"Development and Application of Numerical Models for Non-point Source Pollution Control"

A Discussion of the Nutrient Sub-Model (NSM) and the Contaminant Transport, Transformation, and Fate Sub-Model (CTT&F)
Discussion

- Nutrient Sub-Model (NSM)
- Contaminant Transport, Transformation, and Fate (CTT&F) Sub-Model
- On-going Model Test Studies
  - Eau Galle, WI. (NSM)
  - Black River Test Site, Vicksburg, MS. (CTT&F)
NSM Features

- Overland/Soils Module
  - NH4, NO3, Organic Nitrogen (Dissolved and Adsorbed)
  - PO4 and Organic Phosphorus (Dissolved and Adsorbed)
- Channel Module
  - NH4, NO3, Organic Nitrogen (Dissolved and Adsorbed)
  - PO4 and Organic Phosphorus (Dissolved and Adsorbed)
  - Algae Groups
    - Phytoplankton (Floating Algae)
    - Benthic or Periphyton (Submerged Attached Algae)
- Plant Module
  - EPIC formulations based upon the Heat Index Method
NSM Features

Overland/Soils Nitrogen Cycle

Overland flow

- Advection
- Dispersive

Nitrate → Nitrification → Ammonium → Mineralization → Dissolved Organic N → Hydrolysis → Particulate Organic N

- Mass transfer
- Volatilization

Inorganic fertilizer or air deposition

Plant uptake

Soils

- Nitrification
- Denitrification
- Leaching

Nitrate → Ammonium → Sorbed Ammonium → Inorganic Pool

Mineralization

Active Organic N → Decay → Stable Organic N → Organic Pool

ERDC

System Wide Water Resources Research Program
NSM Features
Overland/Soils Phosphorus Cycle

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NSM Features
Channel Phosphorus Cycle

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NSM Features

Algae Group and Dissolved Oxygen

Water → Growth → Algae Group → Respiration

Sediment → Setting → Bottom Algae

Water → NH4 → Nitrification → Dissolved Oxygen → DOC

Sediment → Sediment Oxygen Demand

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NSM – Mass Transfer

\[ S_d = k_e \left( \frac{SIP}{\phi} - DIP \right) \]

\( S_d = \text{mass transfer (ML}^2 \text{T}^{-1}) \)

\[ k_e = k_m + \frac{ai \theta}{\rho_b} \]  
\( (\text{L/T or meters/day}) \)

Based on diffusion processes

Based on soil detachment processes
CTT&F Features

- Spatial Grid Discretization
- Four Phases Partitioning:
  - dissolved
  - bound to DOC (Dissolved Organic Carbon)
  - sorbed to sediment particles
  - separate solid particles
- 2D Overland Flow Transport with mass transfer between the Upper Soil Layer
- 1D Channel Flow Transport with mass transfer between the Bed Sediments
- Seven Biochemical Transformation Processes:
  - biodegradation
  - hydrolysis
  - oxidation
  - photolysis
  - dissolution of solid phase
  - user-defined extra reaction
  - transformations and daughter products
Chemical Partitioning

Equilibrium partitioning of contaminants among dissolved phase, sediment sorbed phase, and DOC bound phase.

\[ C_d = f_d C_T \]
\[ C_b = f_b C_T \]
\[ C_p = \sum_{n=1}^{N} f_{pn} C_T \]

Fourth phase must account for the effect of “melting” of solids (dissolution) for explosive compounds as reactive particles.
Eau Galle Watershed

Upper Eau Galle Demonstration Sites

French Run ~ 25 acres
1 gage at outlet

Eight Mile Creek ~ 1 mi²
2 gages — One at confluence of upper streams and one at the outlet

Upper Eau Galle ~ 60 mi²
5 gages — 4 along the Eau Galle River (see figure) and one along Carr Creek
Elevations

- 100 m grid elevations were developed from NED 30 m data
- Elevation data are used for
  - overland flow calculations
  - surface/groundwater interactions
  - stream bed elevations
Land Use

- Number of land uses reduced from 13 to 7:
  - 2 - residential
  - 4 - commercial
  - 6 - forest
  - 8 - grass
  - 10 - wetland
  - 12 - row crop
  - 14 - open water

- Predominate land uses in the basin are pasture (8 – light green) and row crops (12 – beige).

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SWWRP
Soil Type

- Soil types reduced from 13 to 6 types
  - Coarse
  - Sandy loam
  - Loam
  - Silty loam
  - Rocky
  - Water
- The predominate soil type is silty loam
Initial Discharge Calibration

Peak Mean Absolute Error (MAE) – 3%
Total Discharge Error – 1.5%

Flow and Sediment Calibration performed by Dr. Chuck Downer (CHL)
Final Discharge Calibration

Peak (MAE) – 42%
Total Discharge – 7%
Sediment Discharge Calibration

- Sediment measurements for selected events.
- Calibration to two June events
- MAE – 12% and 4%, respectively
Eau Galle Watershed

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Water Quality Calibration - DIP
Summary

• The Eau Galle watershed upstream of the Spring Valley Dam was successfully simulated with the GSSHA model.
• Stream discharge was reproduced within normal standards.
• Reservoir stage and discharge were also simulated within acceptable standards.
• The model helped identify problems with the rating curve.
Summary

- Sediment discharge (TSS) was very accurately simulated.
- Simulating sediment discharge requires accurate simulation of hydrologic processes.

By coupling the hydrologic processes together, along with the erosion and sediment transport processes, we are able to more accurately model the system and changes in the system.
Summary

• Observations from WQ analysis
  – Need a dynamically changing landuse capability in order to better model the fate and transport of nutrients and contaminants across seasons.
  – Need a Management Module to allow for temporal mass loading of nutrients throughout the simulation. Currently the nutrient pools are initialized and the plant module allows for additions to the pools but there is not a mechanism for adding farm management scenarios (fertilizer loading, dairy loading, etc.) to the nutrient pools.
The experimental procedure was designed to mimic rainfall-driven surface runoff and transport of explosives residuals deposited on surface soils at firing ranges.

The experimental plot was 9.0 ft x 7.5 ft.

The plot had a bed slope 2% and was designed to collect runoff water and sediment.

Experiments were conducted to simulate two different surface roughness conditions: (1) “disturbed” (unvegetated); and (2) “undisturbed” (vegetated).

The soils for these experiments were obtained from the Camp Shelby, Mississippi military firing range.
The simulated rainfall intensity for the overall plot area averaged 2.8 in/hr (7.1 cm/hr) and ranged from 2.7 to 2.9 in/hr (6.8 to 7.4 cm/hr). The simulated rainfall event lasted 30 ± 60 ± 90 min.

Runoff and suspended sediment samples were collected at the downstream end of each plot. Runoff rates and volumes were determined by collecting samples every minute of a 30 minute rainfall simulation and every minute after rainfall was discontinued until it was noted that runoff had ceased.

Total suspended sediment (TSS) samples were collected every minute for the first 15 minutes of runoff, then every five minutes during the 30 minutes rainfall simulations and every minute afterward.
For the contaminant transport and transformation experiments, this study focused on Comp B, one of the primary explosive formulations used in munitions since World War II for its high explosive yield.

Range activities can result in locally scattered chunks of Comp B on the soil surface with particles having a variety of surface textures and RDX/TNT ratios.

500 grams of Comp B in particles of various sizes (less then 1 cm in diameter and 2 mm in thickness to 3.5 cm in diameter and 2.5 cm thickness) was applied onto the soil surface.

The Comp B used for this study was a 60/39 mixture of RDX and TNT with 1% wax and in the form of crystalline solids.
The experimental plot was modeled using a domain consisting of 30 grid cells with a grid cell resolution of 1.5 ft by 1.5 ft (0.46 m by 0.46 m).

In this study various transformation parameters for RDX and TNT were calibrated empirically to reproduce the measured concentrations of RDX and TNT from the experiment based on their ranges in previous studies.

Parameters included the following: dissolution rate, adsorption kinetics, soil to water partition coefficients, and transformation rate coefficients.

Given the small scale of the test plot and the short duration of simulated rainfall, the focus of this study was the dissolution of Comp B, sorption with sediments, and associated multiphase transport of the contaminants.
CTT&F Testing
Black River Test Site - Results

Unvegetated

![Unvegetated Graph](image)

Vegetated

![Vegetated Graph](image)
CTT&F Testing
Black River Test Site - Results

Unvegetated

Vegetated

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Black River Test Site - Results

Unvegetated

Vegetated

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Black River Test Site - Results

Unvegetated

Vegetated
The comparisons showed that the model was capable of simulating the explosive contaminants from the field with reasonable accuracy. Contaminants released from surface sources were generally simulated within 10% of observed measurements.

Overall comparisons were encouraging, and showed promise for the potential use of the CTT&F sub-model for predicting the fate of distributed sources at watersheds.

More tests are needed at the watershed scale to assess the variability in the model parameters, to confirm the predicted time sequences, and to improve confidence in predicted concentrations.
Eau Galle Watershed, WI
Modeled by GSSHA
Eau Galle Water Quality
Questions?