# DEVELOPMENT OF A DISTRIBUTED SOURCE CONTAMINANT TRANSPORT MODEL FOR MILITARY INSTALLATIONS

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**Abstract**

Given the complex nature of surface water and groundwater interaction, as well as the spatial nature of contaminant distribution, a distributed source contaminant transport model is needed to accurately account for the movement of water and contaminants through the various landscape media where more simplistic models are not applicable, or are homogeneous which is not appropriate for the heterogeneous nature of distributed sources. This paper will discuss the current state of contaminant fate and transport development activities, by the Engineer Research and Development Center (ERDC), for the overland, upper soil zone layer, and channel regimes for inclusion within the Gridded Surface Sub-Subsurface Hydrologic Analysis (*GSSHA*) model. The contaminant modules are being developed to specifically handle Cyclotrimethylenetrinitramine (RDX) and Trinitrotoluene (TNT), however, the formulations are being described in a physical way such that other contaminants of concern will be able to be modeled by the system. The contaminant modules will account for each contaminant in the solid, adsorbed, dissolved, and vapor phases. In addition, parent and child products will be accounted for in the formulations. Finally, model validation studies for Camp Shelby are currently underway. This paper will discuss the current state of these validation studies and any future development activities being planned.

## INTRODUCTION

Ecosystem management to provide for sustained and future sustainable mission capacity remains the DoD goal for military installations. The ecosystem management expectation can only be met by providing the tools necessary to actively manage the landscape on a watershed basis. Water quality and related aquatic ecosystems are major endpoints and are insufficiently understood components of natural resource management, particularly for military installations. Many military installations contain soil, sediment, surface water, and groundwater environments contaminated with explosives (Brannon and Myers, 1997). These installations require usable and effective models that can be implemented for compliance as well as long-term watershed planning and management. Current watershed models are largely confined to conceptual and pseudo-distributed surface water simulation and thus are unable to account for the transport and fate of distributed sources of contamination. Models that reflect hydrologic and aquatic impacts from military contaminants and training scenarios are rare. Watershed models that enable diagnostic, predictive, and operational applications in conjunction with monitoring and data collection programs are virtually non-existent and again are required to meet the growing needs of the military community.

To meet this need, physically based, distributed source Contaminant Transport, Transformation and Fate (CTT&F) modules were developed to simulate both point and non-point sources across a watershed. The watershed domain is divided into cells that comprise a uniform finite difference grid. The spatial variability of soil, depth of the topsoil, and land use are allowed among cells. Potential chemicals are routed through cells from the watershed divide to the outlet. The distributed, process-oriented structure of the modules can be used for identifying critical source areas of distributed sources within the watershed. The CTT&F modules can be linked to any fully physically-based distributed hydrologic models such as the Gridded Surface Subsurface Hydrologic Analysis (*GSSHA*) model. The hydrologic model provides the required hydrological and sediment variables needed to perform the transport and fate of the military contaminants of concern. The expectation is that a modeling system of this type will facilitate the assessment of the fate of distributed source contaminants and lead to better management of the watershed environment for military installations. The ability of the model to simulate explosive compound transport is being demonstrated by a site-specific model application to the Camp Shelby Training Site watershed.

## MODEL METHODOLOGY

To simulate the chemical transport processes in watersheds, it is necessary to estimate beforehand the hydrological variables. The hydrological variables required to drive CTT&F can be calculated using any physically-based distributed model capable of producing a reasonable simulation of the flow and sediment transport fields in the watershed. These include: 1.) for surface transport: overland flow depth, flow in the coordinate directions, sediment load, and sediment concentration; and 2.) for subsurface transport: soil moisture and hydraulic head at various depths in the soil. The hydrologic model being used in this development effort is the *GSSHA* model. This section will discuss the flow and sediment methodologies found within *GSSHA*, in addition to the current overland and channel contaminant process descriptions found within the CTT&F.

### ***GSSHA***

*GSSHA* is a multi-dimensional physically based distributed watershed model that encompasses the full hydrologic cycle. The processes related to the overland and channel regimes are: 1) Precipitation Distribution; 2) Interception; 3) Infiltration; 4) Evaporation and Evapotranspiration; 5) Overland Flow; 6) Channel Flow; 7) Overland Erosion; and 8) Channel Sediment Routing.

Rainfall is always a required input within any hydrologic model. Rainfall may be input as spatially and temporally uniform, at a specified rate for a specified duration, for a single event, or rainfall may be input as spatially and temporally varying for any number of rainfall events. The rainfall interpolation techniques available for spatially varied rainfall is: 1) Inverse Distance Squared Method; or 2) Thiessen Polygon Method. NEXRAD precipitation estimates can be used in *GSSHA*, by formatting the data into a *GSSHA* precipitation file using the RADAR precipitation type card. When using NEXRAD rainfall estimates, *GSSHA* assigns a rain gauge at the center of each radar data pixel. When combined with Thiessen polygon rainfall interpolation, this reproduces the original radar pixels.

The interception of rainfall by the vegetation is modeled in *GSSHA* using the two parameter method published by Gray (1970). An initial quantity of rainfall (mm), entirely intercepted by foliage and a storage capacity are specified within the model for each landuse type.

The evaporation and evapo-transpiration models incorporated in *GSSHA* allow calculation of the loss of soil water to the atmosphere, improving the determination of soil moistures. Two different evapo-transpiration options are included: 1) bare-ground evaporation from the land-surface using the formulation suggested by Deardorff (1978); and 2) evapo-transpiration from a vegetated land-surface utilizing the Penman-Monteith equation.

Water ponded on overland flow plane cells will infiltrate into the soil as conditions permit. Infiltration is dependent upon soil hydraulic properties and antecedent moisture conditions, which may be affected by previous rainfall, run on, ET, and the location of the water table. In *GSSHA*, the unsaturated zone that controls infiltration may be simulated with a 1-D formulation of Richards' equation (RE), which simulates infiltration, ET, and soil moisture movement in an integrated fashion. Infiltration may also be simulated using traditional Hortonian Green and Ampt (GA) approaches which are simplifications of RE. There are three optional GA based methods to calculate infiltration for Hortonian basins: 1) traditional GA infiltration, 2) multi-layer GA, and 3) Green & Ampt infiltration with redistribution (GAR). The traditional GA and multi-layer GA approaches are used for single event rainfall when there are no significant periods of rainfall hiatus. The GAR approach is used when there are significant breaks in the rainfall, or for continuous simulations.

Overland flow in *GSSHA* employs the diffusive wave approximation in two dimensions (x and y). Flow is routed in two orthogonal directions in each grid cell during each time step. The watershed boundary represents a no flow boundary for the overland flow routing and when a grid cell lies on the watershed boundary, flow is not routed across the boundary. Inter-cell fluxes in the $x$ and $y$ directions, $p$ and $q$, respectively, are computed in cell $ij$ from the depth, $d_{ij}$, at the $n^{th}$ time level using the Manning equation for the head discharge relationship in the $x$ and $y$ directions. Once water enters a "channel" grid cell, then the volume of water is added to the channel system and routed to the watershed outlet. The overland flow routine does allow for depression storage, thus water can pool in a depression until it is able to either build up enough head to overcome the topography, infiltrate into the ground, or evaporate into the air.

*GSSHA* solves the diffusive wave equation using two-step explicit finite volume schemes to route water for both 1-D channels and 2-D overland flow, where flows are computed based on heads, and volumes are updated based on the computed flows. Compared with more sophisticated implicit finite difference and finite element schemes, the algorithm used in *GSSHA* is simple. The friction slope between one grid cell and its neighbors is calculated as the difference in water surface elevations divided by the grid size. Compared with the kinematic wave approach, this diffusive wave approach allows *GSSHA* to route water through pits or depressions, and regions of adverse slope. The Manning formula is used to relate flow depth to discharge. Use of the Manning formula implies that the flow is both turbulent and that the roughness is not dependent on flow depth. Neither of these assumptions may be valid on the overland flow plane. While being simple, the method is powerful because it allows calculations to proceed when only portions of the stream network or watershed are flowing. This is an important attribute as rainfall may occur on only a portion of the watershed. The channel routing scheme was developed to allow water to remain in the channel after channel routing ends, and for water to be present in the channel when channel routing begins. Because groundwater may discharge to the stream at anytime, channel routing is initiated anytime a minimum amount of water is in the channel network. If the channel routing scheme indicates there is no flow in the channel, channel routing is halted during periods outside precipitation events. Fluxes between the stream and the groundwater are still computed and adjustments to the stream volumes are made without routing. If groundwater discharges to the stream, channel routing will resume, but at the groundwater time step, which is typically larger than the channel routing time step.

In order to estimate overland erosion, *GSSHA* employs an equation based on the work of Kilinc and Richardson (1973). Their investigation resulted in a sediment transport equation of uniform flow sheet and rill erosion on bare sandy soil. Julien (1995) modified the original Kilinc-Richardson equation to expand the applicability of the equation to non-uniform flow with consideration of soil and land-use specific factors (i.e., USLE factors, K, C, and P). The *K*, *C,* and *P* factors are empirical coefficients with the same conceptual meaning as those used in the Universal Soil Loss Equation. The surface of each grid cell is either eroded or aggraded depending upon the quantity of sediment in suspension and the potential sediment transport rates. This determination is made for three grain sizes, sand, silt, and clay. Conservation of mass of sediment determines what amount of sediment entering each grid cell stays in suspension, and what amount is deposited. The sediment transport capacity is satisfied by sediments already in suspension, previously deposited sediments, and then sediments in the parent material, respectively. If sediments in suspension are unable to satisfy the potential transport rate, the previously deposited sediment is used to satisfy the demand. If there is insufficient previous deposition, then the surface is eroded to meet the demand. If the potential sediment transport rates calculated are insufficient to transport the sediment already in suspension within a grid cell, sediment is deposited on the surface, Johnson (1997).

The present version of *GSSHA* employs the unit stream power method of Yang's (1973) for routing sand-size total-load in stream channels. Unit stream power is defined as the product of the average flow velocity, $U$, and the channel slope $S_o$. The rate of work done per unit weight of water in transporting sediment is assumed directly related to the rate of work available per unit weight of water. Thus, the total sediment concentration or total bed-material load must be directly related to the unit stream power. In the channels, silt and clay size particles are assumed to be in suspension, and are transported as wash load. This treatment implies that the flow is turbulent, and the travel time to the outlet of the catchment is short compared to the settling time, such that particles do not settle in the channel network. This assumption, combined with no bank erosion, results in the channels being neither a source nor sink of fines. Routing of suspended fines is a natural extension of the explicit diffusive-wave channel routing method. Suspended fine sediments are routed as concentrations. The concentration changes as a function of gradients in both concentration and velocity.

**CTT&F**

This section will discuss the chemical transport and fate processes found within the CTT&F.

*Chemical Transport*

A variety of processes determine the fate of chemicals within the watershed environment. Physical transport mechanisms affect the location of chemical mass and the movement of this mass across the overland planes, through the channel system, and ultimately to the watershed outlet. Partitioning and bio-chemical reactions, meanwhile, determine the distribution of chemical mass among different phases and thereby affect the amount of mass available for transport. In consideration of these important processes, the governing equations for chemicals are established over a differential control volume through which the fluid is flowing (Johnson and Zhang, 2005). A basic principle of contaminant transport models is the conservation of mass. In addition, when diffusion effects are significant, the use of Fick's law of dispersion results in the appearance of additional terms. A generalized conceptual framework for the CTT&F model is presented in Figure 1, where the system is represented as two compartments: water column and sediment deposition.

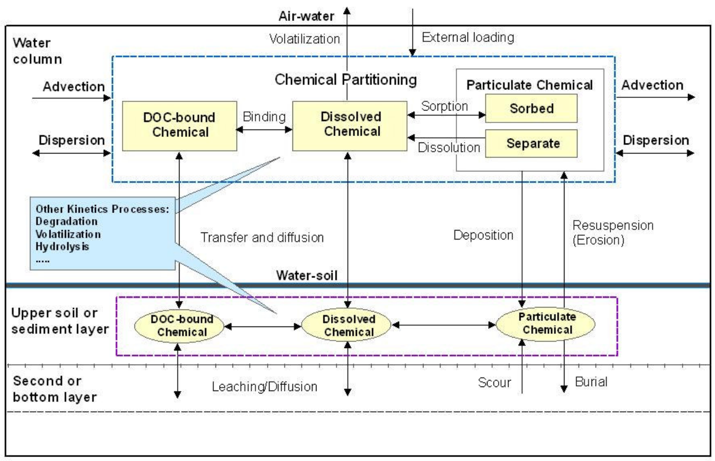


Figure 1 - Schematic chart of the key processes of CTT&F

*Chemical Transport in 2D Overland Regime*

Overland transport of chemicals is vital for quantifying a distributed source. Mathematically modeling for chemical transport involves the solution of governing equations of both overland flow and upper soil layer simultaneously.

Overland Flow:

$$\frac{\partial(hC_T^r)}{\partial t} = -\frac{\partial(q_x C_T^r)}{\partial x} - \frac{\partial(q_y C_T^r)}{\partial y} + \frac{\partial}{\partial x}\left(hD_x \frac{\partial C_T^r}{\partial x}\right) + \frac{\partial}{\partial y}\left(hD_y \frac{\partial C_T^r}{\partial y}\right) - J_{df} + J_{dm} + J_{pe} - J_{pd} + \sum S_k \quad (7a)$$

Upper Soil Layer:

$$\frac{\partial(z_m C_{T2}^r)}{\partial t} = J_{df} - J_{dm} - J_{pe} + J_{pd} + \sum S_k \quad (7b)$$

where $C_T^r$ is total chemical concentration in the overland flow [M/L$^3$], $C_{T2}^r$ is total chemical concentration in the upper soil layer [M/L$^3$], $z_m$ is depth of the upper soil layer [L], $D_x$, $D_y$ is chemical dispersion coefficient in the x- or y-direction [$L^2$/T], $J_{df}$ is dissolved chemical infiltration flux [M/$L^2$/T], $J_{dm}$ dissolved chemical mass transfer flux between surface water and upper soil layer [M/$L^2$/T], $J_{pe}$ is sorbed chemical erosion flux [M/$L^2$/T], $J_{pd}$ is sorbed chemical deposition flux [M/$L^2$/T], $\Sigma S_k$ is total chemical kinetics transformation flux, positive indicates a source, negative a sink [M/$L^3$/T].

*Chemical Transport in 1D Channel/Stream*

The model of the cross-sectionally averaged concentrations of chemicals in channels is formed by writing mass conservation equations for two conceptual areas: the channel and the bed sediments as follows.

Channel Flow:

$$\frac{\partial C_T^w}{\partial t} + \frac{Q}{A}\frac{\partial C_T^w}{\partial x} = \frac{1}{A}\frac{\partial}{\partial x}\left(AD_x \frac{\partial C_T^w}{\partial x}\right) + \frac{q_l}{A}\left(C_T^r - C_T^w\right) + \frac{1}{h}\left(J_{pe} - J_{pd} - J_{dt}\right) + J_{dd} + \sum S_k \quad (8a)$$

Bed Sediments:

$$\frac{\partial (z_m C_{T2}^w)}{\partial t} = -J_{pe} + J_{pd} - J_{dd} + \sum S_k \quad (8b)$$

where $C_T^w$ is total chemical concentration in the channel flow [M/$L^3$], $C_{T2}^w$ is total chemical concentration in the bed sediments [M/$L^3$], $J_{dt}$ is dissolved chemical transmission loss flux [M/$L^2$T], $J_{dd}$ is pore water diffusion flux of dissolved chemicals [M/$L^3$/T].

*Chemical Transformations*

Beyond partitioning and mass transport processes, the fate of chemicals is potentially influenced by a number of bio-chemical transformation processes that include, but are not limited to, biodegradation, hydrolysis, oxidation, photolysis, volatilization, and user-defined reaction. However, these processes may not be operative in all environmental settings. Some chemicals undergo a complex set of reactions, while others behave in a more simplified manner. The importance of any particular process is highly dependent on the chemical of interest and environmental settings. The chemicals may be independent or they may be linked with reaction yields, such as a parent compound-daughter product sequence. The CTT&F modules allows the simulation of a variety of processes that may affect chemicals, which were adapted, in part, from the WASP model (Ambrose, et al., 1993) and IPX model (Velleux, et al., 2000).

*Solution of the Governing Equations*

The coupled set of CTT&F differential equations is solved by numerical techniques. The general procedure follows the techniques used for the hydrologic and sediment routing equations, from *GSSHA*, which uses a finite difference control volume solution scheme. A watershed system is discretized into a mesh of square grids, the locations of which are described in terms of rows, columns, and layers. The finite differential equations for chemical transport are solved on the square DEM map representing the watershed land surface and the equations evaluated at each point in space over the temporal evolution of the landform. DEM-derived local drainage directions are used as the basis for channel routing. By using a finite-difference algorithm, solution of the model yields a general equation of the form:

$$C(x, y, t) = \left(Hydrologic\ Transport\right) + \left(Chemical\ Transformation\right) \quad (9)$$

where $C(x,y,t)$ is the chemical concentration at location *x, y* and time *t*.

## MODEL APPLICATION

In order to verify the general features of the CTT&F modules, a case study is being done to investigate the contamination of RDX in the impact area at Camp Shelby, MS. The Camp Shelby Training Site is the largest reserve component training site, covering 136,000 acres, allowing up to battalion level maneuver training, excellent FA Firing Points, and a wide range of support facilities. This is the normal Annual Training location for National Guard and Reserve units located in Mississippi, Alabama, and Tennessee. However, units from across the country use its excellent assets to support a variety of missions. The impact area at Camp Shelby is used for the firing of small and large caliber weapons and it consists of approximately 17 square kilometers of gently rolling grassland, Figure 2. A number of streams drain the impact area, and riparian wetlands are common along these streams. The Impact Area is utilized year-around and averages in excess of 190 firing days each year; there are approximately 170 troop-firings per day, and the range-firing list includes M1A1 tanks, Bradleys, self-propelled and towed artillery, mortars, laser-guided weapons, and small arms.

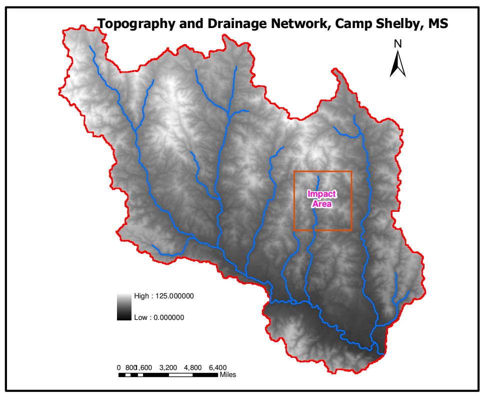


Figure 2 - Topology, stream network and watershed boundary in the Camp Shelby Fire Range

Currently, no reliable field or laboratory data for the RDX sources is available on the Camp Shelby firing range. A GIS analysis and field investigation is currently being done to try and estimate crater locations and estimates of surface loads and soil concentrations for use in the case study. In conjunction with the United Stated Geological Survey (USGS), flow, sediment, and contaminant observations are being made at the Middle Creek and Pearces Creek gage sites along Tank Road. As these data become available, then calibration and validation of the modeling system will be done.

Using CTT&F, current data sources, and engineering judgment, we can infer and trace the sources of RDX transport and how much erosion each source area contributes. This is important in investigating the loss of RDX due to the transport of distributed source contaminants. *GSSHA* generates time series outputs of model state variables at specified points in space over time in addition to providing temporal and spatial distribution, across the landscape, of contaminant source transport in different phases. A more detailed presentation of the Camp Shelby case study will be presented at the conference.

## CONCLUSIONS

Physically based mathematical modules have been developed for simulating transport, transformation and fate of distributed source contaminants in watersheds. Theses modules can be coupled with any fully distributed hydrological model which provides the required hydrological and sediment variables. The physical basis is important since it provides the link between the simulations and physical property measurements. CTT&F has a modular, process-oriented structure that allows the user to select from a library of contaminant transport and transformation processes either as a whole or as a sub-set of processes suitable for a particular application. CTT&F is currently being tested on a military firing range watershed in Camp Shelby, MS using raster GIS data with 30m x 30m grid dimensions. Conceptual simulations will be initially made to evaluate the contaminant transport and fate modules , however, once more realistic contaminant surface loadings, contaminant soil concentrations, and flow, sediment, and contaminant runoff data become available, then calibration and validation of the modeling system will be done for flow, sediment, and contaminant runoff.

The algorithms for the chemical transformation processes, used in CTT&F, were adapted from surface water quality models due to transformation reaction mechanisms and their interrelations being poorly understood for explosive compounds. Translating these understanding and algorithms into quantitative mathematical process descriptors for explosives is impeded by the nature of the information available and will require additional process level research. Further development is needed to add a series of spatially and temporally varying time functions to represent environmental conditions, existing in the watershed, which can give insight on both the persistence of explosives as well as the fate of explosives.

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