility	Obtained from constituent database although it won't affect Tier 1 results
WZ-GHALF	years	Half-life of constituent in groundwater	Set to 1.0 E20

Note: Turquoise shaded parameters must be provided by the user; green shaded parameters are optional inputs by the user

The sensitivity analysis was begun by first creating a spreadsheet of all the input parameters in the RECOVERY Surface Water model. The parameters are listed in Table 5. Next, a base case was created with typical values for the input parameters and assuming no decay of the constituent (RDX, CASRN 121824, was assumed for the base case) and which would reach a steady-state constituent concentration in the water column and sediment bed faster. No decay was assumed in order to yield a conservative estimate of the concentration of contaminant in the water column and sediment. Next, literature and the FRAMES constituent database were canvassed in order to determine a typical range of values for the given input parameters. Note that since the application of TREECS is intended to cover all possible MCOC, parameter values were obtained across many constituents where applicable. Using the range of values obtained, low and high values were determined for each parameter and then a FRAMES test case was created for each. These test cases were run individually and compared to the base test case and the effect on the surface water dissolved concentration and sediment total concentration noted. A list was formulated based on those results for potential parameters which could be sensitive. That list is shown in Table 6.

Table 5. RECOVERY surface water model input parameters.

Parameter Name	Units	Description
rHKEnhancedDiff	cm^2/sec	Enhanced diffusion
rHKenhancedMixDepth	cm	Enhanced mixing depth
rMolecularDiffusivity	cm^2/sec	Molecular diffusivity
rHLC	$Atm-m^3/g-mole$	Henry's Law Constant
rMW	g-mole	Molecular weight

Parameter Name	Units	Description
rKow	(mg/m^3 octanol)/ (mg/m^3 water)	Octanol-water partition coefficient
rDecayCoeffDissContInH2O	1/yr	Decay coefficient for dissolved contaminant in water
rDecayCoeffDissContInMixed	1/yr	Decay coefficient for dissolved contaminant in mixed layer
rDecayCoeffDissContInDeepSed	1/yr	Decay coefficient for dissolved contaminant in deep sediment
rDecayCoeffPartContInH2O	1/yr	Decay coefficient for particulate contaminant in water
rDecayCoeffPartContInMixed	1/yr	Decay coefficient for particulate contaminant in mixed layer
rDecayCoeffPartContInDeepSed	1/yr	Decay coefficient for particulate contaminant in deep sediment
rContamConcInH2O	µg/L	Initial contaminant concentration in water
rWaterInflowConc	µg/L	Water inflow contaminant concentration
rExternalLoad	kg/yr	Additional contaminant constant external loading rate
rInitConcMixedLyr	mg/kg	Initial contaminant concentration in mixed sediment
rCs0	mg/kg	Initial contaminant concentration in deep sediment
rKdwPartitionCoeff	L/kg	Partition coefficient for the water column
rKdmPartitionCoeff	L/kg	Partition coefficient for the mixed sediment pore water
rKdsPartitionCoeff	L/kg	Partition coefficient for the deep sediment pore water
rInitConcDeepSed	mg/kg	Deep sediment profile concentration
rSuspSolidsConcInH2O	mg/L	Suspended solids concentration
rWghtFracCarbonSolidsInH2O	Fraction	Weight fraction carbon in solids in water column
rWaterSurfaceArea	m^2	Water surface area
rWaterDepth	m	Surface water depth
rFlowThrough	m^3/yr	Water flow through
rTau	Yr	Residence time
rL_contamSedDepth	m	Contaminated sediment depth
rZ_depthOfMixedLayer	m	Depth of mixed sediment layer
rMixedLyrSurfaceArea	m^2	Mixed sediment layer surface area
rMixedSedPorosity	Fraction	Mixed sediment layer porosity
rMixedSedParticleDen	g/cm^3	Mixed sediment specific gravity
rWghtFracCarbonSolidsInMixed	Fraction	Mixed sediment layer weight fraction carbon in solids
rDeepSedPorosity	Fraction	Deep sediment porosity

Parameter Name	Units	Description
rDeepSedParticleDen	g/cm^3	Deep sediment specific gravity
rWghtFracCarbonSolidsInSed	Fraction	Deep sediment layer weight fraction carbon in solids
rWindSpeed	m/sec	Wind speed
rSettlingVelocity	m/yr	Settling velocity
rBurialVelocity	m/yr	Burial velocity
rResusVelocity	m/yr	Resuspension velocity
rCalcSettlingVel	m/yr	Calculated velocity (i.e., the one chosen to be calculated – burial velocity for this case)

Table 6. Tentative list of significant RECOVERY surface water model input parameters based on manual sensitivity analysis.

Parameter Name	Description
rKow	Octanol-water partition coefficient
rFlowThrough	Water flow through
rWghtFracCarbonSolidsInMixed	Mixed sediment layer weight fraction carbon in solids
rMixedSedPorosity	Mixed sediment layer porosity
rWindSpeed	Wind speed
rSettlingVelocity	Settling velocity
rHLC	Henry’s Law Constant
rMolecularDiffusivity	Molecular diffusivity
rWaterSurfaceArea	Water surface area
rTau	Residence time
rMixedLyrSurfaceArea	Mixed sediment layer surface area (equal to water surface area)

The list in Table 5 was narrowed down in order to allow the MEPAS S/U module to be used. Finally, a FRAMES test case was created where the MEPAS S/U module was used to perform 500 realizations in order to determine whether there are any statistically significant parameters in which variations affect the constituent concentration in the water column and sediment bed. Table 7 shows the list of input parameters that were treated as uncertain in the MEPAS S/U module. A few of the input parameters (i.e. burial velocity, mixed layer sediment surface area, and residence time) were calculated from other parameters. Mixed layer sediment surface area was set equal to the water column surface area. The distributions of the input parameters that were not calculated or assumed were all set as normal distributions with the exception of the resuspension velocity, which was set to a uniform distribution and only allowed to vary between 1.0E-20 and 1.1E-20 m/yr. Resuspension velocity was done in this manner in order to keep it essentially constant and near zero, but to still allow it to be used in the equation for calculating the burial velocity within the S/U module. Excluded from the S/U module was all of decay rate parameters, which were assumed would be fixed at zero values in order to achieve no decay and therefore provide a conservative estimate of the concentration of contaminant in the water column and sediment bed.

Table 7. List of RECOVERY input parameters treated as uncertain in the MEPAS S/U module.

Parameter Name	Description
rMolecularDiffusivity	Molecular diffusivity
rKow	Octanol-water partition coefficient
rSuspSolidsConcInH2O	Suspended solids concentration
rWghtFracCarbonSolidsInH2O	Weight fraction carbon in solids in water column
rWaterSurfaceArea	Water surface area
rWaterDepth	Surface water depth
rFlowThrough	Water flow through
rTau	Residence time
rZ_depthOfMixedLayer	Depth of mixed sediment layer
rMixedLyrSurfaceArea	Mixed sediment layer surface area
rMixedSedPorosity	Mixed sediment layer porosity
rMixedSedParticleDen	Mixed sediment specific gravity
rWghtFracCarbonSolidsInMixed	Mixed sediment layer weight fraction carbon in solids
rDeepSedPorosity	Deep sediment porosity
rDeepSedParticleDen	Deep sediment specific gravity
rWghtFracCarbonSolidsInSed	Deep sediment layer weight fraction carbon in solids
rSettlingVelocity	Settling velocity
rResusVelocity	Resuspension velocity
rCalcSettlingVel	Calculated velocity (i.e. the one chosen to be calculated – burial velocity for this case)

Results of the S/U analysis indicated that variance of certain input parameters could have more significance than others on the constituent concentration in the water column and sediment bed. Table 8 shows the list of parameters which the S/U analysis determined as sensitive. The primary parameters showing significance were residence time, deep sediment porosity, mixed sediment layer weight fraction of carbon in solids, molecular diffusivity, weight fraction of carbon in solids in the water column, depth of mixed sediment layer, flow through, mixed sediment layer porosity, surface water area, and settling velocity. Note that for the values shown in the last column of Table 8, the lower numbers indicate greater significance. It is possible that some significant parameters were determined to be significant as a result of the simulation not reaching steady state, whereas, if steady state conditions had been reached early in the simulation, those parameters may not have been determined as significant.

Table 8. S/U module results of significant RECOVERY surface water model input parameters.

Parameter Name	Description	Significance Rating (Pr(>|t|))*
rTau	Residence time	4.42E-05
rDeepSedPorosity	Deep sediment porosity	0.000212
rWghtFracCarbonSolidsInMixed	Mixed sediment layer weight fraction carbon in solids	0.014121
rMolecularDiffusivity	Molecular diffusivity	0.02567
rWghtFracCarbonSolidsInH2O	Weight fraction carbon in solids in water column	0.025795
rZ_depthOfMixedLayer	Depth of mixed sediment layer	0.03688
rFlowThrough	Flow through	0.040968
rMixedSedPorosity	Mixed sediment layer porosity	0.043263
rWaterDepth	Surface water depth	0.087289
rWaterSurfaceArea	Water surface area	0.087433
rSettlingVelocity	Settling velocity	0.089088

* Lower values indicate greater significance of the variation of the parameter on the output

Comparison of Tables 6 and 8 reveals that several input parameters showed up as sensitive in the manual assessment but not in the S/U analysis, and vice-versa. The reasons for these differences could not be fully explained, but in some cases, the reason may have been a result of the S/U simulation not reaching steady state. The full list of potentially sensitive input parameters includes all of Table 8, plus the addition of K_{ow}, wind speed, Henry's law constant, and the mixed sediment layer surface area. The mixed sediment layer surface area will be set equal to the water surface area. The previous three inputs are related to sorption and volatilization, where K_{ow} and Henry's law constant are chemical-specific parameters that will be supplied by the constituent database. Wind speed will be set to a typical average default value of 6 m/s in the user interface, but users can change this value to better fit their site. The map shown in Figure 8 can be used as a guide for selecting average wind speed values. The user may also visit the Web site, http://www.awea.org/faq/usresource.html, to get a better view of this map and the legend.

Residence time was one of the most sensitive parameters, which is expected. The TREECS surface water model will calculate the residence time based on water volume and flow rate. In a Tier 1 analysis, the user must provide information regarding surface water dimensions. The user must also provide the water flow rate. If the receiving water is an enclosed water body, such as a lake, wetland, or pond, then the user must input the water surface area and average depth, and the residence time will be computed by the model. If the receiving water is a stream, then the user must input the stream average width and depth, and the model will calculate the stream reach length such that the water residence time is approximately 0.1 year, as explained in Appendix A.

The deep sediment porosity was sensitive as well according to the S/U analysis, but it was not sensitive according to the manual sensitivity analysis. Sensitivity based on the S/U analysis may have been due to not having reached steady state. For the Tier 1 TREECS surface water model, a default value of 0.5 will be set, which is a typical value for deep sediment.

The mixed sediment layer weight fraction of carbon in solids was sensitive, and the TREECS surface water model will require the user to provide a value for this parameter. The molecular diffusivity was sensitive, but the TREECS surface water model will use the value from the constituent database.

The weight fraction of carbon in solids in the water column was sensitive according to the S/U analysis, but not according to the manual sensitivity analysis. It will be assumed that this parameter value is equal to the mixed sediment layer weight fraction of carbon in solids.

The depth or thickness of the mixed sediment layer was sensitive according to the S/U analysis, but not according to the manual sensitivity analysis. The TREECS surface water model will use a default value for this parameter of 0.07 m. Flow through was sensitive, and, as mentioned above, the TREECS surface water model will require the user to provide a value.

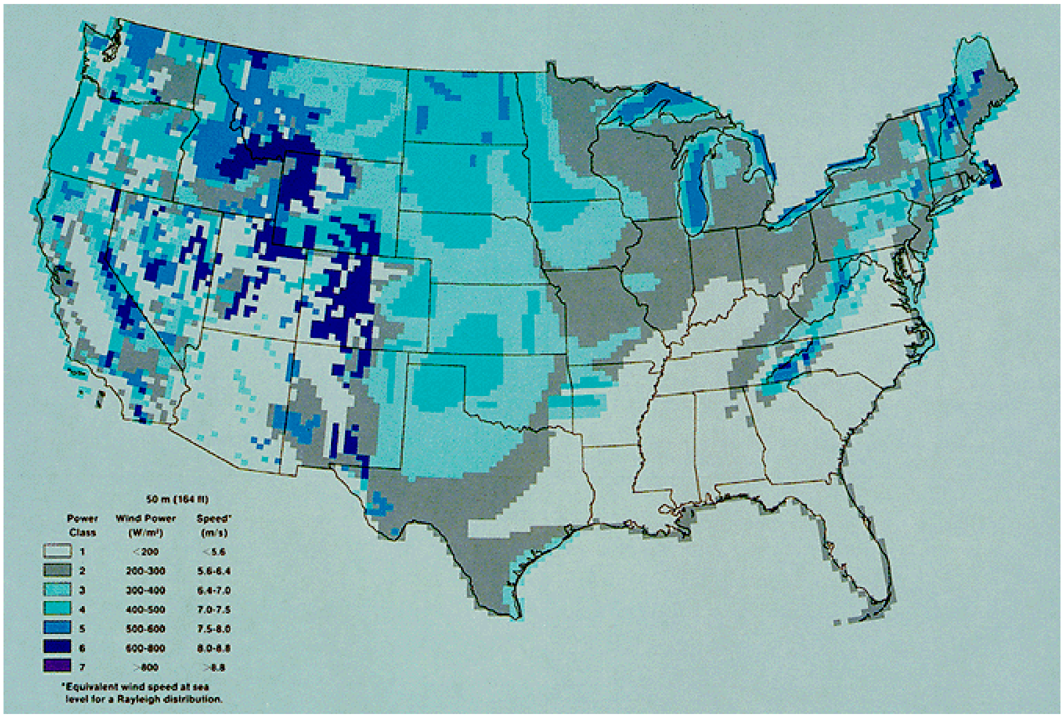


Figure 8. Average wind speeds for the United States (from Renewable Resource Data Center, National Renewable Energy Laboratory).

Mixed sediment layer porosity was sensitive, and the TREECS surface water model will assume a default value of 0.7, which is reasonable for surficial sediments. Also, this value produces a conservative (high) estimate of mixed sediment concentration. The user will have the option to change this parameter. The steady-state contaminant concentration in the water column was not sensitive to values of the mixed sediment porosity.

Water depth and surface area were sensitive, and the user will be required to input a value for depth as discussed previously. Surface water area will also be required input for enclosed water bodies, but stream width will be required for streams and rivers.

The settling velocity was sensitive, but a default value of 0.1 m/day (36 m/yr) will be set for the TREECS surface water model. This value is typical for fine grain sediment that is more likely to hold sorbed contaminants, but users will be able to change this value if they wish.

In the TREECS surface water model, the resuspension velocity will be fixed to a very small value (e.g. 1.0E-20 m/yr), or essentially zero, so that the user will not have to supply a value for it. Results are insensitive to resuspension at steady-state. With values for settling and resuspension velocities specified, the burial velocity can and will be calculated.

Table 9 summarizes RECOVERY surface water model inputs and how they will be handled with Tier 1 TREECS. This list has been reduced to only four input parameters that must be provided by the user. Six additional inputs are optional for specification by the user. The length of the simulation in years is also a RECOVERY model input, but it will be set to 100 years, which is long enough to reach steady state.

Table 9. Methods for setting Tier 1 RECOVERY surface water model inputs.

Parameter Name	Units	Description	Method of Obtaining Input
rHKEnhancedDiff	cm^2/sec	Enhanced diffusion	Set to 0.0
rHKenhancedMixDepth	cm	Enhanced mixing depth	Set to 0.0
rMolecularDiffusivity	cm^2/sec	Molecular diffusivity	Obtained from constituent database
rHLC	Atm-m^3/ g-mole	Henry's Law Constant	Obtained from constituent database
rMW	g-mole	Molecular weight	Obtained from constituent database
rKow	(mg/m^3 octanol)/ (mg/m^3 water)	Octanol-water partition coefficient, K_{ow}	Obtained from constituent database*
rDecayCoeffDissContInH2O	1/yr	Decay coefficient for dissolved contaminant in water	Set to 0.0
rDecayCoeffDissContInMixed	1/yr	Decay coefficient for dissolved contaminant in mixed layer	Set to 0.0
rDecayCoeffDissContInDeepSed	1/yr	Decay coefficient for dissolved contaminant in deep sediment	Set to 0.0
rDecayCoeffPartContInH2O	1/yr	Decay coefficient for particulate contaminant in water	Set to 0.0
rDecayCoeffPartContInMixed	1/yr	Decay coefficient for particulate contaminant in mixed layer	Set to 0.0
rDecayCoeffPartContInDeepSed	1/yr	Decay coefficient for particulate contaminant in deep sediment	Set to 0.0
rContamConcInH2O	μg/L	Initial contaminant concentration in water	Set to 0.0
rWaterInflowConc	μg/L	Water inflow	Set to 0.0

Parameter Name	Units	Description	Method of Obtaining Input
		contaminant concentration	
rExternalLoad	kg/yr	Additional contaminant constant external loading rate	Provided by soil model as computed erosion and runoff flux to surface water
rInitConcMixedLyr	mg/kg	Initial contaminant concentration in mixed sediment	Set to 0.0
rCs0	mg/kg	Initial contaminant concentration in deep sediment	Set to 0.0
rKdwPartitionCoeff	L/kg	Partition coefficient for the water column	Computed from K_{ow} and fraction organic carbon in solids in water for organic constituents; input by user for inorganic constituents.
rKdmPartitionCoeff	L/kg	Partition coefficient for the mixed sediment pore water	Computed from K_{ow} and fraction organic carbon in solids in mixed layer for organic constituents; input by user for inorganic constituents.
rKdsPartitionCoeff	L/kg	Partition coefficient for the deep sediment pore water	Computed from K_{ow} and fraction organic carbon in solids in deep sediment for organic constituents; input by user for inorganic constituents.
rInitConcDeepSed	mg/kg	Deep sediment profile initial concentration	Set to 0.0
rSuspSolidsConcInH2O	mg/L	Suspended solids concentration	Set to 100 although it has little affect Tier 1 results
rWghtFracCarbonSolidsInH2O	fraction	Weight fraction carbon in solids in water column	Set equal to weight fraction carbon in solids in mixed sediment layer
rWaterSurfaceArea	m^2	Water surface area	Specified by user for enclosed water bodies; calculated from width and length of reach for streams where width is input by user and length is calculated to yield residence time of 0.1 yr
rWaterDepth	m	Surface water depth	Specified by user
rFlowThrough	m^3/yr	Water flow through	Specified by user
rTau	yr	Residence time	Calculated or assumed to be 0.1 yr for streams
rL_contamSedDepth	m	Contaminated sediment depth	Set to 1.0
rZ_depthOfMixedLayer	m	Depth of mixed sediment layer	Set to 0.07
rMixedLyrSurfaceArea	m^2	Mixed sediment layer surface area	Set equal to the water surface area
rMixedSedPorosity	fraction	Mixed sediment layer porosity	Default set to 0.7

Parameter Name	Units	Description	Method of Obtaining Input
rMixedSedParticleDen	g/cm^3	Mixed sediment specific gravity	Set to 2.65
rWghtFracCarbonSolidsInMixed	fraction	Mixed sediment layer weight fraction carbon in solids	Specified by user
rDeepSedPorosity	fraction	Deep sediment porosity	Set to 0.5
rDeepSedParticleDen	g/cm^3	Deep sediment specific gravity	Set to 2.65
rWghtFracCarbonSolidsInSed	fraction	Deep sediment layer weight fraction carbon in solids	Set equal to mixed sediment layer weight fraction carbon in solids
rWindSpeed	m/sec	Wind speed	Default value of 6.0 with option for user to change the value; only used for volatile MC
rSettlingVelocity	m/yr	Settling velocity	Default value of 36.0 with option for user to change the value
rBurialVelocity	m/yr	Burial velocity	Computed by the model
rResusVelocity	m/yr	Resuspension velocity	Set to 1.0 E-20
rCalcSettlingVel	m/yr	Calculated velocity (i.e., the one chosen to be calculated – burial velocity for this case)	Burial velocity selected

Note: Turquoise-shaded parameters must be provided by the user; green-shaded parameters are optional inputs by the user

*If a value of the organic carbon to water partition coefficient (K_{oc}) is found in the constituent database, then K_{oc} will be used to compute K_d from $K_d = f_{oc}K_{oc}$ where f_{oc} is the fraction of organic carbon in sediment solids. The input value of K_{ow} for RECOVERY will be adjusted to yield the same computed K_d from the relation used in the model, which is $K_d = 0.6 f_{oc}K_{ow}$. Thus, the adjusted RECOVERY input value of K_{ow} is the database value of K_{oc} divided by 0.6.

5 Summary

The Tier 1 approach for TREECS is based on highly conservative steady-state (time-invariant) assumptions where MC loadings to the range are constant over time, and receiving water media reach a constant MC concentration that can be compared with ecological and human protective health benchmarks for compliance forecasting. Furthermore, it is assumed that MC does not degrade or decay. This approach allows rapid assessments that can be conducted with minimum training or modeling expertise and limited data input requirements. Tier 1 should prove useful during Phase II of ORAP. If a Tier 1 assessment indicates a potential concern, the analysis should proceed to a Tier 2 assessment and/or site data collection. Results from a Tier 1 assessment can also be used to consider the effects of different range usage strategies on compliance. Tier 2 will be better suited than Tier 1 for assessing metals fate since weathering and subsequent dissolution processes can take many years to occur, and thus, steady-state assumptions can lead to overly conservative projections.

TREECS Tier 1 will include an analytical range soil model with its computed leaching flux linked to a semi-analytical-numerical aquifer model and with its computed runoff and erosion fluxes linked to a numerical surface water model. This report primarily describes the basis for the models and how they will be implemented.

An MC loading module will be provided to estimate mass loadings of MC into the range soil. A hydro-geo-chemical toolkit will also be provided for estimating key site- and constituent-specific input parameters. Constituent databases will be available to provide chemical-specific properties, and a database of ecological and human protective health benchmarks, which are being gathered by the DoD services, will be included for compliance determinations. All components will be packaged within a user-friendly PC client-based application with an emphasis on ease of use.

It is envisioned that a range-specific application should not take more than a few hours to set up and to provide output indicating whether or not a particular range operation will ever cause MC concentrations at target media locations, such as groundwater wells or a down-gradient receiving stream/pond/lake/wetland, to exceed protective health benchmarks.

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Appendix A: Surface Water Testing

In the RECOVERY model, the system to be modeled is idealized as a well-mixed surface water layer underlain by a vertically stratified sediment column. However, RECOVERY was not conceptually designed as a model for streams. Because of this, an effort was undertaken to determine whether it could still be used in TREECS Tier 1 with sufficient accuracy, given a range of flow rates and pre-defined stream lengths. In this modeling comparison effort, RECOVERY and the Contaminant Model for Streams (CMS, a model designed for simulating streams) were set up in a manner such that model results of each for stream lengths of 10, 100, 1,000, and 10,000 m could be compared at four different flow rates of 3,000, 1,000,000, 3,000,000, and 30,000,000 m^3/yr. Both models were run to steady state for comparisons. Additionally, CMS output was generated at stream length mid-points and terminus in order to determine whether CMS model results vary appreciably along the stream length.

The CMS model indicated that at steady state, there were no appreciable differences (less than about 0.05 percent) in water or sediment concentrations between mid-reach and terminus for most of the simulated stream lengths and flow rates, indicating fairly uniform conditions longitudinally for the conditions evaluated. Longitudinal gradients were computed by CMS for the lowest flow condition and the longer stream lengths.

RECOVERY-computed concentrations were compared with CMS-computed concentrations located at the terminus for all stream lengths and flows, as shown in Tables A1 and A2. The sediment total and surface water dissolved concentrations for RECOVERY and CMS differed by less than 5 percent at the lowest simulated flow rate and for the 10-m length, but varied substantially (see Tables A1 and A2) at the lowest flow rate for the 100, 1,000, and 10,000 m lengths. However, RECOVERY and CMS compared very closely for the remaining flow rates with all stream lengths, with differences between RECOVERY and CMS ranging from 0 to about 13.4 percent (see Tables A1 and A2). In all cases, RECOVERY concentrations were the same as or slightly higher than CMS, or more conservative. The concentration differences increased in order from the shortest to longest stream length, but differences decreased when comparing lower to higher flow rates for a given reach length. Therefore, it was concluded that RECOVERY can provide reasonable and conservative estimates for receiving water concentrations within the vicinity and downstream (at least up to 10 km) of the MC influx for a wide range of expected flow conditions in the receiving streams.

Table A1. Water column dissolved concentration.

Reach Length, m	Flow Rate, m^3/yr							
	3,000		1,000,000		3,000,000		30,000,000	
	CMS, mg/L	RECOVERY, mg/L	CMS, mg/L	RECOVERY, mg/L	CMS, mg/L	RECOVERY, mg/L	CMS, mg/L	RECOVERY, mg/L
10	6.11E-02	6.40E-02	2.00E-04	2.00E-04	6.67E-05	6.67E-05	6.67E-06	6.67E-06
100	3.49E-02	4.70E-02	1.99E-04	2.00E-04	6.66E-05	6.66E-05	6.67E-06	6.67E-06
1,000	5.62E-03	1.29E-02	1.95E-04	1.98E-04	6.61E-05	6.64E-05	6.66E-06	6.66E-06
10,000	3.21E-07	1.56E-03	1.57E-04	1.78E-04	6.11E-05	6.40E-05	6.61E-06	6.64E-06

Table A2. Sediment total concentration.

Reach Length, m	Flow Rate, m^3/yr							
	3,000		1,000,000		3,000,000		30,000,000	
	CMS, mg/kg	RECOVERY, mg/kg	CMS, mg/kg	RECOVERY, mg/kg	CMS, mg/kg	RECOVERY, mg/kg	CMS, mg/kg	RECOVERY, mg/kg
10	2.78E-02	2.91E-02	9.11E-05	9.10E-05	3.04E-05	3.03E-05	3.04E-06	3.03E-06
100	1.59E-02	2.14E-02	9.08E-05	9.09E-05	3.03E-05	3.03E-05	3.04E-06	3.03E-06
1,000	2.56E-03	5.85E-03	8.86E-05	8.98E-05	3.01E-05	3.02E-05	3.03E-06	3.03E-06
10,000	1.46E-07	7.08E-04	7.15E-05	8.08E-05	2.78E-05	2.91E-05	3.01E-06	3.02E-06

Residence times for each stream reach length and flow are shown in Table A3. Residence time is defined as the reach volume divided by the flow rate. The residence times varied from 1.0 E-4 to 1,000 years with the lowest times associated with the higher flows and shorter reaches. By comparing Tables A1 or A2 with Table A3, it is evident that for residence times on the order of a year or less, RECOVERY compares closely with CMS and thus should be suitable for modeling streams.

The stream flow rate will be a required input for any specific application. RECOVERY also requires the water body surface area and depth, which yields a water volume. The surface area is the product of the water body width and length. For enclosed standing surface water, such as ponds, wetlands, or lakes, the surface area can be easily estimated and should be used as input. The computed concentrations will be the total water body average. However, for a stream or river, the stream length and width define the surface area, which can affect the stream reach average concentrations computed by RECOVERY. Thus, with a single reactor CSTR model like RECOVERY, it is important to provide an appropriate stream reach for the analysis when the choice of length may be subjective. The objective is to pre-set or calculate the stream length within Tier 1 so that the user does not have to worry about choosing an appropriate stream length. The user will still be required to enter the stream width and depth.

From examination of Tables A1-A3, it is obvious that at steady state, the stream length has little to no effect on the concentration for a given flow, as long as the residence time is a year or less and no effect when residence time is 0.1 year or less. Thus, the stream reach should be calculated within the surface model interface such that the residence time is equal to 0.1 year. Once the user has entered the stream width, depth, and annual average flow, the user interface can calculate the required stream reach length required to yield a water residence time of 0.1 year.

Table A3. Residence time, years.

Reach Length, m	Flow Rate, m^3/yr			
	3,000	1,000,000	3,000,000	30,000,000
10	1	0.003	0.001	0.0001
100	10	0.03	0.01	0.001
1,000	100	0.3	0.1	0.01
10,000	1,000	3.0	1.0	0.1

Appendix B: Hydro-geo-chemical Toolkit

A hydro-geo-chemical toolkit (HGCT) will be developed and incorporated within TREECS for estimating site-specific parameters and properties that are related to hydro-geologic factors and chemical-specific properties. Methods to be initially implemented within the HGCT are described within this appendix.

Fate parameters

The only soil fate parameter required for Tier 1 of TREECS is the soil-water partition coefficient K_d for sorption of aqueous phase constituents. For organic constituents K_d can be estimated from fraction by weight of organic matter in the soil and the organic carbon to water partition coefficient K_{oc} as follows

$$K_d = 0.0001\, K_{oc}\left(57.735\,OM + 2.0\,clay + 0.4\,silt + .005\,sand\right) \qquad \text{(B1)}$$

where OM, clay, silt, and sand are the percent by weight of organic matter, clay, silt, and sand, respectively (Streile et al. 1996). If K_{oc} is not known, it will be estimated from $K_{oc} = 0.6\ K_{ow}$. If OM is not known, it can be estimated as $OM = 170\ f_{oc}$, where f_{oc} is the fraction by weight of organic carbon in the soil. The soil composition must be known, or at least a texture classification, such as loamy sand, must be known, and the composition (texture) can be determined from Table B1. A utility with a user interface for implementation of Equation B1 exists within FRAMES, as mentioned in Chapter 4, and that utility will be used within the HGCT.

The partition coefficient for some inorganic constituents can be determined from a lookup table as related to soil composition (total percent of clay, OM, and iron and aluminum oxyhydroxides) and pH as discussed by Strenge and Peterson (1989). The lookup table has been digitized, and a lookup algorithm exists for estimating the K_d value given the constituent, the soil composition, and the pH. K_d values for MC from the literature will also be tabulated and made available to the user.

As stated in Chapter 4, K_d is computed within the RECOVERY MUI for organic constituents in surface waters/sediments. Sediment-water K_d

values for inorganic constituents, such as metals, is more problematic and beyond the scope of this report. Values will need to found and tabulated from the literature and made available to the user.

Table B1. Representative soil properties, part a.

Soil-Texture Classification	Soil Composition (based on USDA Textural Diagram)			Saturated Hydraulic Conductivity, (cm/s)	Representative Root- Zone Depth, cm	Porosity %
	% Sand	% Silt	% Clay			
Sand	92	5	3	6.6E-03	73	38.0
Loamy Sand	83	11	6	1.9E-03	76	43.7
Sandy Loam	65	25	10	7.2E-04	79	44.2
Loam	42	38	20	3.7E-04	55	46.6
Silty Loam	20	65	15	2.0E-04	31	46.3
Silt	7	88	5	1.3E-04	44	44.2
Sandy Clay Loam	60	14	26	1.1E-04	57	39.8
Clay Loam	32	35	33	6.2E-05	70	47.7
Silty Clay Loam	10	57	33	4.6E-05	64	49.0
Sandy Clay	52	7	41	3.4E-05	57	43.0
Silty Clay	7	46	47	2.6E-05	50	48.6
Clay	20	20	60	1.9E-05	43	47.5

Soil properties

The HGCT will provide digitized tables to look up values for soil properties required within TREECS. At this time, only those soil properties required for Tier 1 analyses will be covered, which include volumetric soil moisture content (θ_w) and soil dry bulk density (ρ_b). Tables B1 and B2 list soil properties for different soil compositions as provided within FRAMES, where the values were collated from various information sources. Dry bulk density and field capacity are included in Tables B1 and B2. Volumetric soil moisture content can be assumed to equal the field capacity on an annual average basis.

Table B2. Representative soil properties, part b.

Soil-Texture Classification	Dry Bulk Density, g/cm^3	Field Capacity, %	Available Water Capacity, %	Soil-Type Coefficient	USLE K-Factor by Organic Matter Content		
					<0.5%	2%	4%
Sand	1.64	9.0	5.0	4.05	0.05	0.03	0.02
Loamy Sand	1.49	12.0	6.0	4.38	0.12	0.10	0.08
Sandy Loam	1.48	17.5	8.5	4.90	0.27	0.24	0.19
Loam	1.42	23.5	11.0	5.39	0.38	0.34	0.29
Silty Loam	1.42	27.5	15.5	5.30	0.48	0.42	0.33
Silt	1.48	28.0	19.0	5.30	0.60	0.52	0.42
Sandy Clay Loam	1.60	24.0	8.3	7.12	0.27	0.25	0.21
Clay Loam	1.39	34.0	14.0	8.52	0.28	0.25	0.21
Silty Clay Loam	1.35	37.5	15.0	7.75	0.37	0.32	0.26
Sandy Clay	1.51	32.0	9.0	10.40	0.14	0.13	0.12
Silty Clay	1.36	42.0	14.5	10.40	0.25	0.23	0.19
Clay	1.39	40.0	10.0	11.40	0.25	0.23	0.19

Groundwater parameters

The only groundwater parameter required within Tier 1 of TREECS is the Darcy velocity, which is the bulk velocity of groundwater flow (i.e., the groundwater flow rate per unit area of media perpendicular to the flow). If no value is available from the site data, Darcy velocity (V_d) can be estimated by

$$V_d = K\frac{(H_1 - H_2)}{L_x} \tag{B2}$$

where K is the saturated hydraulic conductivity (L/T), and $(H_1\text{-}H_2)/L_x$ is the hydraulic gradient, defined as the difference in hydraulic head at two points in the aquifer, divided by the distance (L_x) between the two points. This gradient can be obtained from water table or potentiometric surface maps. If no value is available for saturated hydraulic conductivity, a typical value can be selected from Table B1 for a given soil texture.

Hydrologic parameters

Three hydrologic parameters must be estimated for use in a Tier 1 analysis that will be addressed within the HGCT, average annual runoff (Q), infiltration (q_w), and erosion (E) rates. The methods that will be used to estimate these three parameters are described below.

Runoff and infiltration rate

The infiltration rate may be known from other work and will not have to be estimated. The following procedures can be used when it must be estimated.

Monthly infiltration depths $I(m)$ will be computed based upon monthly average precipitation $P(m)$, runoff $Q(m)$, evapotranspiration $ET(m)$, and initial abstraction $I_a(m)$ depths,

$$I(m) = P(m) - Q(m) - ET(m) + I_a(m) \tag{B3}$$

The monthly averages will be accumulated to yield annual averages, which in turn are averaged over the period of record to give annual average values that are used in the models discussed in Chapters 3 and 4. The annual average infiltration depth I divided by 1 year is the same as q_w (m/yr) discussed in the model descriptions after unit conversions.

The monthly average runoff depth $Q(m)$ is an accumulation of the event based (daily) runoff Q_e in inches divided by the number of precipitation days in the month. Q_e can be estimated using the Soil Conservation Service (SCS) curve number (CN) method (Ponce 1989) as follows,

$$Q_e = \frac{(P - 0.2S)^2}{(P + 0.8S)} \tag{B4}$$

where S is the cumulative average annual retention depth in inches. Equation B4 assumes an initial abstraction of 0.2S. Thus, $I_a(m)$ is an accumulation of the event based initial abstractions divided by the number of precipitation days in the month. Retention S is computed from

$$S = \frac{1000}{CN} - 10 \tag{B5}$$

The curve number, *CN*, can be determined from cover type, hydrologic condition, and hydrologic soil group (see Tables B3 - B6).

Hydrologic soil groups include A, B, C, or D, which describe runoff potential. For example, group A soils are characterized as having low runoff potential with high infiltration rates. Such soils are primarily deep, very well drained sands and gravels. In contrast, group D soils have high runoff potential with a very slow infiltration rate when thoroughly wetted. Such soils are primarily clay with a high swelling potential, or soils with a permanent high water table, or soils with a clay layer near the surface, or shallow soils overlying impervious material.

The runoff area of the site can be partitioned into sub-areas for computing a composite *CN*, or

$$CN = \sum_{i=1}^{n} CN_i \times p_i \tag{B6}$$

Where CN_i is the *CN* estimated for each sub-area i, p_i is the fraction of total runoff area taken by sub-area i, and n is the total number of sub-areas.

Table B3. Runoff curve numbers for urban areas[1] (USDA SCS 1986).

Cover description		Hydrologic Soil Group			
Cover type and hydrologic condition	Average Percent Impervious Area[2]	A	B	C	D
Fully developed urban areas (vegetation established)					
Open space (lawns, parks, golf courses, cemeteries, etc.):[3]					
Poor condition (grass cover < 50%) ..		68	79	86	89
Fair condition (grass cover 50% to 75%) ...		49	69	79	84
Good condition (grass cover > 75%) ..		39	61	74	80
Impervious areas:					
Paved parking lots, roofs, driveways, etc. (excluding right-of-way)		98	98	98	98
Streets and roads:					
Paved; curbs and storm sewers (excluding right-of-way)		98	98	98	98
Paved; open ditches (including right-of-way) .		83	89	92	93
Gravel (including right-of-way) .		76	85	89	91
Dirt (including right-of-way) .		72	82	87	89
Western desert urban areas:					
Natural desert landscaping (pervious areas only)[4] ...		63	77	85	88
Artificial desert landscaping (impervious weed barrier, desert shrub with 1- to 2-inch sand or gravel mulch and basin borders)		96	96	96	96
Urban districts:					
Commercial and business	85	89	92	94	95
Industrial	72	81	88	91	93
Residential districts by average lot size:					
1/8 acre or less (town houses)	65	77	85	90	92
1/4 acre	38	61	75	83	87
1/3 acre.	30	57	72	81	86
1/2 acre	25	54	70	80	85
1 acre	20	51	68	79	84
2 acres	12	46	65	77	82
Developing urban areas					
Newly graded areas (pervious areas only, no vegetation)[5]		77	86	91	94
Idle lands (curve numbers (CN's) are determined using cover types similar to those in Table 5-2(c)).					

[1] Average runoff condition, and I_a = 0.2S.

[2] The average percent impervious area shown was used to develop the composite *CN*'s. Other assumptions are as follows: impervious areas are directly connected to the drainage system, impervious areas have a *CN* of 98, and pervious areas are considered equivalent to open space in good hydrologic condition. *CN*'s for other combinations of conditions may be computed using Fig. 5-16 or 5-17.

[3] *CN*'s shown are equivalent to those of pasture. Composite *CN*'s may be computed for other combinations of open space cover type.

[4] Composite *CN*'s for natural desert landscaping should be computed using Figs. 5-16 or 5-17 based on the impervious area percentage (*CN* = 98) and the pervious area *CN*. The pervious area *CN*'s are assumed equivalent to desert shrub in poor hydrologic condition.

[5] Composite *CN*'s to use for the design of temporary measures during grading and construction should be computed using Figs. 5-16 or 5-17 based on the degree of development (impervious area percentage) and the *CN*'s for the newly graded pervious areas.

Table B4. Runoff curve numbers for cultivated agricultural lands[1] (USDA SCS 1986).

Cover Description			Curve Numbers for Hydrologic Soil Group			
Cover Type	Treatment[2]	Hydrologic Condition[3]	A	B	C	D
Fallow	Bare soil	—	77	86	91	94
	Crop residue cover (CR)	Poor	76	85	90	93
		Good	74	83	88	90
Row Crops	Straight row (SR)	Poor	72	81	88	91
		Good	67	78	85	89
	SR + CR	Poor	71	80	87	90
		Good	64	75	82	85
	Contoured (C)	Poor	70	79	84	88
		Good	65	75	82	86
	C + CR	Poor	69	78	83	87
		Good	64	74	81	85
	Contoured and terraced (C&T)	Poor	66	74	80	82
		Good	62	71	78	81
	C&T + CR	Poor	65	73	79	81
		Good	61	70	77	80
Small grain	SR	Poor	65	76	84	88
		Good	63	75	83	87
	SR + CR	Poor	64	75	83	86
		Good	60	72	80	84
	C	Poor	63	74	82	85
		Good	61	73	81	84
	C + CR	Poor	62	73	81	84
		Good	60	72	80	83
	C&T	Poor	61	72	79	82
		Good	59	70	78	81
	C&T + CR	Poor	60	71	78	81
		Good	58	69	77	80
Close-seeded or broadcast legumes or rotation meadow	SR	Poor	66	77	85	89
		Good	58	72	81	85
	C	Poor	64	75	83	85
		Good	55	69	78	83
	C&T	Poor	63	73	80	83
		Good	51	67	76	80

1 Average runoff condition, and Ia = 0.2S.

2 Crop residue cover applies only if residue is on at least 5% of the surface throughout the year.

3 Hydraulic condition is based on combination factors that affect infiltration and runoff, including (1) density and canopy of vegetative areas; (2) amount of year-round cover; (3) amount of grass or close-seeded legumes; (4) percent of residue cover on the land surface (good hydrologic condition is greater than or equal to 20%); and (5) degree of surface roughness. Poor: Factors impair infiltration and tend to increase runoff. Good: Factors encourage average and better than average infiltration and tend to decrease runoff.

Table B5. Runoff Curve Numbers for Other Agricultural Lands[1] (USDA SCS 1986).

Cover Description		Curve Numbers for Hydrologic Soil Group			
Cover Type	Hydrologic Condition	A	B	C	D
Pasture, grassland, or range—continuous forage for grazing[2]	Poor	68	79	86	89
	Fair	49	69	79	84
	Good	39	61	74	80
Meadow—continuous grass, protected from grazing and generally mowed for hay	—	30	58	71	78
Brush—brush-weed-grass mixture with brush the major element[3]	Poor	48	67	77	83
	Fair	35	56	70	77
	Good	30[4]	48	65	73
Woods—grass combination (orchard or tree farm)[5]	Poor	57	73	82	86
	Fair	43	65	76	82
	Good	32	58	72	79
Woods[6]	Poor	45	66	77	83
	Fair	36	60	73	79
	Good	30[4]	55	70	77
Farmsteads—buildings, lanes, driveways, and surrounding lots	—	59	74	82	86

1 Average runoff condition, and $Ia = 0.2S$.

2 Poor: <50%) ground cover or heavily grazed with no mulch.
Fair: 50 to 75% ground cover and not heavily grazed.
Good: > 75% ground cover and lightly or only occasionally grazed.

3 Poor: <50% ground cover.
Fair: 50 to 75% ground cover.
Good: >75% ground cover.

4 Actual curve number is less than 30; use $CN = 30$ for runoff computations.

5 *CN*'s shown were computed for areas with 50% woods and 50% grass (pasture) cover. Other combinations of conditions may be computed from the *CN*'s for woods and pasture.

6 Poor: Forest litter, small trees, and brush are destroyed by heavy grazing or regular burning.
Fair: Woods are grazed but not burned, and some forest litter covers the soil.
Good: Woods are protected from grazing, and litter and brush adequately cover the soil.

Table B6. Runoff curve numbers for arid and semi-arid rangelands[1] (USDA SCS 1986).

Cover Description		Curve Numbers for Hydrologic Soil Group			
Cover Type	Hydrologic Condition[2]	A[3]	B	C	D
Herbaceous—mixture of grass, weeds, and low-growing brush, with brush the minor element.	Poor		80	87	93
	Fair		71	81	89
	Good		62	74	85
Oak-aspen—mountain brush mixture of oak brush, aspen, mountain mahogany, bitter brush, maple, and other brush	Poor		66	74	79
	Fair		48	57	63
	Good		30	41	48
Pinyon-juniper—pinyon, juniper, or both; grass understory	Poor		75	85	89
	Fair		58	73	80
	Good		41	61	71
Sagebrush with grass understory	Poor		67	80	85
	Fair		51	63	70
	Good		35	47	55
Desert shrub—major plants include saltbush, greasewood, creosotebush, blackbrush, bursage, palo verde, mesquite, and cactus	Poor	63	77	85	88
	Fair	55	72	81	86
	Good	49	68	79	84

[1] Average runoff condition, and I_a, = 0.2S. For range in humid regions, use Table 5-2(c).

[2] *Poor*: <30% ground cover (litter, grass, and brush overstory).
Fair: 30 to 70% ground cover.
Good: > 70% ground cover.

[3] Curve numbers for group A have been developed only for desert shrub.

The event based runoff Q_e is computed for each daily rainfall event over a period of record, such as a 30 year record of daily rainfall, and the values are used to compute monthly and annual average runoff depths Q.

ET will be computed on a monthly basis using the Thornthwaite Method. This method is based upon a heat index method whereby knowing the monthly average air temperature and the latitude of the geographic area of interest, one can compute the ET for the site. Thus, the approaches described above for hydrology will require site- or area-specific daily rainfall and air temperature data.

The above method will be built into a friendly user interface so that a user can easily estimate the CN, Q, P, and I (q_w) with a minimal amount of effort. However, the user will need to have some basic ideas regarding the site characteristics so that CN can be estimated.

Erosion rate

The Universal Soil Loss Equation (USLE) can be used to estimate annual average sheet and rill erosion, A (tons/acre-yr), from the equation

$$A = R \times K \times L \times S \times C \times P \tag{B7}$$

where:

R = rainfall factor
K = soil erodibility factor
L = slope-length factor
S = slope-gradient factor
C = crop management factor
P = conservation practice factor.

The parameters in Equation B7 can be estimated as follows.

R is the rainfall erosivity index, which is equal to the mean annual erosivity value divided by 100: $R = eI30/100$. By definition, the value of eI30 for a given rainstorm equals the product of total storm energy (e) times the maximum 30-min intensity ($I30$), where e is in hundreds of foot-tons per acre and $I30$ is in inches per hour (in/h). A map of R for the United States is shown in Figure B1 for determining R for a specific site.

K is a measure of the resistance of a soil surface to erosion, and it is defined as the amount of soil loss (tons per acre per year) per unit of rainfall factor R from a *unit plot*. A unit plot is 72.6 ft long, with a uniform lengthwise gradient of 9 percent, in continuous fallow, tilled up and down the slope. Values of K for various soil classifications are shown in Tables B2 and B7.

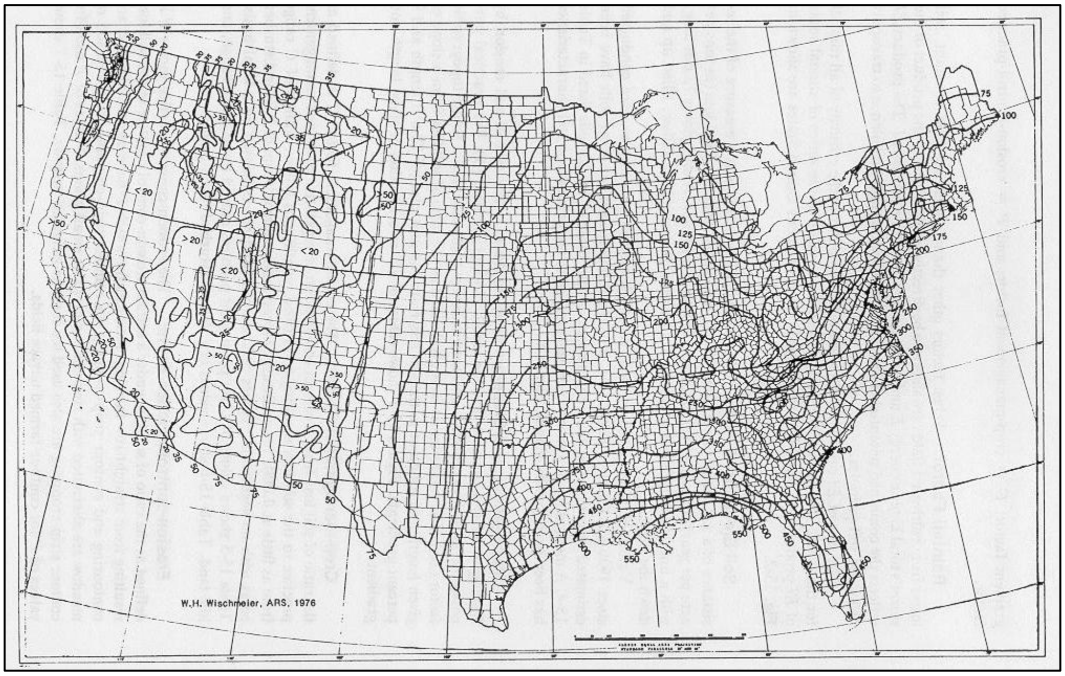
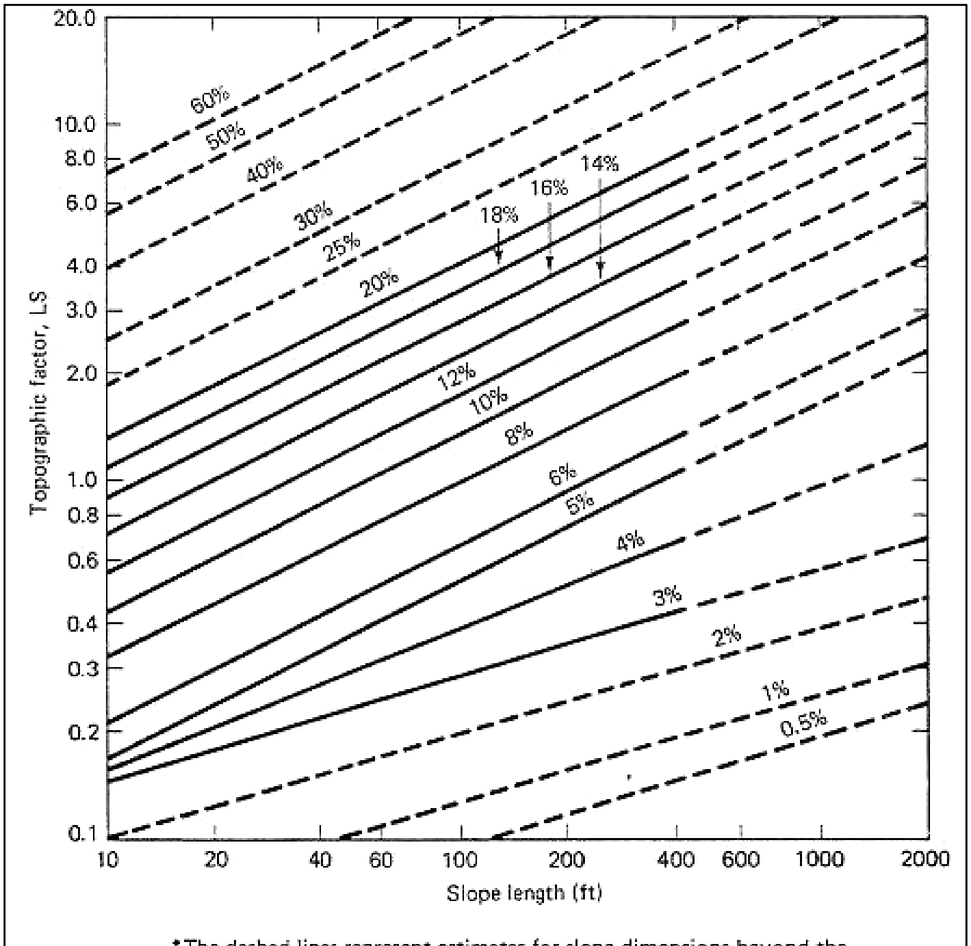


Figure B1. Rainfall factor, *R*, for the U.S. (USDA SCS 1983)

Table B7. Soil erodibility factors, *K*, for various soil classifications and percent organic matter content (USLE Fact Sheet 2008).

Textural Class	Average	Less than 2 %	More than 2 %
Clay	0.22	0.24	0.21
Clay Loam	0.30	0.33	0.28
Coarse Sandy Loam	0.07	–	0.07
Fine Sand	0.08	0.09	0.06
Fine Sandy Loam	0.18	0.22	0.17
Heavy Clay	0.17	0.19	0.15
Loam	0.30	0.34	0.26
Loamy Fine Sand	0.11	0.15	0.09
Loamy Sand	0.04	0.05	0.04
Loamy Very Fine Sand	0.39	0.44	0.25
Sand	0.02	0.03	0.01
Sandy Clay Loam	0.20	–	0.20
Sandy Loam	0.13	0.14	0.12
Silt Loam	0.38	0.41	0.37
Silty Clay	0.26	0.27	0.26
Silty Clay Loam	0.32	0.35	0.30
Very Fine Sand	0.43	0.46	0.37
Very Fine Sandy Loam	0.35	0.41	0.33

The rate of soil erosion by flowing water is a function of slope length (*L*) and gradient (*s*). For practical purposes, these two topographic characteristics are combined into a single topographic factor (*LS*). The topographic factor is defined as the ratio of soil loss from a slope of given length and gradient to the soil loss from the unit plot (72.6-ft length and 9-percent gradient). Topographic factors are shown in Figure B3 for various *L* and *s* values.



*The dashed lines represent estimates for slope dimensions beyond the range of lengths and steepnesses for which data are available.

Figure B3. Topographic factor, *LS*, in USLE (USDA SCS 1983).

Crop management factor, *C*, is defined as the ratio of soil loss from a certain combination of vegetative cover and vegetative canopy to the soil loss resulting from tilled, continuous fallow. Values of *C* range from as little as 0.0001 for undisturbed forest land to a maximum of 0.45 for disturbed areas with no vegetation. Tables B8 and B9 show values of *C* for various cover characteristics.

Table B8. Crop management factors, *C*, for use in USLE[1] (USDA SCS 1983).

Vegetative Canopy		Cover That Contacts the Soil Surface						
			Percent Ground Cover					
Type and Height[2]	% Cover[3]	Type[4]	0	20	40	60	80	100
No appreciable canopy		G	0.45	0.20	0.10	0.042	0.013	0.003
		W	0.45	0.24	0.15	0.091	0.043	0.011
Tall grass, weeds or short brush with average drop fall of 20 in. or less	25	G	0.36	0.17	0.09	0.038	0.013	0.003
		W	0.36	0.20	0.13	0.083	0.041	0.011
	50	G	0.26	0.13	0.07	0.035	0.012	0.003
		W	0.026	0.16	0.11	0.076	0.039	0.011
	75	G	0.17	0.10	0.06	0.032	0.011	0.003
		W	0.17	0.12	0.09	0.068	0.038	0.011
Appreciable brush or bushes, with average drop fall height of 6.5 ft	25	G	0.40	0.18	0.09	0.040	0.013	0.003
		W	0.40	0.22	0.14	0.087	0.042	0.011
	50	G	0.34	0.16	0.08	0.038	0.012	0.003
		W	0.34	0.19	0.13	0.082	0.041	0.011
	75	G	0.28	0.14	0.08	0.036	0.012	0.003
		W	0.028	0.17	0.12	0.078	0.040	0.011
Tree, but no appreciable low brush. Average drop fall height of 13 ft	25	G	0.42	0.19	0.10	0.041	0.013	0.003
		W	0.42	0.23	0.14	0.089	0.042	0.011
	50	G	0.39	0.18	0.09	0.040	0.013	0.003
		W	0.39	0.21	0.14	0.087	0.042	0.011
	75	G	0.36	0.17	0.09	0.039	0.012	0.003
		W	0.36	0.20	0.13	0.084	0.041	0.011

[1] The listed *C* values require that the vegetation and mulch be randomly distributed over the entire area. For grazed forest land, multiply these values by 0.7.

[2] Canopy height is measured as the average fall height of water drops falling from canopy to ground. Canopy effect is inversely proportional to drop fall height and is negligible if fall height exceeds 33 ft.

[3] Portion of total area surface that would be hidden from view by canopy in a vertical projection.

[4] G: cover at surface is grass like plants, decaying compacted duff, or litter. W: cover at surface is mostly broad-leaf herbaceous plants (weeds) or un decayed residues or both.

Table B 9. Crop management factors C used in USLE for undisturbed forest lands[1] (USDA SCS 1983).

Percentage of Area Covered by Canopy of Trees and Undergrowth	Percentage of Area Covered by Litter[2]	C Value[3]
100-75	100-90	0.0001-0.001
70-45	85-75	0.002-0.004
40-20	70-40	0.003-0.009

[1] Where litter cover is less than 40% or canopy cover is less than 20 %, use Table 15-5. Also use Table 15-5 when woodlands are being grazed, harvested, or burned.

[2] Percentage of area covered by litter is dominant. Interpolate on basis of litter, not canopy.

[3] The ranges listed in C values are caused by the ranges in the specified forest litter and canopy cover, and by variations in effective canopy height.

The computed value of *A* from Equation B7 in units of tons/acre-yr must be converted to erosion units for *E* in m/yr. This conversion can be made by dividing *A* by the soil dry bulk density and multiplying by the appropriate conversion units. The complete conversion equation is as follows

$$E(m/yr) = \frac{A(T/acre-yr)x2000(lb/T)x454(g/lb)x10^{-6}(m^3/cm^3)x10.76(ft^2/m^2)}{43{,}560(ft^2/acre)x\rho_b(g/cm^3)}$$

$$E(m/yr) = \frac{2.24E-4}{\rho_b}A \qquad \text{(B8)}$$

As discussed previously, soil dry bulk density can be estimated based upon soil composition. As with the methods for estimating runoff and infiltration, the methods of the USLE for estimating *E* will be incorporated into a user-friendly interface to facilitate ease of use.

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14. 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 and risk of 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 the range manager with tools to assess range management strategies to meet environmental compliance goals. Tier 1 will consist of screening-level methods that require minimal data input requirements and can be easily and quickly applied by range managers or their local environmental staff to assess whether or not there is potential for MC compliance concern, such as predicted surface water and/or groundwater MC concentrations exceeding protective health benchmarks at receptor locations.

(Continued)

15. SUBJECT TERMS

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14. ABSTRACT (Concluded)

This report describes the Army’s existing and perceived future requirements for TREECS Tier 1 tools and provides recommendations and a plan for technology developments to meet those needs. The information provided in this report is sufficient to serve as design and specifications for development of models and software that will comprise Tier 1 of TREECS. The details of the model formulations provided herein can also serve as documentation for the Tier 1 TREECS models.

The highly conservative assumptions of steady-state (time-invariant) conditions and no MC degradation are used. Thus, MC loadings to the range are constant over time, and fluxes to and concentrations within receiving water media reach a constant MC concentration for comparison to protective ecological and human health benchmarks. Tier 1 will include an analytical range soil model with its computed leaching flux linked to a semi-analytical-numerical aquifer model and with its computed runoff-erosion flux linked to a numerical surface water model. Tier 1 will also include an MC loading module, a hydro-geo-chemical toolkit for estimating input parameters, constituent databases for chemical-specific properties, and a database of ecological and human protective health benchmarks. All components will be packaged within a user-friendly PC client-based application with an emphasis on ease of use.