Predicting the Transport and Fate of Military Contaminants Using a Distributed Source Model

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Abstract

The CTTF model was developed as a physically-based, distributed watershed contaminant transport model, transformation and fate sub-model for existing hydrological modeling systems. This model builds upon the latest advances in the various landscape-scale physical, biogeochemical, and ecological processes taking place in the watershed. Physical processes of contaminant transport are included in the CTTF model through the integration of new hydrologic (FLUX-96) and ecological (ELM) models. The sub-models describing transport and transformation processes in CTTF are simulated for each cell and thus in the watershed outlet. For update CTTF simulates contaminant erosion and transport processes at the watershed scale. For the simulation of transport and transformation processes of this material together with that supplied by overland flow. The net rate of transport equations governing the watershed systems are solved to yield the site-specific contaminant concentrations for the various landscape-scale physical, biogeochemical, and ecological processes. The CTTF models for simulating transport and transformation processes in the sub-models of contaminant transport and partitioning, portion of truly dissolved phase, dissolved organic carbon (DOC) phase and sediment-adsorbed phase of the contaminant. To evaluate the performance of the models, CTTF model was compared with the analytical solution for steady-state transport and transformation processes of a linearly adsorbed contaminant. The result shows that the model simulations agree with the measured data set. Validation of the model, however, is based on a comparison with limited laboratory experiment data. Proper validation would require extensive experimentation, preferably in the field which is, up to now, unattainable.

1. Introduction

Many U.S. Department of Defense (DoD) installations contain soil, sediment, surface water, and groundwater environments contaminated with explosives and energetic materials (Brannon and Myers, 1997). To assist with compliance with water quality regulations as well as long-term watershed planning and management for these contaminated sites, there is a corresponding interest, therefore, in developing techniques which predict, at the watershed scale, the effects of distributed contaminant sources. Given that these models should address various contaminant processes in the context of the watershed environment, it has motivated the development of a physically-based, distributed-source Contaminant Transport, Transformation and Fate (CTTF) sub-model, by the U.S. Army Engineer Research and Development Center (ERDC). To describe the transport and transformation of contaminants through the various landscape media in a watershed, it is important to model processes on a cell by cell basis, allowing each cell to have different flow characteristics, as well as the spatial transport and transformation of multiple contaminants and thus the assessment of the fate of distributed sources and lead to better management of the watershed environment for military installations.

2. Model Description

To simulate the contaminant transport processes in watersheds, it is necessary to estimate both hydrological and hydrochemical factors. The basic model components include hydrology, erosion, and sediment and contaminant transport. The hydrological variables are obtained through deterministic or stochastic processes. The hydrochemical includes advective/dispersive transport, dispersion, chemical reactions, and equilibrium processes. The model uses a combination of macro- and micro-scale simulations providing a realistic estimation of the simulation of the flow and sediment transport fields as follows:

- Precipitation and interception
- Evapotranspiration
- Groundwater flow
- Channel routing
- Stream/surface water interaction
- Sediment transport

The calculations for each process at every time step is independent and information is transferred from one process to the other. The results are then used to compute the fluxes of contaminants from the transport sub-model to the sediment transport sub-model of the contaminant transport sub-model.

3. Contaminant Partitioning and Distribution

The CTTF incorporates "four phase partitioning", where a contaminant may partition between solid particles, sediments, DOC, and soil water. Two solid chemicals are assumed to be an

\[ C = C_{\text{sol}} + C_{\text{diss}} + C_{\text{DOC}} + C_{\text{sed}} \]

where \( C \) = dissolved phase concentration of the contaminant (\( \mu \text{g/L} \)), \( C_{\text{sol}} \) = solid sorbed phase concentration of the contaminant (\( \mu \text{g/L} \)), \( C_{\text{diss}} \) = dissolved sorbed phase concentration of the contaminant (\( \mu \text{g/L} \)), \( C_{\text{DOC}} \) = DOC-bound phase concentration of the contaminant (\( \mu \text{g/L} \)), \( C_{\text{sed}} \) = sediment-adsorbed phase concentration of the contaminant (\( \mu \text{g/L} \)). The partitioning between the truly dissolved (aqueous), particle sorbed, and DOC-bound phases is assumed. The equilibrium partition coefficient can be used to describe the fraction of the total chemical that is associated with each phase. The concentration of the chemical in truly dissolved, bound, and particle phases can then be calculated by:

\[ C = \frac{C_{\text{sol}}}{K_{\text{diss}}} + \frac{C_{\text{diss}}}{K_{\text{DOC}}} + \frac{C_{\text{sed}}}{K_{\text{sed}}} \]

where \( K \) = partition coefficient.

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4. Contaminant Transport Equations

Within a watershed, the erosion and transport processes of contaminants can be divided into those acting on the upland and those acting in the channel. Overland contaminant transport equation concerns the downslope movement of contaminants over land surface by overland flow. The overland flow is important in the transport process in the overland flow or transported through the flow of water that is transported by overland flow. The mass transfer between overland flow and the upper soil. Contaminants partition process of contaminant processes of contaminants occur in the channel are the advective and dispersive movement, sedimentation, resuspension, and mass transfer between water and sediment. The foundation of channel transport processes is the flow and transport processes affecting the fate and transport of explosives on firing ranges.

The simulated rainfall event lasted 30 ± 0.30 min. Runoff and sediment were collected at the downslope end of the plot and measured volumetrically. Runoff rates and volumes were determined by collecting runoff every minute of a 30 minute rainfall event. The runoff was measured by a tipping bucket rain gauge that run off that ceased. The total suspended sediment (TSS) samples were collected every five minutes, from the peak of the runoff until the end of the event, every five minutes, and measured for 30 minutes rainfall simulations and every minute afterward. For each sample, a composite sample was collected by a total of 550 g. The composite sample was dried at 60°C, then every minute five minutes, and every five minutes, then measured and analyzed. The composite samples were analyzed for contaminants by using a variety of different methods. The experiment was conducted using a domain consisting of 30 grid cells, the size of the grid was 2.5 by 2.5 m (0.625 by 0.625 m). Different Manning roughness coefficients were used for the unvegetated and vegetated surfaces. The focus of this study was the generation of the sediment, the vegetated plots, and associated multiphasic transport of the contaminates due to smaller field plots and shorter experimental time. The contamination transport from the field plots on the 30 grid cells in the model is two-dimensional (2D) advection-dispersion equation (ADE). The model used in this study was calibrated by comparing the simulated and measured surface runoff, sediment concentrations, and contaminant concentrations that do not the errors between simulated and measured values were minimum. Comparison of the overall trends and measured concentrations results over time for surface runoff and sediment concentrations for the vegetated plots. The results show that the model is well calibrated to predict the contaminant transport processes affecting the fate and transport of explosives on firing ranges.

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5. Summary

The contribution of CTTF governing equations could be solved using any one of numerical techniques. In this study, the general procedure follows that for the CUSK hydro-logic and sediment routing equations, which use a different control volume solution scheme. A watershed system is discretized into a mesh of square grids, each corresponding to grid cell 30 m by 30 m. The horizontal and vertical exchange of toxicants is modeled by using the exchange of toxicants, management strategies which model distributed contaminant source effects both on the upland and through the channel. CTTF is still a research and development model that has much room to grow. Future research is expected to enhance the capability of CTTF, which including other transformations, environmental conditions, and unsaturated soil capabilities. The work reported here was supported by the Environmental Quality Technology Research Program of the U.S. Army Corps of Engineers.