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Extension of Capabilities for the Tier 1 and Tier 2 Approaches within the Training Range Environmental Evaluation and Characterization System (TREECS™)

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Environmental Laboratory
U.S. Army Engineer Research and Development Center
3909 Halls Ferry Road
Vicksburg, MS 39180-6199

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Abstract

The Training Range Environmental Evaluation and Characterization System (TREECS™) is being developed for the Army with varying levels of capability to forecast the fate of and risk from munitions constituents (MC), such as high explosives (HE), within and transported from firing/training ranges to surface water and groundwater. The overall objective is to provide environmental specialists with tools to assess the potential for migration of MC into surface water and groundwater systems and to assess range management strategies to protect human and environmental health. Initial development consisted of two tiers. Tier 1 included screening-level methods that assume highly conservative, steady-state MC loading and fate, with no MC loss due to degradation. Tier 2 provides time-varying analyses. Thus, media concentrations computed with Tier 2 should be closer to those expected under actual conditions. The present work as summarized in this report focused on extending the capabilities of the Tier 1 and 2 methods in TREECS™. The requirements and specifications for including these extended capabilities are described in this report as well as various technical analyses that were conducted to support the work.

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Preface

This study was funded by the U.S. Army's Environmental Quality and Installations (EQI) Research Program. The work reported herein was conducted by staff within 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 WQCMB staff that conducted this work and prepared this report including the following: Dr. Mark Dortch of MSD Engineering Consulting under contract to Los Alamos Technical Associates, which was under contract to ERDC; and Dr. Billy Johnson and Jeffrey Gerald of the WQCMB.

The study was conducted under the general direction of Dr. Beth Fleming, Director of the EL; Dr. Warren Lorentz, Chief, EPED; Dr. Quan Dong, prior Chief, WQCMB; and Dr. Patrick Deliman, Acting Chief, WQCMB. Dr. Elizabeth Ferguson was Technical Director of military environmental research, and John Ballard was Program Manager for the EQI Research Program.

Personnel from the U.S. Army Environmental Command (AEC) and the U.S. Army Public Health Command (Provisional), Army Institute of Public Health (AIPH) provided valuable information, review, comment, and recommendations during this study that helped to improve and refine the Tier 2 methods. Personnel from AEC and AIPH also provided technical peer review of this report. Their assistance and participation are greatly appreciated.

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

Unit Conversion Factors

Multiply	By	To Obtain
acres	4,046.873	square meters
English tons	907.2	kilograms

1 Introduction

Background

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

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

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

After Tiers 1 and 2 of TREECS™ were completed, follow-on work was initiated that includes enhancing the Tier 1 and Tier 2 methods and tools. This work also includes adding a spatially explicit analysis capability so that the installation landscape can be modeled with varying levels of MC contamination along the landscape as well as spatially explicit landscape fate and transport processes. This report presents the Tier 1 and 2 enhancements being conducted as part of this work unit.

Scope

This report describes enhancements to the Tier 1 and 2 approaches of TREECS™. At the time of this writing, these enhancements were ongoing. However, all of the recommended enhancements, with the exception of time-varying hydrology and erosion, were completed and implemented into TREECS™ by the time this report was published. The details of the developed Tier 1 and Tier 2 modeling approach are not repeated in this report; they can be found in the reports by Dortch et al. (2009, 2011a). Enhancements are discussed in separate chapters that follow.

2 Calculating Erosion of Solid Phase MC

Background and present Tier 2 approach

The Tier 2 version of TREECS™ accounts for the mass export rate from the area of interest (AOI) due to erosion of solid phase MC. Thus, solid phase particles of MC can move from the AOI into surface water as a result of this process. The method for estimating this process that was implemented in Tier 2 of TREECS™ is described in Appendix A of the report by Dortch et al. (2011a). This method consists of multiplying the fraction of soil mass that is solid phase MC by the soil erosion rate as computed by the Universal Soil Loss Equation (USLE). Mathematically, this is stated as

$$F_{es} = f_{MC} \rho_b A E \tag{1}$$

where

F_{es} = solid phase MC mass erosion export rate, g/yr
f_{MC} = fraction by weight of soil mass that is solid phase MC mass
ρ_b = soil dry bulk density, g/m^3
A = AOI surface area, m^2
E = soil erosion rate as determined from the USLE, m/yr

It is recognized that f_{MC} can be computed from

$$f_{MC} = \frac{M_s}{A Z_b \rho_b} \tag{2}$$

where M_s (g) is the solid phase MC mass in the AOI, and Z_b (m) is the thickness of the active layer of the surface soil where all of the MC residue resides. Combining Equations 1 and 2 results in Equation 3.

$$F_{es} = M_s \frac{E}{Z_b} \tag{3}$$

The fundamental problem arising from this approach is the assumption that the soil erosion is adequately modeled with the USLE when solid phase MC is present. This assumption is probably suitable for MC that has a density and size similar to that of the soil particles. However, the assumption is questionable when MC with much different properties is involved, such as lead particles, which have a density about five times greater than that of soil particles. The next section describes an approach that can account for the effects on erosion rate due to a mix of disparate particle types.

Einstein and Brown equations

The Einstein and Brown (E-B) equations were used to evaluate the effect of a mix of disparate particle types on erosion rate. The basic E-B method is described in this section. Application of this approach to laboratory and field conditions is described in the following section to show the relevancy of using the E-B approach for soil erosion, since the method was developed for sediment erosion in surface waters.

The E-B method is an empirical approach to estimating bottom sediment erosion in surface waters. However, the approach requires the input of physical variables associated with hydraulics and associated bottom shear; thus, the approach does have a physical basis. The primary advantage of this approach over other similar approaches for estimating sediment erosion is that it does not require estimation of a critical shear stress.

The E-B method is described in the text by Julien (1995). There is a non-linear relationship for dimensionless volumetric unit (per unit width of flow) sediment discharge (q_{bv^*}) versus the dimensionless Shields parameter τ_*. The variable q_{bv^*} is defined as

$$q_{bv^*} = q_{bv} \left\{ \sqrt{(G-1) g d_s^3} \left[\sqrt{\frac{2}{3} + \frac{36 \nu^2}{(G-1) g d_s^3}} - \sqrt{\frac{36 \nu^2}{(G-1) g d_s^3}} \right] \right\}^{-1} \tag{4}$$

where

q_{bv} = dimensional volumetric sediment discharge per unit width of flow, m^2/sec
d_s = particle diameter, m
G = specific gravity of the sediment (or MC solid particles)
g = acceleration of gravity, 9.815 m/sec^2
ν = kinematic viscosity of water, approximately 1.0E-6 m^2/sec

The dimensionless Shields parameter is defined as

$$\tau_* = \frac{\tau_o}{(\gamma_s - \gamma) d_s} \tag{5}$$

where

τ_o = shear stress of the flow, Pa (Pascal = 1.0 Nt/m^2)
γ_s = specific weight of sediment (solid particles), Newton (Nt)/m^3
γ = specific weight of water, Nt/m^3

Three non-linear equations are used to relate q_{bv^*} to τ_* depending on the value of τ_*:

$$q_{bv^*} = 2.15 \exp\left(-\frac{0.391}{\tau_*}\right) \quad when\, \tau_* < 0.18 \tag{6}$$

$$q_{bv^*} = 40\tau_*^3 \quad when\, 0.52 > \tau_* > 0.18 \tag{7}$$

$$q_{bv^*} = 15\tau_*^{1.5} \quad when\, \tau_* > 0.52 \tag{8}$$

After determining the value of τ_* from Equation 5, the value of q_{bv^*} is computed from one of Equations 6 through 8. With a value for q_{bv^*}, q_{bv} is computed from Equation 4. The value of q_{bv} is multiplied by the width of flow to obtain the total volumetric sediment discharge (m^3/sec). The volumetric sediment discharge is converted to mass discharge (g/sec) by multiplying by the dry sediment particle density (g/m^3), which can be computed from the product of G and the density of water, 1.0E6 g/m^3.

Evaluation of the Einstein and Brown equations

The E-B equations were applied to laboratory and field conditions to evaluate their relevance to predicting soil erosion. The laboratory application is described first, followed by the field application. The laboratory application is compared to measured eroded sediment mass, while the field application is compared to results computed with the ULSE.

Laboratory application

The E-B equations were applied to a laboratory rainfall lysimeter test described by Larson et al. (2005). The soil in the lysimeter had no amendment other than loading of lead from fired bullets. The results from this laboratory study were used for other model comparisons and are described by Dortch et al. (2011b).

The lysimeter test cells were filled with test soil and were placed under a rainfall simulator on a slope of 0.0625 to create runoff. The lysimeter test cell was 78.7 cm on each side with approximately 23 cm of soil depth. Each lysimeter was configured to allow collection of runoff water and leachate water. Rainfall, which was water treated through reverse osmosis (RO), was applied for 16 weeks at a rate of 18 L per week, which amounted to an annual rainfall rate of 0.467 m/yr. Rainfall was applied weekly over a period of about 26 minutes once per week.

The amount of runoff was measured each week over the 16 weeks, and the average runoff was determined to be 5.17 L per week. This is considerably less than the amount of rainwater applied, because infiltration and evaporation occurred.

The results from the sand B test were used. The silty sand B soil consisted of 77.2% sand and 22.3% fines. The measured specific gravity was 2.62. Since measurements of soil porosity and/or dry bulk density were not available and other information on soil texture (percent silt and clay) was lacking, assumptions had to be made for further definition of soil characteristics. It was assumed that the silty sand B soil was similar to a loamy sand texture, which has about 83, 11, and 6% of sand, silt, and clay, respectively. These percentages were adjusted to allow 77.2% sand with a total percentage of 100% for all three types; thus, the texture was assumed to be 77.2, 14.8, and 8% sand, silt, and clay, respectively. This soil texture has a sediment dry bulk density of about 1.49 kg/L.

The measured cumulative total suspended solids (TSS) mass in runoff from the sand B soil test cell over the 16 weeks was 125.9 g. This value for measured TSS mass eroded over 16 weeks for 26 minutes per week was used to compute the instantaneous mass erosion rate of 1.3E-5 g/sec. This erosion rate, with a soil dry bulk density of 1.49 kg/L, a surface area of the test cell of 0.619 m^2, and conversion from second to year, results in an erosion rate of 4.45 E-4 m/yr.

The E-B equations were applied to the above laboratory test conditions to predict an erosion rate for comparison to the measured rate. The first step was to estimate the water flow rate over the test cell soil surface when rainfall is applied. The weekly (event) runoff volume of 5.17 L was converted to cubic meters and then divided by the duration of rainfall each week (26 min converted to seconds), yielding a weekly rainfall event flow of 3.31E-6 m^3/sec. This flow was then used with Manning's equation, the flow width and slope prescribed above, and a Manning's n value of 0.05 to determine the depth of flow, which is 2.27E-4 m. The average grain size for the sand B soil using the texture percentages described above is about 198 μm. Using the flow depth, the specific weight of water, and the slope, the shear stress of the flow was computed to be 0.139 Pa. With the shear stress, the specific weight of water, the G value, and the grain size, the dimensionless Shield's parameter was computed to be 0.044. This means that Equation 6 must be used to calculate q_{bv^*} resulting in a value of 3.12E-3. Equation 4 was then solved to produce q_{bv} = 1.58E-9 m^2/sec. This value was multiplied by the cell width and the dry soil density to produce a mass erosion rate of 3.25E-3 g/sec for each rainfall event. This value was multiplied by the number of events (16) and the duration of each to produce a total mass of soil eroded equal to 81.1 g. This mass erosion rate is equivalent to a land erosion rate of 2.86E-4 m/yr. A C factor as used in the USLE equation was not applied to this result since the soil was bare, and C factors may not be appropriate for flume and laboratory studies. Thus, the C factor was assumed to be 1.0.

The computed eroded mass of 81.1 g and erosion rate of 2.86E-4 m/yr should be compared to the measured amount of 125.9 g and associated erosion rate of 4.45E-4 m/yr. It is encouraging that the computed mass and rate are within one order of magnitude of that measured, considering that the E-B equations were developed for sediments rather than soil.

There may be another reason that the measured runoff of soil is greater than that computed. Soil surfaces exhibit negative charge with a force field around each soil particle. The size of the field is called the Debeye screening length and is inversely proportional to the salt concentration in the system. For normal soil conditions that contain salts, the Debeye length is small, and so repulsive forces between other soil particles are small. Therefore, the soil is able to aggregate together. However, when the system is washed with low salt water, like rainwater or RO water, the salts rinse out of the system, which decreases the ionic strength. Thus, during rainfall, the Debeye length increases and the repulsive field around the particles expands to the extent that the particles cannot approach each other closely enough to aggregate, and so a stable suspension or dispersion forms. It is possible that the laboratory rainwater could have caused some stripping of salts with increased soil dispersion and suspension, resulting in increased runoff of soil particles in addition to the soil runoff associated with erosive forces. Sediment dispersion can also occur in freshwater lakes after a heavy rainfall, causing increased lake turbidity. Eventually the turbidity will decrease as excess waters drain off, the lake reverts back to normal, and the salt concentration returns to normal. The E-B equations do not account for the effects of soil dispersion and suspension.

Field application

The E-B equations were applied to conditions at Fort A.P. Hill, and the results were compared to those computed with the USLE. The average annual rainfall runoff at Fort A.P. Hill has been estimated to be 0.306 m/yr (Dortch et al. 2011b). The ground surface slope for the AOI is approximately 0.06. Based on local site conditions, the USLE factors were set to R = 225, K = 0.24, LS = 1.335, C = 0.1, and P = 1.0. The surface area of the AOI is 10,775,905 m^2, and AOI soil bulk density was estimated to be 1.48 g/mL. With the above factors, the USLE yields a soil erosion rate of 7.21 tons/acre/yr. This translates into a land erosion rate of 0.00109 m/yr. These rates are without any correction for the sediment delivery ratio (SDR).

As discussed by Dortch et al. (2010, 2011b), daily rainfall was used to compute the long-term annual average runoff for Fort A.P. Hill. The annual average runoff rate of 0.306 m/yr was multiplied by the AOI surface area of 10.776E6 m^2, divided by the average number of runoff events per year of 14, and divided by the conversion of 86,400 sec/day (since a rainfall event was for the day), yielding an average event runoff flow rate of 2.73 m^3/sec. This flow rate was used with the AOI runoff flow width of 4715 m, a Manning's n of 0.05, and slope of 0.06 to compute the depth of flow of 0.0044 m. The soil texture at Fort A.P. Hill is sandy loam with the estimated composition of 65, 25, and 10% sand, silt, and clay, respectively, with an average soil particle diameter of 170 μm. The specific gravity of the soil was assumed to be 2.65.

With the above information, the E-B equations were applied, yielding a computed erosion rate of 22 tons/acre/event after using the appropriate conversions. A crop management factor C, which includes the effects of vegetative cover, was set to 0.1 for the USLE, and a C factor of 1.0 is implied for the E-B equations since this method does not normally include this factor as applied to river bottom sediments. If a C factor of 0.1 is multiplied by the rate computed with the E-B equations, then the rate is decreased to 2.2 tons/acre/event. This yield must be multiplied by 14 events per year, yielding 30.8 tons/acre/yr, which is about four times the value of 7.21 tons/acre/yr computed with USLE. The fact that the result with the E-B equations is within an order of magnitude of the USLE-computed sediment yield lends some support to using the E-B equations for estimating soil erosion for a field site.

The above analysis can be refined by considering the exceedence frequency of the annual maximum daily runoff and the associated erosion of each. Annual average erosion unit yield Y_a (tons/acre/yr) can be estimated from return period maximum runoff and associated erosion unit yield rates (Simons and Senturk 1992) as follows,

$$Y_a = R_a \frac{0.4Y_2 + 0.06Y_{10} + 0.02Y_{25} + 0.01Y_{50} + 0.01Y_{100}}{0.4R_2 + 0.06R_{10} + 0.02R_{25} + 0.01R_{50} + 0.01R_{100}} \quad (9)$$

where Y_2, Y_{10}, etc., and R_2, R_{10}, etc., are the event soil erosion unit yields (tons/acre/event) and the event rainfall runoff depth (m/event), respectively, for the 2-year, 10-year, etc., return periods; R_a is the annual average runoff depth (m/yr). An event is a day since runoff was computed using daily rainfall (Dortch et al. 2010, 2011b).

The daily runoff (m) was computed for a 25-year record of rainfall, and the maximum daily runoff for each year was determined. A frequency analysis was performed on the annual maximum daily runoff using the log Pearson Type III probability distribution. From this distribution, the maximum daily runoff values for return periods of 2, 10, 25, 50, and 100 years were determined for use in Equation 9. With the return period maximum runoff, the associated erosion was computed using the E-B equations and multiplying the result by a C factor of 0.1. With the return period runoff and erosion and the annual average runoff of 0.306 m/yr, Equation 9 gives an average annual erosion yield of 27.2 tons/acre/yr. This value is close to the average annual erosion yield of 30.8 tons/acre/yr computed with the E-B equations using the average annual runoff event, which is the average annual runoff divided by an average of 14 runoff events per year. Thus, the two estimates of the average annual erosion using the E-B equations are consistent, but the rates are about four times greater than that computed with USLE.

Implications of using E-B equations to compute erosion

The primary reason for considering the E-B equations was to provide a means to estimate soil erosion with the presence of substantial MC concentrations that could alter the composite soil characteristics, such as can occur with high concentrations of lead. Another potential benefit of considering the E-B equations is that they could be used to estimate soil erosion rates for short-term, event-based runoff, whereas the USLE is not appropriate for that. This section describes applications of the E-B equations for various concentrations of lead to determine the impacts of lead concentrations on erosion.

Solid phase lead was used for these analyses. It was assumed that the erosion rate is determined by the characteristics of the average particle representing the mixture of soil and lead. Thus, the first step was to compute the characteristics of the mixture. A spreadsheet was used to conduct the calculations.

The specific gravity values of the soil and lead were fixed at 2.65 and 11.35, respectively. The average diameters of the soil and lead particles were set to 170 and 500 μm, respectively. The concentration of lead in soil was treated as an input and was converted to percent by weight of lead in the mixture. With this information and assuming the particles are spherical, it was possible to compute the composite density and specific gravity of the mixture and the average particle diameter of the mixture. With known runoff flow rate, an n value, and flow width, the depth of flow can be computed as described previously. The average event flow rate (average annual runoff divided by 14 runoff events/year) and depth of flow for the E-B application to Fort A.P. Hill as described above were used. With depth of flow, flow rate, composite particle diameter, and composite particle specific gravity, the E-B equations can be solved to estimate the erosion for the composite sediment-lead particles.

Assuming a lead concentration of 20,000 mg/kg gives a percent of lead by weight of 2%. With this input and the other inputs described above, the sediment yield of the mixture was computed to be 39.8 tons/acre/yr, which is about 30% greater than the yield for pure soil (30.8 tons/acre/yr). Thus, adding lead to soil increases the erosion rate of the composite mixture for the imposed runoff rate of 0.0219 m/day (based on 0.306 m/yr for 14 events per year). A lead concentration of 1% resulted in a sediment yield of 37 tons/acre/yr.

It was surprising that the addition of lead increased the sediment yield. Thus, a lower runoff rate was imposed to investigate the effect. For a runoff rate of 0.00612, which is the average annual runoff of 0.306 m/yr divided by 50 runoff days per year, the sediment yield is 27 tons/acre/yr for pure soil. For the composite mixture of soil and lead with 2% lead, the sediment yield drops to 17.5 English tons/acre/yr. For 1% lead, the sediment yield of the mixture is 21.2 tons/acre/yr. Therefore, it appears that there is a threshold runoff rate above which the sediment yield increases with increasing lead concentration, and below which sediment yield decreases with increasing lead concentration. Through iterative solutions for Ft. A.P. Hill, this threshold runoff was determined to be 0.0133 m/day, which is the average annual runoff divided by 23 days/yr of runoff.

Conclusions

Use of the E-B equations to predict annual soil erosion produces rates that are about four times greater than those computed with USLE. Although use of the E-B equations would provide more conservative results (i.e., greater erosion) than use of USLE, the E-B equations were developed for bottom sediment erosion in rivers, and there is no history of using the E-B equations for overland soil erosion. Thus, results from using the E-B equations for overland soil erosion should be viewed with caution. More testing of the E-B equations against observed overland soil erosion data is required before this method could be considered.

The use of the E-B equations to estimate erosion of soil-MC mixtures indicates that the erosion rate can be about 30% more or less for a mixture than for pure soil, depending on whether the runoff rate is greater or less than a threshold runoff rate. Thus, for some sites and hydrology, treating the particles as a composite mixture of soil and MC is more conservative than assuming pure soil. However, for other sites and hydrology, treating the particles as a mixture can be less conservative than treating the particles as pure soil. A series of trial solutions are required for a particular site and hydrology to determine the threshold runoff, above or below which the effect of a soil-MC mixture switches from increasing to decreasing the erosion rate.

Recommendations

It is recommended at this time that soil-MC mixtures be treated as pure soil for erosion computations. Alternatively, for sediments with high concentrations of a heavy metal, such as lead, model results can be assessed for uncertainty in the erosion rate. For such assessments, the erosion rate should be varied plus and minus about 30% of the input value within the Monte Carlo simulations.

Although computing soil erosion with the E-B equations is more physically based than using USLE, the USLE has a long history of acceptance for computing annual soil erosion, while the appropriateness of using the E-B equations for computing soil erosion has not been demonstrated. Given these facts, it is recommended that the USLE continue to be used in TREECS™, including soil containing rather high concentrations of MC. Thus, Equation 3 will continue to be used to compute the mass export rate of MC due to solid phase MC erosion, and the erosion rate E in that equation will continue to be estimated with USLE.

As discussed later in this report, there is a need to be able to compute soil erosion for single events or on a daily basis. USLE is not the appropriate method for this; an alternative method, the Modified ULSE or MUSLE, is evaluated for that purpose.

3 Adding Firing Points as a Source of MC

Background

Firing points could contribute to MC loading within an AOI. TREECS™ presently does not include this feature although place-holders were used to accommodate a future extension to include this feature. The main requirement for adding this feature is to have access to a database of munitions particulate matter emission factors. This database would allow estimation of MC loading rates (g/yr) based on the types of munitions used and their emission factors (g of particulate MC mass emitted/item fired). There is an Army emission factors database for gaseous release of MC at firing points for various munitions. However, it has since been determined that the gaseous emissions are not nearly as important for long-term human and ecological health as the particulate emissions that are deposited on the soil. Thus, there is a need for emission factors for particulates. Some work has been conducted to quantify particulate emission from munitions. It remains necessary to determine the status and availability of such data. For now, the firing point feature will be added to TREECS™, but the user must specify the emission factor or similar input so that the loading can be defined.

Approach for implementation

The modifications required to add firing points as a source of MC were not substantial and involve the following:

1. The *Firing Point* button on the *Site Conditions/Operational Inputs* screen must be activated. If the Firing Point button is selected, one or more other new screens must be developed that will be launched.
2. An input dialog must be added for firing point usage on the *Site Conditions/Operational Inputs* screen, similar to the one for impact zone, which allows the user to input the number of items fired per year for each firing point munition used.
3. An input dialog must be added on the *Site Conditions/Operational Inputs* screen for particulate emissions for each munitions item and MC pair. In the absence of an emission factor database, two options are recommended. One option is to have the UI compute the emission factor (g/item) based on the product of the firing point content (g) of each MC of interest and a

user-specified percentage of unexpended MC when fired, such as propellant that was not fully burned upon firing. Munitions firing point MC content information is contained within the TREECS™ munitions database. The other option is for the user to enter the emission factor for each munitions item and each MC.

4. A mass loading calculation and display screen must be added similar to the one for the impact zone that shows the loading rate (g/yr) for each MC summed over all munitions used. The firing point MC loading is simply the emission factor for each munitions item – MC pair times the number of those items fired per year, and then summing the item – MC pair loading rates for all firing point munitions items.

Once the munitions use and MC loading functions are performed for the firing point, then everything else within TREECS™ should work the same as before. However, if an impact zone and a firing point are both of interest, then two separate applications (.TRP files) are required, one for firing point and one for impact zone. The firing point and impact zone can be in the same AOI or different AOIs. Recall that TREECS™ Tier 1 and 2 applications have been constrained to a single AOI. It is possible for the same AOI location and site characteristics to be applied for the two applications (impact zone and firing point), but the loadings would be different. As discussed in the next chapter, the Multiple AOI Tool can be used to combine the AOI exports from multiple applications to assess impacts on a common receiving water (groundwater or surface water).

4 Multiple AOI Tool

Background

The original design of TREECS™ Tiers 1 and 2 was restricted to assessing a single AOI for each application (.TRP file). Furthermore the AOI could have only one target surface water and aquifer, with up to five target receptor wells. However, there can be situations that warrant assessing the effects of multiple AOIs that can contribute MC to the same surface water body and/or receptor well. Thus, a tool is under development to allow assessment for multiple AOIs.

Basic approach

The basic approach for developing a tool to assess multiple AOIs is to constrain this tool as a separate auxiliary application that resides under the Tools tab on the TREECS™ main menu bar. All of the applications within the Tools tab are stand-alone applications that are run independently. However, applications within the Tools tab may require inputs from previously developed TREECS™ application files (.TRP files) or may provide output to those files. Structuring the multiple AOI tool in this manner greatly reduces the effort required to address this need.

Previous TREECS™ model application outputs serve as inputs to this tool. Thus, each model application has a single AOI that exports MC to either groundwater or surface water or both. Each AOI application has no more than one aquifer and one target surface water body, the same as the original design for Tiers 1 and 2. The receiving water concentrations caused by each AOI are independent, since receiving water concentrations are linearly related to loading. Thus, the Multiple AOI Tool (MAT) superimposes the results of the individual AOI applications by simply adding together the receptor well and surface water and sediment MC concentrations produced for each AOI application.

Specifications and requirements

Figure 1 provides a schematic of how multiple AOIs can be addressed with MAT. In this example, four AOIs are assessed. There is a single target lake that is potentially affected by AOIs 1 and 2. There is also a single target receptor well that is potentially affected by AOIs 3 and 4. AOIs 1 and

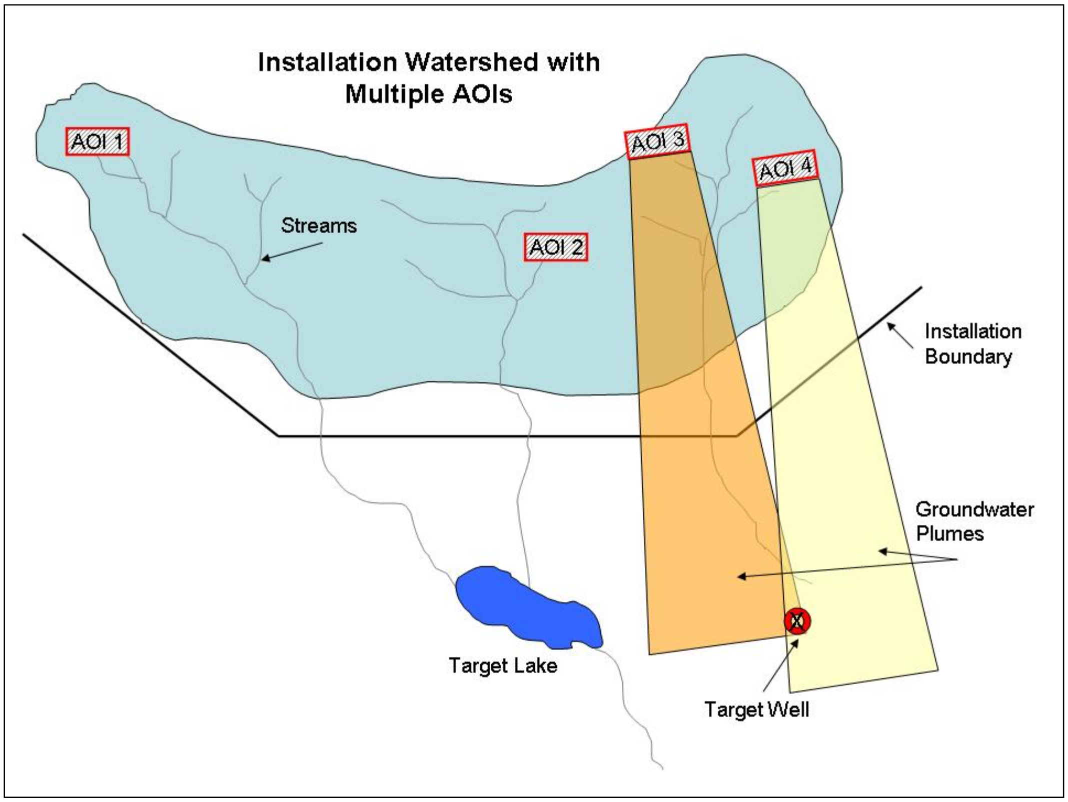

Figure 1. Example schematic of an installation watershed with multiple AOIs that can be addressed with MAT.

2 can be assessed together in a single MAT project to determine the combined surface water/sediment concentration in the lake. AOIs 3 and 4 can be assessed together in a different MAT project to determine the combined groundwater concentration at the target well. AOIs 3 and 4 each include the same common well and its distances (longitudinal, lateral, and vertical) relative to the center of the AOI for that application. For this particular scenario, the user would not be able to assess the combined effects on both the lake and target well in a single MAT project because the MAT requires that if groundwater is present in one AOI, then it must be included in all of the AOIs used in a given MAT project. Additionally, the AOIs selected must be limited to a single common target well (recall that TREECS™ allows up to five wells to be included in a Tier 2 scenario). The MAT does not require that surface water be included in each AOI used in a MAT project. Therefore, the user is free to select AOIs for a MAT project that may or may not include the surface water media.

Suppose that AOI 2 in Figure 1 also included the groundwater media and that its plume affected the same target well as in AOIs 3 and 4. Then AOIs 2, 3, and 4 could be selected in a given MAT project to assess the combined effect of these three AOIs on the target well. However, this would preclude the user from selecting AOIs 1 and 2 in a different MAT project because AOI 1 does not include groundwater, whereas AOI 2 now would, and this would violate the requirement that all AOIs selected in the MAT project must include the groundwater media (and be limited to one target well) or all must not include the groundwater media. If AOI 1 and AOI 2 each included the groundwater media and if each potentially affected the same groundwater well as in AOIs 3 and 4, then all four AOIs could be selected in a given MAT project to determine the combined surface water/sediment concentrations in the target lake due to AOIs 1 and 2 as well as the combined groundwater concentration at the target well due to AOIs 1, 2, 3, and 4.

The assumptions, requirements, and constraints for the MAT development are listed below:

1. Only Tier 2 applications can be addressed with the MAT.
2. The MAT is a stand-alone tool in TREECS™. As such, the MAT uses information generated from previously run applications (.TRP files), and no new .TRP file is generated from the MAT application.
3. The number of AOIs (.TRP files) that can be combined is limited to 10.
4. Each AOI application (.TRP file) must assess the same MCs and must have the same health benchmarks. However, each AOI can have different munitions usage, soil characteristics, hydrology, and other inputs.
5. Each AOI application should extend over the same time period.
6. Each AOI application must be fully completed and executed (from soil through receiving water) before using MAT.
7. Each AOI application must have the same common groundwater target well, which must be limited to 1 due to system design constraints. The spatial coordinates of the target well must be input within each AOI application as distances relative to the center of the AOI for that application. If the user attempts to select an AOI application with more than one well, then the MAT will display an error message.
8. Each AOI application must have the same receiving surface water body or no surface water due to system design constraints.
9. Surface water modeling is limited to use of the RECOVERY model at this time, but work is planned to include the Contaminant Model for Streams, CMS.

10. If soil interflow and/or groundwater discharge to surface water are included in an AOI application, then those features are preserved in the MAT results.
11. The MAT inputs and outputs are saved such that the MAT application can be viewed later following initial application.
12. The MAT uses only the graphical viewers for water concentration files (WCF) and sediment concentration files (SCF) with health benchmarks to display MAT results.
13. Sensitivity and uncertainty (S/U) analysis are not allowed within MAT due to system design constraints.

Implementation

MC concentrations resulting from each AOI impacting each receptor well or surface water body are combined using the Plus Operator. The Plus Operator is a module that combines time series of concentrations or fluxes for various media. This operator is used in TREECS™ to combine the flux of groundwater discharge to surface water carrying AOI soil runoff/erosion fluxes prior to combined fluxes entering the target surface water. The operator combines all of the time points for each entering time series into one time series that contains all of the time points of the entering series. Values for concentration or flux are linearly interpolated at time points of a series that is missing data after consolidating time points. With a value for each contributing data source for each time point of the combined series, the values for each entering concentration/flux can then be added together, producing the total concentration/flux. The combined concentration/flux time series is then written by the operator to the appropriate output file type (WCF and SCF for concentrations and water flux files, WFF, for fluxes), which can then be viewed by the appropriate viewer (i.e., WCF, SCF, and WFF graphical viewers). For the MAT, it will only be necessary to combine concentrations, not fluxes; thus, only the WCF and SCF viewers will be used.

A MAT processor has been developed that uses the number of AOI applications to be assessed and the .TRP file names and their locations as input for each application. The processor gathers the specified .TRP files and their associated output files (WCF and SCF files), reads them, and organizes the information as input for the Plus Operator module. The MAT dynamically creates a project GID file for the given combined scenario based on the individual WCF and SCF files from the individual TREECS™ applications. The processor then executes the Plus Operator module for each media and concentration type, which potentially includes aquifer-dissolved, surface water-total, surface water-dissolved, and surface water sediment-total. The MAT processor also allows the user to view each of the Plus Operator time series outputs, which are also the MAT outputs for each aquifer well, for surface water (total and dissolved), and for sediment.

5 Adding Generic Source Loadings

Background

It is useful to include a generic source loading module so that TREECS™ applications that do not involve firing ranges and munitions can be conducted. These applications have broad applicability for other federal and state agencies, as well as the private sector. Also, these applications potentially address a wide variety of needs, such as evaluating potential for various types of sites to contaminate groundwater and surface water and for evaluating site cleanup.

The Defense Ammunition Center (DAC) developed the munitions database used in TREECS™. DAC restricts the use of this information to registered users with a .mil or .gov internet address. TREECS™ will be useful for non-DoD applications if there is a means for defining the sources of contamination without having to use the TREECS™ munitions database.

Approach and requirements for implementation

Below are the steps for adding this capability.

1. Continue to require a .mil address to use the munitions database.
2. Modify TREECS™ *Site Conditions → Operational Inputs* screen to include an additional option under *Type of loading to be estimated* called *General soil source zone*. A DoD user can select any one of three options under this section: Impact Zone, Firing Point, or General Soil Source Zone. For military range applications, the general soil source zone could represent an open burning/open detonation (OBOD) area or other demolition area that is being used, or other sources of MC loading that are not covered by firing point and impact zone. If an AOI is contaminated from previous use and is not receiving future loadings, then the user will need to choose the *General soil source zone* option and simply enter zero loadings. Existing or initial soil concentrations are entered in the Tier 2 soil model UI.
3. For the non-DoD user, the Impact Zone and Firing Point buttons will be dim and not selectable. Thus, there will be no reason or capability to access the munitions database. A non-DoD user can select the *General soil source zone*. When the user chooses this option, a new dialog will appear for

entering loadings for this option. This new dialog will actually be much shorter and simpler than the ones for *Impact zone* and *Firing point* since no munitions are being used. The dialog will request the user to enter the yearly loading rate (g/yr) for each constituent. These loadings can vary from year to year.

4. As discussed in item (2) above, there may be situations when there are no loadings for the general soil source zone in a non-DoD application, but there is existing contamination from previous activities. For those cases, the user simply puts in two time points and zero loadings. The Tier 2 soil model allows the user to enter initial soil concentrations for each constituent in the event that there is contamination from previous activity, regardless of whether there are future loadings or not.
5. The *General soil source zone* loading capability is being added to both Tier 1 and Tier 2. However, for Tier 1, it is recognized that there is no initial soil concentration since Tier 1 is a steady-state analysis. Also, only a single general loading rate is entered for each constituent, similar to what is done for the impact zone now in Tier 1.
6. After addressing the needs for the revised *Operational Inputs* screen, everything else in TREECS™ will work satisfactorily with few other changes. The only other primary need is for users to provide their own user-defined target health benchmark database if they do not want to use the DoD benchmark database that focuses on MC found on ranges and the associated DoD benchmarks. Also, non-DoD users must develop the loadings to soil with their own preferred methods, which would be external to anything in TREECS™.

6 Adding Soil Interflow and Groundwater Discharge to Tier 1

Background

Soil interflow and groundwater discharge to surface water were implemented into Tier 2, and there is now a requirement to add these features to Tier 1. Below are the approaches and requirements to accomplish this.

Interflow approach and requirements

Interflow through the vadose zone or soil to surface water is a minor pathway in most cases, but it could be a potential pathway for surface soils having a high hydraulic conductivity with an impermeable or semi-impermeable soil layer at a shallow soil depth, thus creating a perched water table. The addition of interflow to Tier 1 follows the same approach as that used for Tier 2. The mass flux of MC associated with interflow is assumed to flow directly into the target surface water without any further transport or fate processes.

Since the TREECS™ Tier 1 and 2 models are based on average annual hydrology, interflow must be added through specification of the fraction of average annual infiltration that is lost to interflow. Interflow is caused by infiltration flow that is greater than the maximum percolation rate (i.e., groundwater recharge rate) of the vadose zone layer, which is the saturated hydraulic conductivity, K_s. A conceptual schematic of flow within the soil, vadose, aquifer system is shown in Figure 2. After prompting the user to enter a value of K_s for the vadose zone layer, the soil model UI will automatically provide an estimate of the interflow fraction as follows. If the average annual water infiltration rate in soil q_w is less than or equal to K_s, the fraction of interflow F_{if} is estimated to be zero. If q_w is greater than K_s, then $F_{if} = \frac{q_w - K_s}{q_w}$. The user can also enter his/her own estimate for F_{if}. In many cases, the interflow fraction should be set to zero, which will send all of the infiltration water to the aquifer.

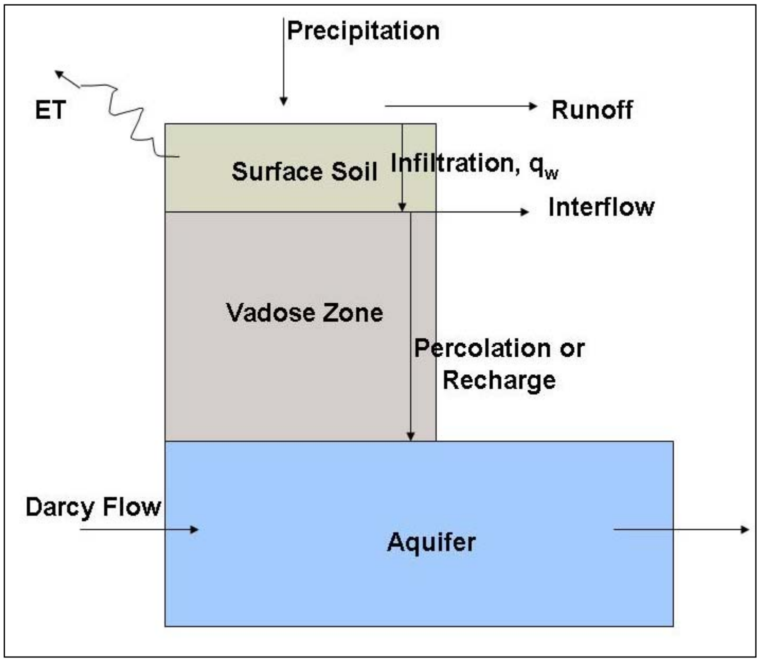

Figure 2. Conceptual schematic of surface and sub-surface hydrology (note: the vadose zone is not actually modeled in Tier 1).

No fate processes, such as sorption or degradation, are applied to the interflow flux. Thus, the fraction of interflow is multiplied times the infiltrating flow rate and mass flux computed by the soil model to produce the interflow water flow rate and mass flux, exactly as done for Tier 2. These values are then added to the surface runoff flow rate and dissolved mass flux computed by the soil model, and the combined results are written to the WFF for surface water. The soil model also reduces the water flow and mass flux exported to groundwater by the same amount before writing to the WFF vadose file.

Two inputs are required and must be added to the Tier 1 soil model UI: the vadose zone saturated hydraulic conductivity K_s (m/yr), and the percent of infiltration diverted to soil interflow. The latter will include the alternative of having the UI estimate the percentage of infiltration diverted to soil interflow based on K_s. A reference note will be available for each input as well. These additional inputs for the Tier 1 soil model UI will be added through a separate and new third tab. The help file for the Tier 1 soil model UI must also be modified to reflect these changes.

Groundwater discharge approach and requirements

During dry seasons when surface stream flows are low, groundwater discharge can contribute a major portion of the stream flow. For some watershed conditions, groundwater discharge can be the primary contributor to flow in small streams. For these reasons, it is necessary to include a contribution of MC loading from groundwater flow to surface water for Tier 1, similar to what is done in Tier 2.

For Tier 2, it was necessary to develop a special module to allow groundwater discharge to surface water. The new module consumes the MEPAS Aquifer model WFF, which contains aquifer flow (m^3/yr) and aquifer mass flux (g/yr) at a flux location, which is specified in the MEPAS Aquifer model UI. The flux location in this case is the distance from the center of the AOI to the point in the landscape where the stream or water body and aquifer have crossed in the landscape. If the target surface water point of interest (i.e., receptor target location) is further downstream, then there are no further mass losses or mass flux attenuation as water travels from the point of groundwater intersection to the water body target location.

The new module serves two functions: it performs an operation on the aquifer WFF for groundwater discharge to surface water; and it combines surface water and aquifer WFFs. The new module is referred to as the Plus operator for Surface water and Groundwater, or Plus-SG for short. The Plus-SG operator or module will be used for Tier 1 just as it is used for Tier 2. The Plus-SG module combines surface water flow and mass flux from soil and aquifer water discharge and mass flux into a single, combined surface water WFF that will be consumed by the Tier 1 surface water model.

The same UI for the Plus-SG module developed for Tier 2 is used in Tier 1 where the user is requested to input either the percentage of total groundwater flow that discharges from groundwater to surface water or a constant groundwater flow rate (m^3/yr) entering the receiving surface water body. The Plus-SG module divides the aquifer WFF mass flux by the aquifer WFF flow rate at the flux location to obtain an aquifer concentration at the location of groundwater discharge to surface water. This concentration is multiplied by the user-input groundwater discharge rate to obtain values for mass flux (g/yr) from groundwater to surface water. The groundwater discharge UI is launched within TREECS™ when the user saves and exits the Tier 1 aquifer UI, which is the same way it is done in Tier 2.

It is noted that groundwater flow in the aquifer model is constant since it is based in part on a user-specified and constant Darcy velocity. Thus, using a percentage of groundwater flow or a constant flow for groundwater discharge to surface water is acceptable.

The surface water WFF dissolved mass flux from soil (including interflow) that enters the Plus-SG is combined with the groundwater-to-surface-water mass flux to obtain a total dissolved mass flux entering the surface water body. The surface water WFF particulate (adsorbed) mass flux from soil that enters the Plus-SG is passed unaltered to the Plus-SG output WFF, which is consumed by the surface water body model. The surface water WFF water flux from soil runoff is combined with the groundwater-to-surface-water flow to obtain the total flow entering the surface water body. Thus, the Plus-SG operator outputs a surface water WFF that is similar to the surface water WFF from soil. The Plus-SG output file will be consumed by the Tier 1 surface water model.

It will also be necessary to add another tab in the Tier 1 aquifer model UI for the user to enter the longitudinal distance from the center of the AOI to the location of groundwater discharge and the associated dispersivities. These are the same inputs required in the Tier 2 aquifer model UI. There will also be an option of either having the UI estimate the dispersivities based on the distance of the flux location or allowing the user to enter dispersivities, the same as for Tier 2. It will also be necessary to modify the GID file templates for Tier 1 to include the Plus-SG operator. The help file for the Tier 1 aquifer model UI will be modified to reflect these changes.

Other changes are required of the TREECS™ UI and framework in order to accommodate these new features for Tier 1 analyses. For example, the TREECS™ GUI will be modified to display the Plus-SG input form. The algorithm that determines the appropriate GID template for a given Tier 1 scenario will have to be modified. Also, the “run model” algorithm must be modified such that it additionally runs the Plus-SG model for Tier 1 analyses.

7 Adding Water Hardness to Correct Ecological Health Benchmarks in Water

Background

Ecological health benchmarks for dissolved metals in freshwater systems should be reported based on water hardness. The U.S. Environmental Protection Agency (EPA) provides equations for ecological health benchmarks as related to chronic exposures to dissolved metals. These equations are part of the EPA National Recommended Water Quality Criteria published in 2006. The capability has been added to TREECS™ Tiers 1 and 2 to compute ecological health benchmarks for metals in surface water using water hardness.

Approach and requirements

The general formula for calculating the ecological benchmark (EBM) is stated as

$$EBM = CF \exp\left[mc\left(\ln hardness\right) + bc\right] \tag{10}$$

where *CF, mc*, and *bc* are values or relationships that vary depending on the metal. These parameter values for various metals are shown in Table 1.

Table 1. Metals and their parameters for computing the EBM.

Metal	CF	mc	bc
Cd-Cadmium	1.101672- 0.041838 ln (hardness)	0.7409	-4.719
CrIII-Chromium III	0.86	0.819	0.6848
Cu-Copper	0.96	0.8545	-1.702
Pb-Lead	1.46203- 0.145712 ln (hardness)	1.273	-4.705
Ni-Nickel	0.997	0.846	0.0584
Ag-Silver	0.85	1.72	-6.59
Zn-Zinc	0.986	0.8473	0.884

Thus, as examples, the benchmark equations for copper, lead, and zinc are, respectively:

$$EBM_{Cu} = 0.96 \exp\left[0.8545 \ln\left(hardness\right) - 1.702\right] \quad (11)$$

$$\begin{gathered} EBM_{Pb} = \left[1.46203 - 0.145712 \ln\left(hardness\right)\right] \\ \exp\left[1.273 \ln\left(hardness\right) - 4.705\right] \end{gathered} \quad (12)$$

$$EBM_{Zn} = 0.986 \exp\left[0.8473 \ln\left(hardness\right) + 0.884\right] \quad (13)$$

The *EBM* is in parts per billion (ppb) or µg/L dissolved metal, and *hardness* is in units of parts per million (ppm) or mg/L as calcium carbonate.

At this time, the ecological benchmark for antimony is a single number that is not dependent on hardness. The numbers for silver are actually acute benchmarks, not chronic. Since there are no chronic benchmarks for silver, the acute value must be used for now. The hardness-dependent formulas are only applicable to freshwater metals. All other freshwater metals not shown in Table 1 and all marine water benchmarks are not hardness dependent.

The hardness feature has been added within the DoD Target Health Benchmarks screen of the TREECS™ GUI. The DoD benchmark database was not altered. The changes to the benchmark UI screen involved adding a dialog that will check to see if a Chemical Abstract Service Registry Number (CASRN) of any of the user-specified MC of concern matches those CASRNs that have an equation to compute the benchmark based on hardness, like the ones above. For the MC values that match, the UI will query for the water hardness and compute the benchmark based on hardness and display the computed value in a new table for each MC that uses hardness. This new table also includes a check box next to each MC to either use the computed value or not. If the computed value is not used, then the value in the database will be used.

8 Capability to Simulate MC Fate with Time-Varying Hydrology and Erosion

Background

Tiers 1 and 2 of TREECS™ presently simulate long-term fate of MC on and exported from firing ranges using average annual hydrology and erosion. The TREECS™ advisory panel expressed interest in having the capability to model short-term, single events associated with individual storms. Additionally, it was deemed beneficial to have the capability to use time-varying hydrology and erosion for the long term. This chapter examines the requirements and specifications to allow for modeling time-varying hydrology and erosion. A daily time increment was selected as the base time unit.

Requirement

The overall requirement is to have the capability to include the effects of time-varying hydrology and erosion on fate and export of MC on ranges. Time-varying hydrology and erosion will be developed for daily updates within the soil model. This capability will facilitate examination of individual storms and first-flush features of a site as well as the impact of varying hydrology on long-term MC fate.

Approach and specifications

Including daily-varying hydrology and erosion will require modification/ extension of the Hydro-Geologic Characteristics Toolkit (HGCT) and the hydrology program used within it, portions of the TREECS™ system and UI, as well as modification of the Tier 2 soil model and its UI. Each component requiring modification is discussed below.

Tier 2 soil model

The Tier 2 soil fate and export model and its UI will be modified to allow simulations with daily-varying hydrology and erosion. The following modifications and/or clarifications for this model are:

1. The hydrologic input parameters (precipitation, infiltration, runoff, and erosion rates) used by the model must be expanded from single, time-invariant inputs to daily-varying inputs. The model unit for time must be changed from a year to a day. Thus, the model time-step must be expressed in units of days and must be limited to a day or less to be compatible with daily hydrologic inputs. If the time-step is less than a day, the hydrologic input values will be held constant within the model simulation until the next daily update. All mass fluxes and rates used to compute mass fluxes must be per day units rather than per year units. The model must be able to identify when the model simulation time has reached the next update day.
2. In addition to reading the daily-varying hydrology input file, the Tier 2 soil model must be modified to read in hourly rainfall data (rainfall intensity in inches/hour), which is required for computing rainfall extraction rates of MC in soil pore water. It will be necessary to modify the rainfall extraction algorithm within the model that is used to compute export due to rainfall and runoff. The rainfall extraction export rate will be computed as described in Appendix A of this report. The revised constituent mass balance equation is also presented in Appendix A.
3. The solid phase MC dissolution flux and volatilization rate equations must be modified in the soil model for daily updates and rates as described in Appendix A.
4. Although the revised Tier 2 soil model for time-varying hydrology will operate with a daily time scale, the model output will still be in annual time units. For example, the mass export fluxes to surface water and vadose zone will be output as g/yr versus time where time is in units of years (with decimal fractions), the same as the existing version of the model. These units are consistent with the TREECS™ system specifications and can still accommodate outputs that vary daily.
5. Modifications and/or clarifications required of the Tier 2 soil model UI are as follows:
    a. The Tier 2 soil model UI must be modified so that the user is required to choose either *Average Annual Hydrology* or *time-Varying Hydrology*. This choice must be made before entering other data and will cause the appropriate screens/fields of the UI to be displayed, depending on the type of analysis. This choice will also result in execution of the appropriate model or routines, depending on the type of analysis.

b. An alternate version of the *Hydrology* screen of the UI must be developed. This new screen for time-varying hydrology will not include any of the inputs for average annual hydrologic variables. Two queries will show on this screen to provide the two input file names for the files containing the daily hydrologic inputs generated by the HGCT daily hydrology model and the observed hourly rainfall data.

c. The soil interflow panel on the new, alternate *Hydrology* screen will include two options: 1) interflow is a constant percentage of the time-varying infiltration rate and is input by the user; and 2) interflow will be computed using vadose zone saturated hydraulic conductivity and the daily-varying infiltration rate. If the second option is selected, then the percent of infiltration going to interflow will not be displayed, since it will vary with time.

d. Although the revised Tier 2 soil model will utilize daily hydrology (e.g., infiltration) and compute daily infiltration mass fluxes, it will be necessary for the soil model UI to average the daily recharge flow rates over the simulation period and write the average annual recharge flow (m^3/yr) into the WFF vadose output file used as input by the vadose zone model. The reason for this need is explained in the section below on “Groundwater.” The recharge flow can be computed within the soil model UI from the difference in the infiltration flow rate and soil interflow rate. Daily mass fluxes of MC associated with the daily-varying recharge flow will still be output to the WFF vadose file.

e. The other inputs involving time in the input units will retain yearly time units in the UI input fields, but will be converted to daily units for use by the model, which has a time basis of days. These conversions can be done either within the UI code or within the model code.

Tests must be conducted to verify that the model is properly computing export fluxes and soil concentrations. For example, one test can consist of applying the model with constant daily inputs and comparing to the previous model that uses average annual inputs. The two results should be nearly the same. In another test the period of record will be run with time-varying hydrology and then compared to previous runs with annual average hydrology to examine the differences and benefits of using daily hydrology.

HGCT

It will be necessary to modify and extend the HGCT and the associated model/routines to provide daily varying hydrology and erosion rates, as well as hourly rainfall as needed for the revised Tier 2 soil model. The required changes to HGCT and the models for daily hydrology and erosion are described in the sections below.

Hydrology

Hourly observed precipitation will be required as input for time-varying hydrology. The user must choose the precipitation recording station and period to be used for modeling and gather the hourly observed data for that period.

The revised HGCT for time-varying hydrology will still query for the precipitation file name, but the file must contain hourly rather than daily precipitation data. The HGCT hydrology model will produce a file of hourly rainfall data for use by the soil model for computing rainfall-extracted export rates. It is noted that this output file must contain rainfall, not precipitation, thus air temperatures are required as before to determine snow versus rain. The hourly rainfall data will be summed by the hydrology model to obtain daily rainfall, which will be used within the HGCT to compute daily erosion rates as described in the next section below. The number of hours of rainfall each day will also be counted within the hydrology model. Hourly precipitation (not rainfall) will also be summed within the hydrology model to obtain daily values, which will be used within the hydrology model to compute daily runoff, evapotranspiration (ET), and infiltration using the methods currently in the HGCT hydrology model (Dortch et al. 2009, 2010, and 2011b). The HGCT hydrology model will write data into two output files for the period of record as follows. One output file will contain hourly rainfall each day. The other output file will contain the number of hours each day that there is rainfall, and daily depths of precipitation, rainfall, runoff, ET, and infiltration. This second file will be used by the HGCT module and will also include the average annual values computed by the hydrology model as before.

The calculation of runoff as implemented in the HGCT hydrology model is briefly summarized again as follows. A slightly modified version of the U.S. Department of Agriculture (USDA) Soil Conservation Service (SCS) curve number (CN) runoff method (USDA SCS 1983) is used to determine the daily runoff depth Q (inches),

$$Q=\frac{(P-0.2S)^2}{P+0.8S}=\frac{[CN(P+2)-200]^2}{CN[CN(P-8)+800]} \tag{14}$$

where potential retention *S* (inches) is defined by

$$S=\frac{1000}{CN}-10 \tag{15}$$

P is rainfall for the day in inches, and CN is the curve number adjusted for antecedent moisture condition (AMC). There is runoff for the day only if $P > 0.2S$. If $P > 0.2S$ for the day and $P > 0.2S$ for the day before, then all of the rainfall runs off, or $Q = P$ for the present day. This AMC approach and threshold runoff condition should be re-examined and possibly revised based upon comparisons with observed rainfall – runoff data. The method used in the Soil and Water Assessment Tool (SWAT) should be considered. SWAT is a watershed model developed by the USDA. The method in SWAT computes a dynamic retention parameter *S* that varies daily and depends on the previous day's value and the current day's rainfall, runoff, and evapotranspiration. The runoff depth *Q* must be converted from inches to meters and multiplied by the AOI surface area *A* (m^2), resulting in runoff volume for the day, Q_v (m^3).

The inputs presently required on the *Hydrology* screen of the HGCT UI will still be required. The query for the precipitation and air temperature file names should probably be moved, since these are needed for erosion and hydrology. Alternatively, the file queries could remain on the *Hydrology* screen with the constraint that the inputs for the *Hydrology* screen must be provided first, and the hydrology model must be executed before proceeding to the *Erosion* screen of the HGCT. The HGCT UI should still display the average annual hydrology as provided by the hydrology model in the existing average annual version; this would be accomplished by summing the daily values for the period of record and dividing by the number of years.

Erosion

The Modified Universal Soil Loss Equation (Modified USLE), or MUSLE, will be used to estimate daily soil erosion rates. The MUSLE equation (Williams 1975) is stated as,

$$A_s = 11.8\left(Q_v\, q_p\right)^{0.56} K\, LS\, C\, P \tag{16}$$

where

A_s = sediment yield from overland soil erosion for a rainfall event, metric tons
Q_v = event runoff volume, m^3
q_p = peak runoff flow rate for an event hydrograph, m^3/sec

The other parameters in Equation 16 (*K, LS, C, P*) are the standard USLE parameters that are used in the HGCT for Tier 1 and Tier 2 of TREECS™. In this implementation of MUSLE, an event consists of a one-day duration in which there is rainfall within the day.

The steps required for estimating the two flow variables in Equation 16 are as follows.

1. The daily runoff Q_v is computed by the HGCT hydrology model from the long-term precipitation record as discussed in the Hydrology section above. In addition to daily runoff, the HGCT hydrology model will also provide daily rainfall and the number of hours of rainfall each day, or the daily rainfall duration t_r (hours).
2. The daily peak runoff flow rate q_p will be estimated by the HGCT using the relation $q_p = \dfrac{Q_v}{t_r}$, which is based on using a triangular hydrograph shape; t_r should have been converted from hours to seconds.
3. With values for q_p and Q_v, the MUSLE equation will be applied within the HGCT to compute sediment yield for each day (metric tons/day; metric ton = 1,000 kg). The sediment yield will be divided by the AOI surface area (m^2), and that result will be divided by the soil dry bulk density ρ_b (metric tons/m^3) to obtain the erosion rate E (m/day). Soil dry bulk density is estimated by the HGCT and is approximately 1.5 metric tons/m^3.

It is emphasized that steps 2 and 3 above will be performed by the HGCT module, so the AOI surface area will be a new input on the HGCT hydrology screen.

For confirmation, the above procedure for computing daily erosion was compared to the USLE results calculated for the AOI at Fort A.P. Hill (Dortch et al. 2011b) with the sediment delivery ratio (SDR) set to 1.0. The daily erosion rates computed with MUSLE were summed for each day over the 26-year record and then divided by 26 to obtain an average annual rate. The rates are compared here as fluxes in English mass units (tons, T) per unit area (acre) per year. The average annual flux computed with MUSLE using daily rainfall was 7.5 T/acre/yr, and the flux computed using USLE was 7.2 T/acre/yr. This excellent agreement confirms that it is acceptable to use daily rainfall to compute daily runoff and it is also acceptable to use daily peak flow rate to compute daily erosion with MUSLE.

The *Erosion* screen of the HGCT UI will query for the same input as the previous version for average annual erosion. All of this information is required for the MUSLE equation, except for the rainfall factor R. However, the rainfall factor and the other inputs will still be used with USLE to compute the average annual erosion rate for comparison purposes. Additionally, the average annual erosion rate will be displayed as computed from the average of the daily values computed using MUSLE for the period of record. The HGCT will append the daily erosion rates to the daily hydrology output file written by the hydrology model for use by the soil model. A flow diagram of data generated for and/or by the HGCT, the hydrology model, and the soil model is shown in Figure 3.

HGCT user interface

As stated above, it is necessary to develop time-varying hydrology before attempting to develop time-varying erosion. Thus, the HGCT UI should be modified to require this sequence of input and execution. Additionally, the HGCT UI must be modified to require choosing either *Average Annual* or *Time-Varying analyses*. It is assumed that if a user decides to compute time-varying hydrology, then time-varying erosion will also be computed. Therefore, the choice of analysis type (average annual or time-varying hydrology and erosion) can be placed on the *Hydrology* screen. This choice will cause the appropriate fields to be displayed on the *Hydrology* and *Erosion* screens that accompany the choice of analysis. The choice would also invoke the appropriate hydrology and erosion model/routines to be

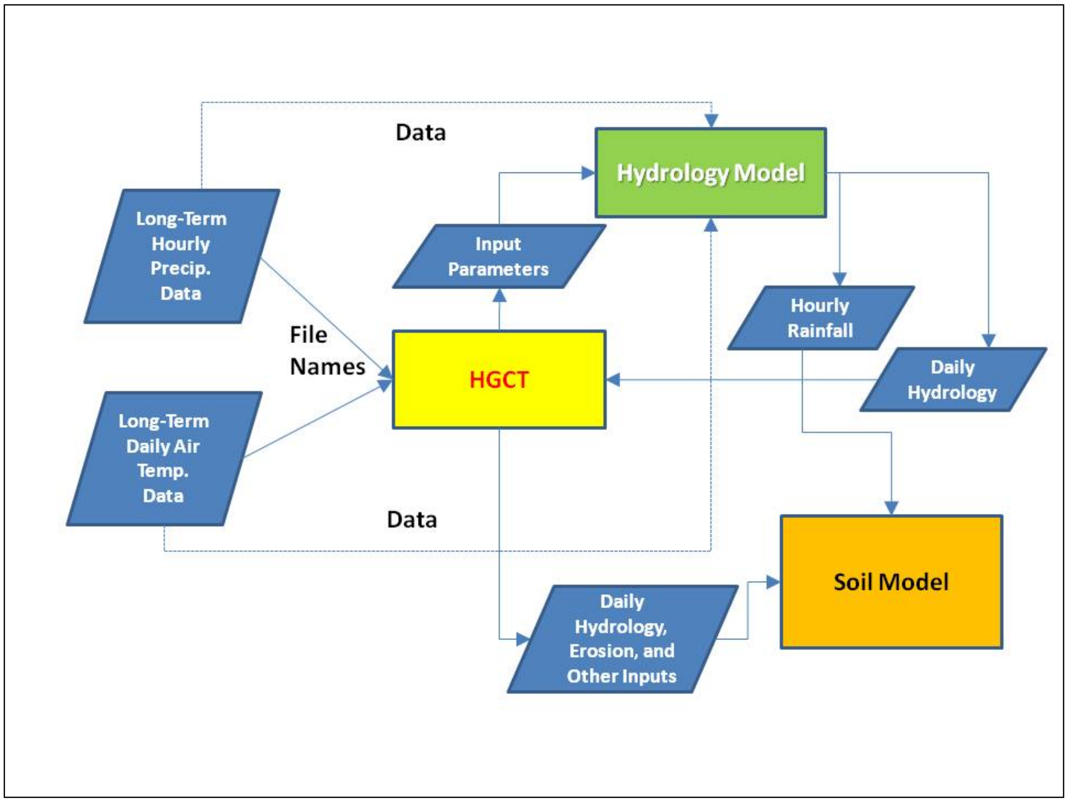

Figure 3. Data flowchart for handling time-varying hydrology.

executed. The Tier 2 soil models may need to verify that time-varying HGCT output is not used with the constant hydrology soil model and that the average annual HGCT output is not used with the time-varying hydrology soil model. AOI surface area will be a new input required on the hydrology screen.

Surface water

Either receiving water model (RECOVERY or CMS) can be used with output from the revised soil model, but CMS is better suited for highly transient inputs stemming from the soil model output, such as daily-varying loadings, since the time basis for solution in CMS is in days. The RECOVERY model uses years for its time basis.

Additionally, the CMS can accurately simulate highly unsteady fate/ transport of contaminants in streams. However, the CMS assumes uniform flow, and there is no flow routing capability. Thus, for each update in the input time series of flow and mass influx, the model takes the input flow rate that enters at the head of the stream and assumes that flow exists instantaneously throughout the entire modeled reach until the next input flow update. This simplified representation of stream flow is not a major concern since flow changes occur fairly rapidly within relatively short stream reaches, and most stream reaches associated with range runoff are expected to be low order and relatively short. Thus, the assumption of instantaneous flow updates throughout the stream reach is not expected to compromise model results to any great degree. Likewise, for relatively short stream reaches, the uniform flow assumption is not unreasonable. These two flow assumptions within the CMS are what make the model fairly easy to use while providing reasonable results. It is emphasized, however, that the CMS does route constituents, i.e., it performs time-varying, one-dimensional, reactive, mass transport (advection and diffusion) along the stream reach, and can simulate quite accurately short-term, highly transient transport, such as that associated with spills (Fant and Dortch 2006, 2007).

The RECOVERY model accepts time-varying MC loadings (g/yr), but water inflow rate (m^3/yr) is constant throughout the simulation and is input by the user. As noted above, CMS can accept both time-varying loadings and time-varying water inflow rates. Thus, it would be better to use the CMS rather than RECOVERY for hydrology that varies substantially over time. It is anticipated that no changes will be required of the CMS or RECOVERY for processing output using time-varying flows and MC loads. It is emphasized again that RECOVERY does not use the time-varying flows.

Groundwater

The MEPAS vadose zone model can read time-varying percolation (recharge) flow rates (m^3/yr) from the soil model, but it only uses the first value in such a time series. That single value is used for transport throughout the vadose zone simulation and is also output for use as input to the aquifer model. Therefore, time-varying hydrology, including infiltration and recharge, will not be reflected in the groundwater simulations. Modifications to these legacy MEPAS models would be required to include the effects of time-varying recharge flow rate. The assumption of a constant recharge rate is not as bad as it might appear considering that constituent transport is very slow in groundwater and can require many years (even centuries) to reach target wells. Thus, assuming an average annual recharge rate is not unreasonable. The soil model UI should output the average annual recharge (determined by averaging the difference in daily infiltration and daily soil interflow rates) to the WFF vadose file used by the vadose model. This average annual value must be written as the first value for flow in the time-varying WFF file used by the vadose model.

Based on these facts, it is recommended that the MEPAS groundwater models not be modified at this time. Although daily recharge and interflow will be used by the revised Tier 2 soil model to compute daily export fluxes to be used as input to the vadose zone and surface water models, the soil model UI must output average annual recharge flow rate (m^3/yr) to the vadose zone model as the first flow entry in the WFF file.

9 Assessing the Effect of MC Particle Size Classes on AOI Export

Background

The Tier 2 soil model presently assumes a single initial particle size of solid phase MC residue on ranges. Thus, the mean initial particle diameter is entered as input. Dissolution of solid phase MC is the only fate process in TREECS™ presently affected by particle size. During the development of Tier 2 of TREECS™, it was recognized that solid phase MC has a distribution of varying particle sizes, but implementing such a feature would have added additional, and possibly unnecessary, model complication. Thus, it was necessary to investigate this feature to determine if it should be added to the soil model. Such an investigation was conducted and is summarized in this chapter.

Objective

The objective of the investigation summarized in this chapter was to determine the relative importance of including multiple classes of initial particle sizes for solid phase MC residue. The term *relative* effect is used since the effects were gauged by comparing results to the present approach; i.e., treating all particles as having one common or average size.

Approach

The existing Tier 2 soil model was applied for a base case and three variations of the base case, where each variation differed from the base according to the prescribed initial particle diameter of MC residue and the amount of MC residue mass loaded and existing initially (at the beginning of the simulation) within the AOI. The three variation cases represented three particle size classes as shown in Table 2. The base case consisted of 10-mm particles that represented 100% of the initial and loaded MC residue mass.

All four applications (base and three variations) were run using RDX and conditions for Fort A.P. Hill as discussed by Dortch et al. (2011b). The four applications were run for varying amounts of MC initial residue mass and non-solid phase MC concentration C_{tt} (g/m^3) to determine any effects that initial conditions might have on results.

Table 2. Variation cases simulated.

Simulation Case	Initial Particle Diameter, mm	Percent of Base Case Total Mass Initially and Loaded
1	20	25
2	10	50
3	1	25
base	10	100

Relative effects were determined by summing the export mass fluxes from AOI soil for the three variation applications and comparing those fluxes to the export fluxes computed for the base case. A set of runs were conducted to validate the approach. This was accomplished by running all four cases with the same particle diameter. The approach was validated since the sum of the AOI exports for the three variation cases equaled the AOI exports for the base case.

Results

The four applications were conducted for three levels (low, moderate, and high) of initial mass of solid phase MC residue. Each of these three levels had the respective values of 7.7E-6, 7.7E-4, and 1.0 for the ratio of initial MC mass to cumulative MC residue mass loaded over a 65-year loading period. These three sets of applications had zero initial non-solid-phase MC concentration.

The AOI relative mass exports from soil after 100 years due to leaching, erosion, and rainfall extraction are shown in Table 3. Relative export is defined as the variation case cumulative exported mass (g) divided by the base case cumulative exported mass (g). As shown by Table 3, the overall relative effect of including three particle size classes is that the individual and total cumulative mass exports are 97% of that computed with one size class. Therefore, there is little difference in results whether modeling involves three size classes or one size class.

Table 3. Relative cumulative mass exports.

Simulation Case	Leaching Relative Export	Erosion Relative Export	Rainfall Extraction Relative Export	Total Relative Export
1	0.186	0.186	0.186	0.186
2	0.500	0.500	0.500	0.500
3	0.283	0.283	0.283	0.283
Totals	0.969	0.969	0.969	0.969

Test results for the other sets of runs with the high and low solid phase MC residue initial mass were similar to those in Table 3, i.e., total relative exports were less than 1% different from those in Table 3. A set of simulations was also run with an initial non-solid-phase MC concentration. The AOI MC mass associated with this concentration was about three times greater than the cumulative residue mass loaded over the 65-year loading period. Thus, this initial C_{tt} concentration had a dominating impact on results. The total relative cumulative export was 1.02 for these runs, or the mass exports with three and one particle size classes were almost the same. Therefore, as before, AOI exports are affected very little whether modeling involves three size classes or one size class.

Other considerations

A portion of solid-phase MC residue particles can be so small that they behave as a colloid. A colloid is a system in which finely divided particles, which are approximately 1 µm or less in size, are dispersed within a continuous medium in a manner that prevents them from being filtered easily or settled rapidly. This phenomenon can be particularly true for lead and other metal particles in impact berms of small arms firing ranges where bullet impact causes smearing of lead/metal fragments into very small particles.

Colloids are mobile and have been known to move with water in runoff and infiltrate through porous media. Results of laboratory lysimeter studies (Larson et al. 2005) indicated that the flux of metal mass in leachate measured as total was found to be considerably greater than the leachate flux measured as dissolved (as filtered through a 0.45-micron filter). This indicates that metal mass greater than 0.45 µm had passed through the soil, sand, geotextile cloth, and pea gravel layers in the lysimeter before being collected as a leachate sample. It is suspected that the particulate metals in the leachate were colloids, which were too small to be filtered by the porous media and geotextile cloth and too large not to be filtered by the 0.45-micron filter during analysis. Total metal concentrations greater than dissolved metal concentrations have been observed in groundwater near firing ranges, such as at Fort A.P. Hill. However, it is possible that stationary soil particles containing adsorbed metal were drawn through the well screen into the sample collection well rather than the occurrence of colloidal transport in groundwater.

The percent of total solid phase MC residue mass that is colloidal is difficult to determine and is not well known. Metal colloids are of primary interest since small organic particles with higher solubility, such as explosives, should dissolve fairly rapidly compared with metals. Adding metal colloids as an additional state variable within the TREECS™ models would be challenging and a sizable effort. It is difficult to justify modifying the models to add additional processes and complication when there is little to no information with which to estimate the input parameters required for modeling colloids, such as the percent of total solid phase metal residue that exists in colloidal form.

Since colloids basically behave like dissolved constituents, the effect of colloids on non-solid phase MC concentrations and export from soil can be imitated by increasing the dissolution flux of solid phase MC and decreasing the soil K_d for the MC. The dissolution flux can be increased by increasing the MC solubility. The adjusted (decreased) K_d is referred to as the apparent distribution coefficient K_d' (L/kg), similar to the approach used to model partitioning of organic constituents when water-dissolved organic carbon (DOC, mg/L) is present in the water (such as soil/sediment pore water) to adsorb the chemical and facilitate transport when DOC moves with the water.

Soil and sediment–water partitioning is modeled in the TREECS™ models with a reversible linear equilibrium distribution coefficient K_d (L/kg), where K_d is defined as the MC concentration adsorbed onto sediment or soil C_a (mg/kg) divided by the water dissolved or liquid concentration C_l (mg/L). In the case of a metal colloid, K_d' can be computed from

$$K_d' = \frac{K_d}{1 + \dfrac{C_c}{C_l}} \tag{17}$$

where C_c is the colloid concentration in water (mg/L), and K_d is the traditional estimate of the partitioning distribution coefficient with the absence of facilitated transport (i.e., colloids in this case). The problem with Equation 17 is that C_c is not known and can't be determined without knowing the rate of source supply (based on percent of solid phase MC residue that is colloidal); nor is the relationship of C_c to C_l (such as their ratio) known. Thus, one must assume the ratio C_c/C_l. A ratio of 1.0 would make the apparent distribution coefficient half of the traditional value.

Facilitated transport of organic MC can be rather easily accounted for by using an apparent distribution coefficient for partitioning between soil/sediment and water. The apparent distribution coefficient for organic MC can be computed from

$$K_d' = \frac{K_d}{1 + 10^{-6} K_{DOC} DOC} \tag{18}$$

where K_{DOC} (L/kg) is the distribution coefficient for partitioning between DOC and water, which can be assumed to equal the organic carbon-water sorption partitioning coefficient K_{oc}; K_{oc} can be estimated from the octonol–water sorption partitioning coefficient K_{ow} (L/kg). In TREECS™, $K_{oc} = 0.617 K_{ow}$.

Conclusions and recommendations

Based on the results of the tests described above, it is concluded that including multiple size classes for the initial particle size of solid phase MC residue will have little effect on dissolution fluxes and computed mass exports from soil. Given this conclusion, it is recommended that the Tier 2 soil model should continue to treat solid-phase MC residue particles as one size, with the size equal to the expected mean particle size based on the mass distribution of particle sizes.

The presence of metal colloids and DOC can facilitate water-phase transport of MC. Although colloids could be a significant contributor to MC residue fate, there is not enough information at this time to warrant implementation of colloids into the TREECS™ models. It is recommended that the potential effects of colloids and DOC on facilitated transport be accounted for by using apparent soil/sediment–water sorption partitioning distribution coefficients. A higher solubility could also be used to increase dissolution, which increases non-solid phase MC, thus mimicking the presence of colloids.

The above recommendations will not require any changes to any of the TREECS™ models or framework. The user must decide whether to adjust the partitioning coefficients. If adjustment is warranted, then Equations 17 and 18 can be used to assist in the adjustment. There is no guidance for increasing the MC solubility; rather this might be treated as an uncertain input during sensitivity/uncertainty analysis.

References

Dortch, M. S., J. A. Gerald, and B. E. Johnson. 2009. *Methods for Tier 1 modeling with the Training Range Environmental Evaluation and Characterization System*. Technical Report ERDC/EL TR-09-11. Vicksburg, MS: U.S. Army Engineer Research and Development Center.

Dortch, M. S., B. E. Johnson, and J. A. Gerald. 2010. Proof-of-Concept Application of Tier 1 Modeling Approach within the Training Range Environmental Evaluation and Characterization System. Technical Report ERDC/EL TR-10-19. Vicksburg, MS: U.S. Army Engineer Research and Development Center.

Dortch, M. S., B. E. Johnson, Z. Zhang, and J. A. Gerald. 2011a. *Methods for Tier 2 Modeling within the Training Range Environmental Evaluation and Characterization System*. Technical Report ERDC/EL TR-11-2. Vicksburg, MS: U.S. Army Engineer Research and Development Center.

Dortch, M. S., B. E. Johnson, J. A. Gerald, and Z. Zhang. 2011b. *Proof-of-concept application of Tier 2 modeling approach within the Training Range Environmental Evaluation and Characterization System*. Technical Report ERDC/EL TR-11-10. Vicksburg, MS: U.S. Army Engineer Research and Development Center.

Fant, S., and M. S. Dortch. 2006. A flexible and easy to use contaminant fate/transport model for streams. *Proceedings of the 3rd Federal Interagency Hydrologic Modeling Conference, Reno, Nevada.*

Fant, S., and M. S. Dortch. 2007. *Documentation of a one-dimensional, time-varying contaminant fate and transport model for streams.* ERDC/EL TR-07-01. Vicksburg, MS: U.S. Army Engineer Research and Development Center.

Gao, B., M. T. Walter, T. S. Steenhuis, W. L. Hogarth, and J. Y. Parlange. 2004. Rainfall induced chemical transport from soil to runoff: Theory and experiments. *J. of Hydrology* 295: 291-304.

Julien, P. Y. 1995. *Erosion and sedimentation*. New York, NY: Press Syndicate of the University of Cambridge.

Larson, S., B. Tardy, K. Rainwater, and J. Tingle. 2005. *Rainfall lysimeter evaluation of leachability and surface transport of heavy metals from six soils with and without phosphate amendment*. Technical Report ERDC TR-05-9. Vicksburg, MS: U.S. Army Engineer Research and Development Center.

Simons, D. B., and F. Senturk. 1992. *Sediment and transport technology – Water and sediment dynamics*. Littleton, CO: Water Resources Publications.

U.S. Department of Agriculture (USDA) Soil Conservation Service (SCS). *1983. National Engineering Handbook, Section 3, Sedimentation, 2d. ed.*

Williams, J. R. 1975. Sediment-yield prediction with Universal Equation using runoff energy factor. In *Present and prospective technology for predicting sediment yield and sources*. ARS-S-40, 244-252. U.S. Department of Agriculture.

Appendix A: Modifying the Tier 2 Soil Model for Daily Time Scale

The Tier 2 soil model equations will be modified to properly handle a daily time scale. The equation modifications discussed below are in addition to the modifications discussed in Chapter 8 that involve changing all time units to days rather than years, reading in daily hydrology and erosion inputs, and reading in hourly rainfall.

Rainfall-induced pore water ejection and runoff flux

Rain-induced pore water ejection and runoff F_r (g/day) must be computed. Chemicals 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/hr) due to rain-induced ejection, as described by Gao et al. (2004) and as modified by Dortch et al. (2011a) for soil total concentration on a total volume basis C_{tt} (g/m^3), can be computed from

$$\mathrm{Re}_{dQ} = \frac{Ad_e}{T}\left(1 - e^{-\beta T}\right)C_{tt} \tag{A1}$$

where A is surface area of the AOI (m^2), d_e is the soil exchange layer thickness (meters), and T is the time-averaging interval or the event duration (hours). Since this version of the soil model will be using hourly rainfall, and the rainfall extraction rates will be computed hourly, T is equal to 1.0 hr. The parameter β (1/hr) is computed from

$$\beta = \frac{aI\phi F_{dp}}{\rho_b d_e \theta_w} \tag{A2}$$

where

a = soil detachability due to rainfall (kg/L)
I = rainfall intensity (m/hr)
ϕ = saturated water content, which is the soil porosity (dimensionless)
ρ_b = soil dry bulk density (kg/L)

θ_w = soil volumetric moisture content (dimensionless)
The factor F_{dp} is computed from

$$F_{dp} = \frac{\theta_w}{\theta_w + (\phi - \theta_w) K_H + \rho_b K_d} \tag{A3}$$

where K_H is the dimensionless Henry's constant for partitioning between air and water, and K_d (L/kg) is the distribution coefficient for partitioning a constituent between soil particles and water.

The parameter θ_w is treated as constant throughout the model simulation and should be set to the annual average value. It is not assumed that θ_w is equal to ϕ during rainfall.

The other variables in Equations A1–A3 are constants with the exception of I and C_{tt}. Assuming that C_{tt} is constant over a day, a daily rainfall extraction rate Re_r (m/day) can be determined for each MC from

$$\mathrm{Re}_r = \sum_1^{24} \left[d_e \left(1 - e^{-\beta} \right) \right] \tag{A4}$$

The duration T shown in Equation A1 has been omitted in the above equation since it has a value of unity (1.0 hr).

The daily rainfall extraction export rates Fr (g/day) can be computed from

$$F_r = A \mathrm{Re}_r C_{tt} \tag{A5}$$

Relating the above equations to the rainfall extraction export flux results in a revised Equation 50 in the report by Dortch et al. (2011a), as follows,

$$\begin{aligned} \frac{dC_{tt}}{dt} = \frac{F_{dis}}{AZ_b} - \Bigg[\frac{\mathrm{Re}_r}{Z_b} + \frac{E}{Z_b} + \frac{q_w}{\theta_w Z_b} F_{dp} + \\ \left(\lambda_l F_{dp} + \lambda_a F_{pp} \right) + F_{ap} \frac{K_v}{Z_b} \Bigg] C_{tt} - \frac{F_{precip}}{AZ_b} \end{aligned} \tag{A6}$$

where all other variables are defined by Dortch et al. (2011a) with the exception that the time units for the rates are 1/day rather than 1/yr for the above equation, and dt is the time-step in days. The export rate Re_r

varies daily and by MC; thus, these must be computed within the soil model and cannot be preprocessed by the HGCT.

Daily runoff will be computed by the HGCT and provided as an input to the soil model. If runoff for the day is zero, then Re_r will be set to zero for that day even if there is rainfall on that day.

Testing of the above method of computing daily rainfall-extracted export using hourly rainfall data revealed that it is more accurate to use hourly rainfall rather than daily rainfall. The above method was also compared with the annualized method in the Tier 2 soil model (Dortch et al. 2011a) with an average annual rainfall of 0.923 m for an average of 99 rainfall days per year. This is equivalent to an hourly rainfall of 0.0153 in./hr for 24 hr 99 days a year. Applying this hourly rainfall with the above method for an example case of RDX in soil at a concentration of 2.16E-4 g/m^3 resulted in a computed rainfall export rate of 400 g/yr for 99 rainfall days per year. This compares favorably with the export rate of 340 g/yr computed by the Tier 2 soil model's annualized formulation.

Dissolution of solid phase MC

Dissolution flux F_{dis} (g/day) must be computed daily rather than computing a single average annual value. The formula for dissolution flux is the same as the one developed by Dortch et al. (2011a) except for the precipitation rate units, which are m/day rather than m/yr. The dissolution flux is computed from

$$F_{dis} = P_t \alpha M_s C_s \tag{A7}$$

where

M_s = MC solid phase mass (g)
C_s = aqueous solubility of the MC (g/m^3)
P_t = precipitation rate (m/day)
α = average specific surface area (m^2/g)

The dissolution flux is updated for each time-step using daily precipitation data. Equations 41–43 in the report by Dortch et al. (2011a) are still used to compute updates for α each time-step.

Volatilization rate

The volatilization rate K_v must be changed from an annual rate to a daily rate (m/day). The equation to estimate the daily rate is simply the annual rate as shown in the report by Dortch et al. (2011a) divided by 365 days/year or

$$K_v = \frac{D_{G_{eff}}}{d_v} \tag{A8}$$

where $D_{G_{eff}}$ is the effective diffusion coefficient (m^2/day) for a vapor in soil, and d_v is the diffusion layer thickness (m) in the top of the soil layer. Dortch et al. (2011a) provide equations for estimating the effective diffusion coefficient; a value for d_v of 0.4 m is also recommended. The volatilization rate is assumed to be constant over time, so it only needs to be computed one time by the revised Tier 2 soil model UI.

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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 of and risk from munitions constituents (MC), such as high explosives (HE), within and transported from firing/training ranges to surface water and groundwater. The overall objective is to provide environmental specialists with tools to assess the potential for migration of MC into surface water and groundwater systems and to assess range management strategies to protect human and environmental health. Initial development consisted of two tiers. Tier 1 included screening-level methods that assume highly conservative, steady-state MC loading and fate, with no MC loss due to degradation. Tier 2 provides time-varying analyses. Thus, media concentrations computed with Tier 2 should be closer to those expected under actual conditions. The present work as summarized in this report focused on extending the capabilities of the Tier 1 and 2 methods in TREECS™. The requirements and specifications for including these extended capabilities are described in this report as well as various technical analyses that were conducted to support the work.

15. SUBJECT TERMS

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