# GLOBAL AND REGIONAL CLIMATE CHANGES CONFERENCE

*Kiev, Ukraine*
*November 16-19, 2010*

## Development of the Distributed Sources Contaminant, Transport, Transformation and Fate (CTT&F) Sub-model

*Billy E. Johnson, PhD, PE, D.WRE*

# What We Do

Develop, modify and apply numerical models to solve hydrologic, sediment, and water quality problems related to:

- Surface water hydrology
- Groundwater hydrology
- Surface Water/Groundwater Interaction
- Sediment Management
- Surface water quality and TMDL's
- Contaminant fate/transport in surface water and groundwater and related health risk assessment

# Discussion Topics

- Watershed Modeling System (WMS)
- Gridded Surface Subsurface Hydrologic Analysis (GSSHA) Model
- Contaminant Transport, Transformation, and Fate (CTT&F) Sub-Model
- GSSHA-CTT&F Experimental Testing

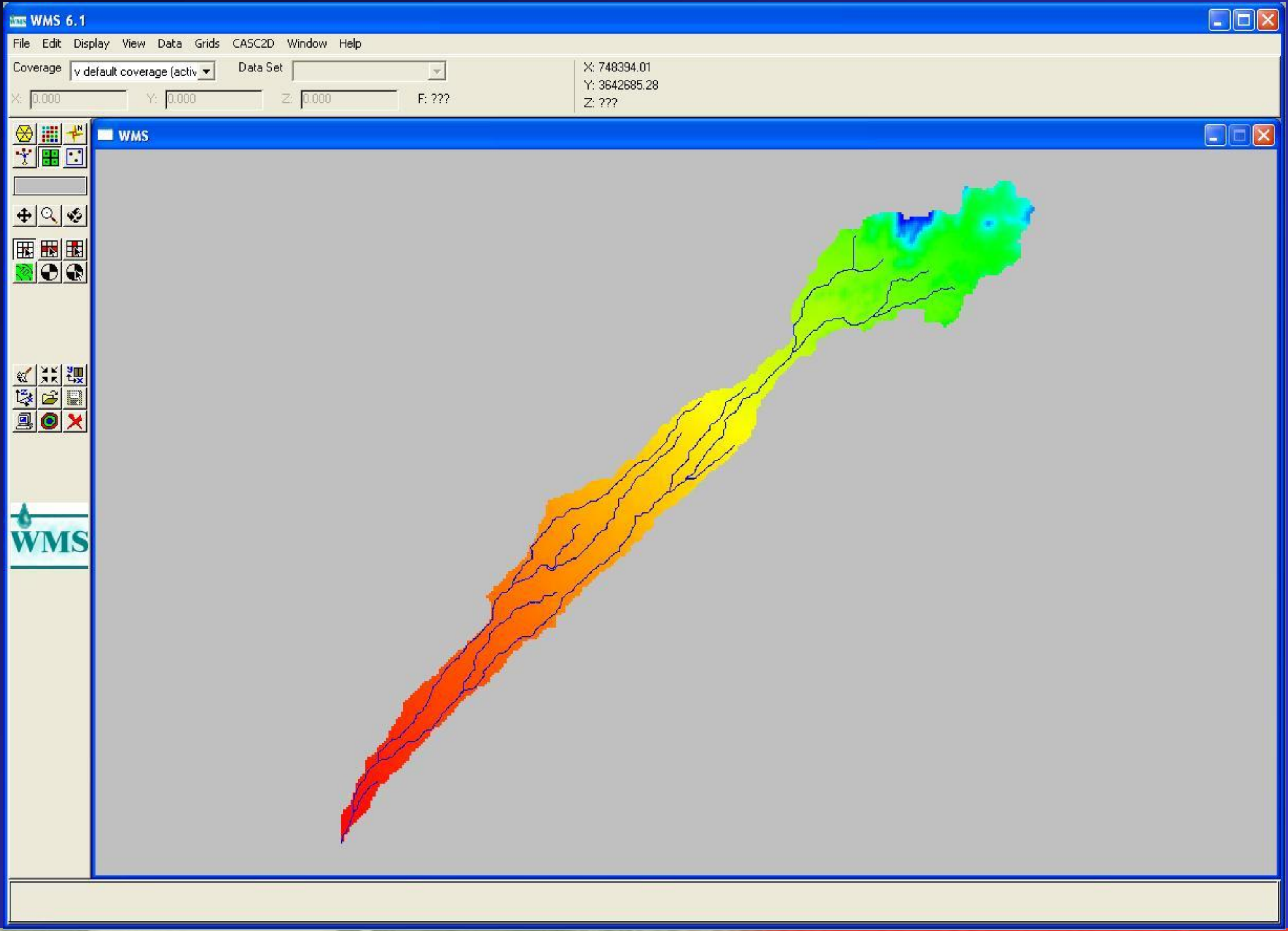
# Watershed Modeling System (WMS) Overview

- Comprehensive system for watershed / reservoir modeling
- Extensive GIS import / export capabilities (ArcGIS, GRASS)
- Supports several models including
  - Rational Method
  - Flood Frequency Analysis
  - TR-20
  - HEC-1, HEC-HMS, and HEC-RAS
  - HSPF
  - GSSHA
  - CE-QUAL-W2
- Widely used for civil and military applications
- Connectivity to surface and groundwater systems

# WMS provides tools to perform the following tasks

- Import and analyze data - USGS and DTEDS DEMS, STATSCO soil data, USGS land use, rainfall, stream data, GIS coverages
- Delineate basins
- Delineate streams
- Provide input for hydrologic / reservoir models
- Create finite difference grids
- Create finite element meshes
- View model output and create animations

# WMS Interface



# Hydrologic Processes Modeled in GSSHA

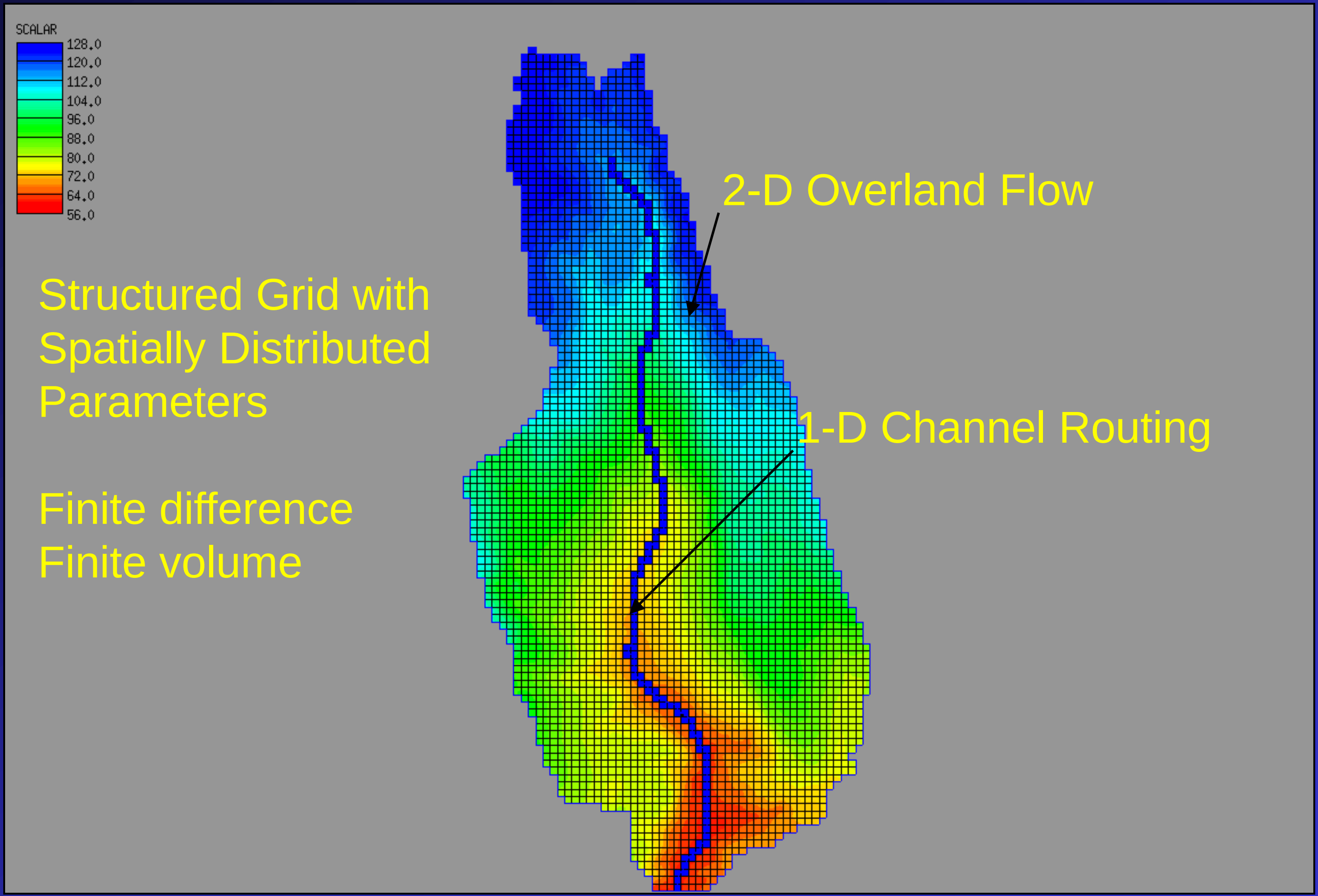
- Spatial distribution of precipitation
- Overland flow
- Channel flow
- Pipe Network and Tile Drainage Network
- Infiltration
- Evapo-transpiration
- Lateral groundwater flow
- Groundwater recharge/discharge
- Snow  accumulation and melting
- Overland and channel erosion and sediment transport
- Soil, Overland, and Channel Contaminant Fate and Transport
- Soil, Overland, and Channel Nutrient Fate and Transport

# GSSHA

## Two-Dimensional, Physically Based, Hydrologic Model

Structured Grid with Spatially Distributed Parameters

Finite difference
Finite volume



# Contaminant Transport, Transformation, and Fate (CTT&F) Sub-Model

The distributed watershed Contaminant Transport, Transformation and Fate (CTT&F) Sub-model was developed to characterize spatial and temporal dynamics of chemicals from both point and non-point sources and has been documented by the Environmental Laboratory of U.S. Army Engineer Research and Development Center.

The sub-model simulates multi-chemical transport and transformation processes across watershed systems.

*Johnson, Billy E., and Zhang, Zhonglong, 2006, "CTT&F: Distributed Sources Contaminant Transport, Transformation and Fate Sub-model", ERDC-TN-EQT-06-1.*

# Contaminant Transport, Transformation, and Fate (CTT&F) Sub-Model

- **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**
- **Vadose Zone Fate and Transport**

# Contaminant Transport, Transformation, and Fate (CTT&F) Sub-Model

- **Seven Biochemical Transformation Processes:**

- ***biodegradation*** *- due to such processes as mineralization, tetoxication, cometabolism, and microbial decay.*

- ***hydrolysis*** *- a reaction in which cleavage of a molecular bond of the chemical and formation of a new bond with either the hydrogen or the hydroxyl component of a water molecule occurs.*

- ***oxidation*** *- in aquatic systems can be a consequence of interactions between free radicals and the contaminants.*

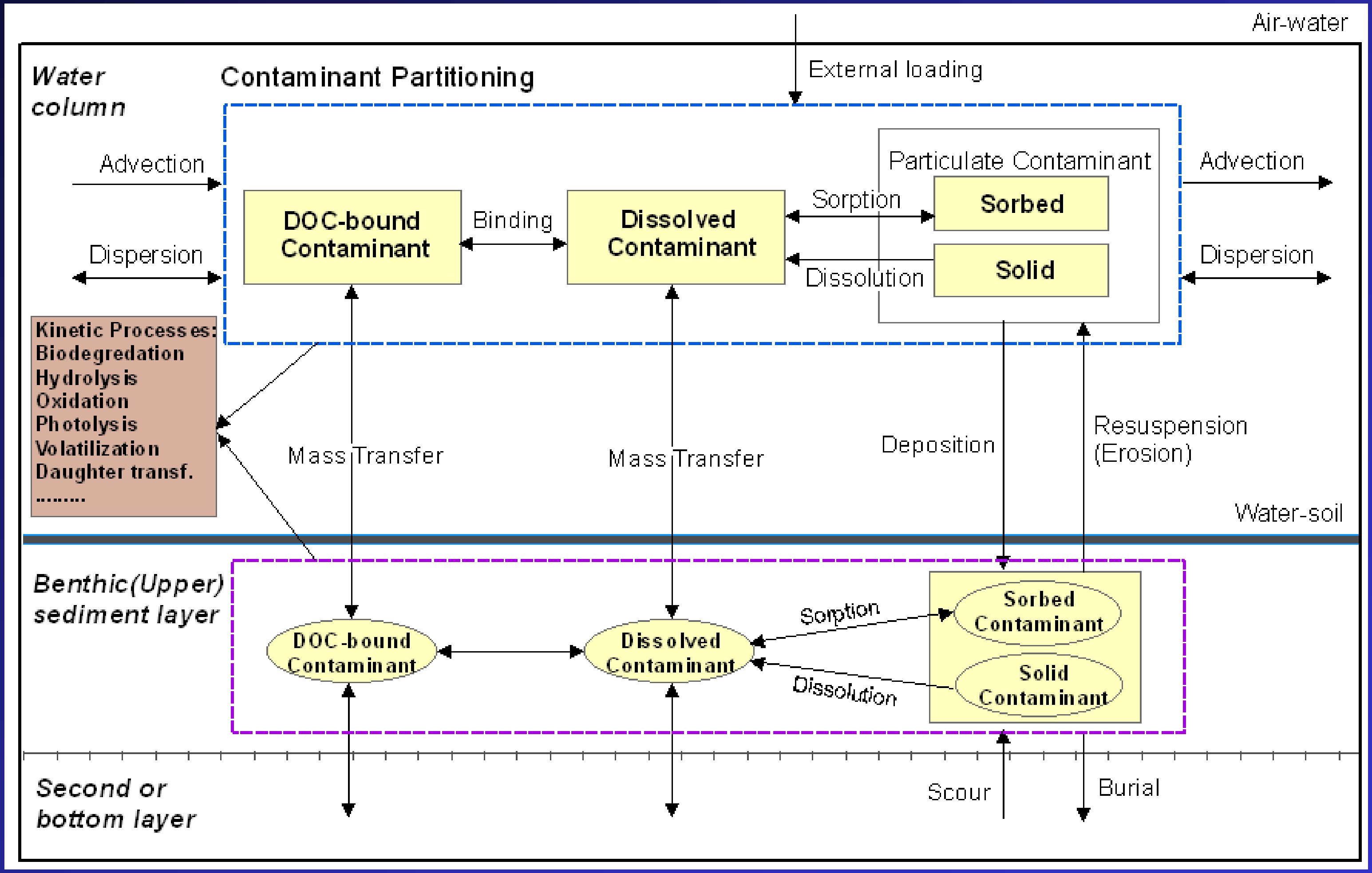
- ***photolysis (photodegradation)*** *- is the transformation or degradation of a chemical that results directly from the adsorption of light energy.*

- ***dissolution of solid phase***

- ***user-defined extra reaction***

- ***transformations and daughter products***

# Contaminant Transport, Transformation, and Fate (CTT&F) Sub-Model



# 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.

# Chemical Transport in Overland

## 2D Overland Flow:

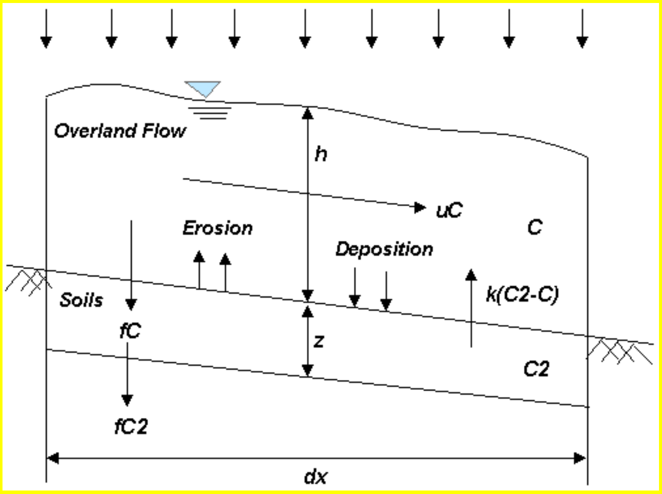
Advection · Dispersion

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

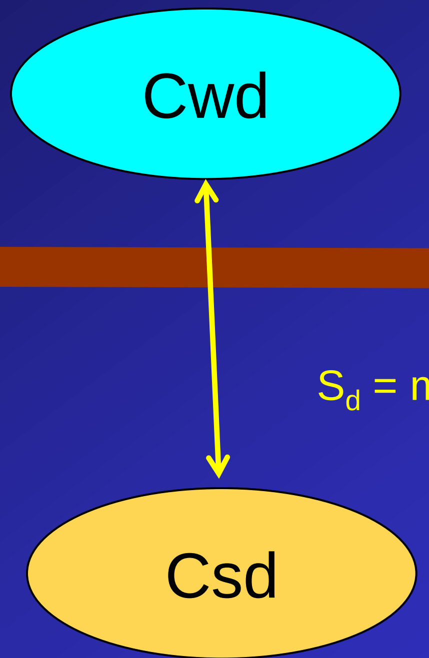
Mass Transfer · Erosion & Deposition · Transformations

## Upper Soil Layer:

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



# Mass Transfer between Water Column and Upper Soil Layer




Soil-WC Interface

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

$$S_d = k_e\left(SIP/\phi - DIP\right)$$

$$k_e = k_m + \frac{ai\theta}{\rho_b}$$

(L/T or meters/day)

Based on diffusion processes

Based on soil detachment processes

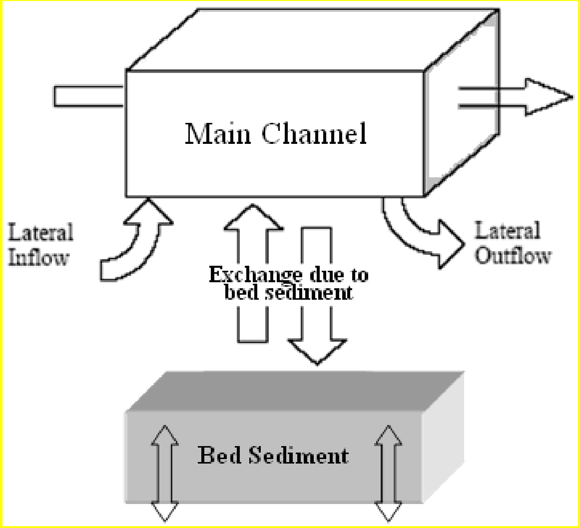
# Chemical Transport in Channel/Stream

1D Channel Flow:

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

Bed Sediments:

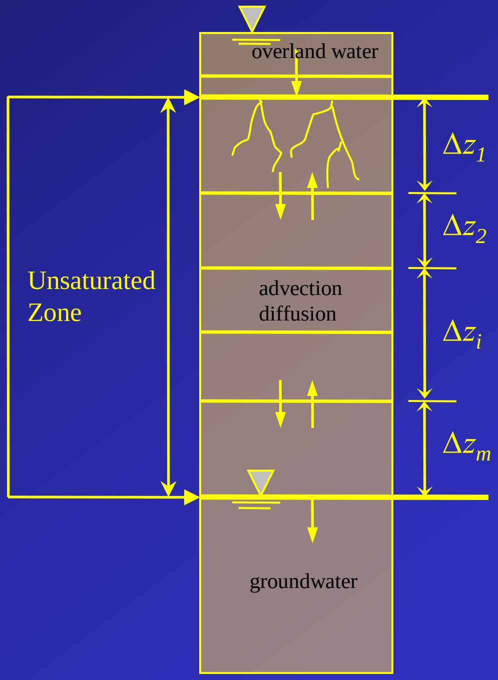
$$\frac{\partial (z_m C_{T2}^w)}{\partial t} = -J_{pe} + J_{pd} - J_{dd} + \sum S_k$$



# Contaminant Transport, Transformation, and Fate (CTT&F) Sub-Model

- **Transport processes**
  - *Advection*
  - *Dispersion*

- **Transformation processes:**
  - *Partitioning*
  - *Biodegradation*
  - *Hydrolysis*
  - *Oxidation*
  - *Photolysis (Photodegradation)*
  - *Dissolution*
  - *User-defined extra reaction*
  - *Transformations and daughter products*




*Chemical Transport in Vadose Zone*

# Experimental Testing of CTT&F

The objective of this application was to illustrate the use of CTT&F to quantify transport, transformation and fate of contaminants in watersheds. Of interest are explosive compounds RDX and TNT used by the military and their resulting presence in the environment.

In order to verify the general performance of the model, an experiment was conducted which simulated rainfall and overland flow in a laboratory.

# Experimental Testing of CTT&F

The discharge, sediment and contaminant were measured and related to the hydraulic transport conditions.

The experiment plot was 9.0'x 7.5'. The bed slope of the plot was 2%.

Two land covers were used for the experiments to simulate two different surface roughness.

Uniform rainfall was simulated. The simulator was supplied with tap water through a rotameter so that the total discharge was measured and kept constant. During the experiment, precipitation intensity was kept constant at 2.8 in/hr, the rainfall event lasted 30 ± 60 min.

# Experimental Testing of CTT&F

Runoff and sediment data were collected at the downstream end of the plot and measured volumetrically.

The RDX and TNT were simulated by spreading explosive composition B (Comp B) over the surface. Comp B is a 60/39 mixture of RDX and TNT that contains 1% wax.

The RDX and TNT concentrations in the runoff were measured by collecting 4 L samples at the measuring points.

# Experimental Testing of CTT&F

The experiment plot domain consisted of 30 grids, the grid cell resolution was 1.5 ft x 1.5 ft.

The computational time step for the simulation was 0.5 sec, with the following values (Table 1) for the relevant parameters, and an initial density of Comp B of 500 g.

Table 1. Model parameters for RDX and TNT in water at 25°C

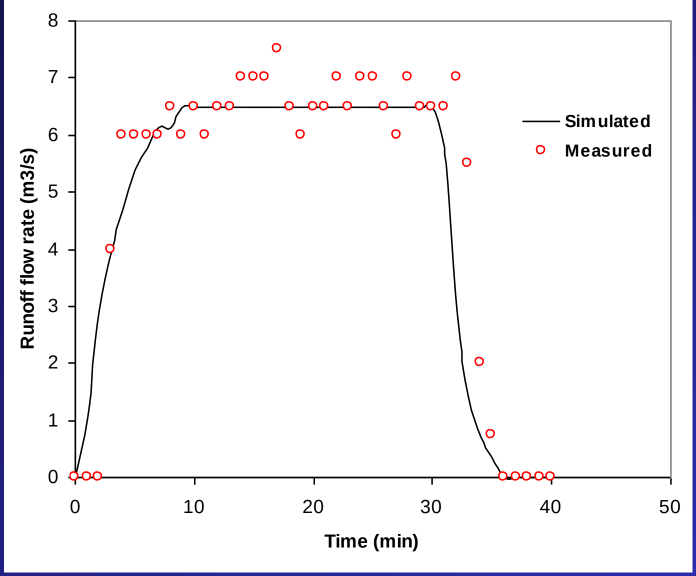
| Parameter | Comp B | RDX | TNT |
|---|---|---|---|
| *S* ($g/cm^3$) | 1.65 | $4.6 \times 10^{-5}$ | $1.3 \times 10^{-4}$ |
| *D* ($cm^2/s$) | | $2.2 \times 10^{-6}$ | $6.7 \times 10^{-6}$ |
| ρ ($g/cm^3$) | | | |

*S* = solubility
*D* = diffusion coefficient
ρ = density

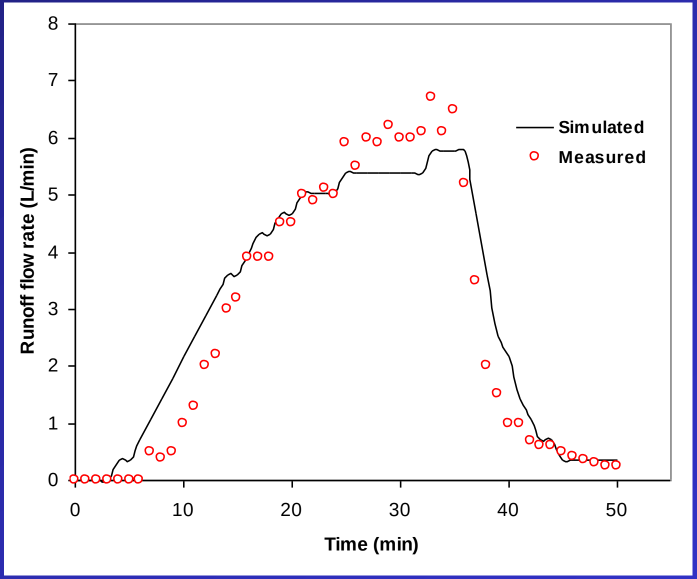
# Experimental Testing of CTT&F - Results

Runoff

## Unvegetated



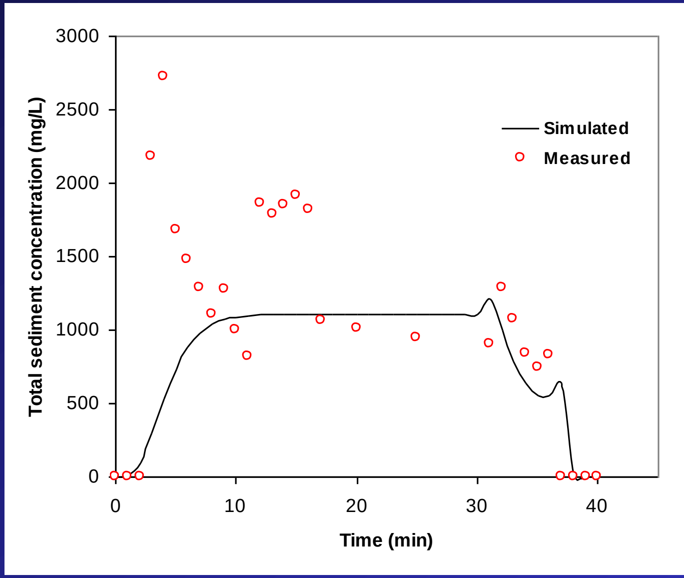

## Vegetated



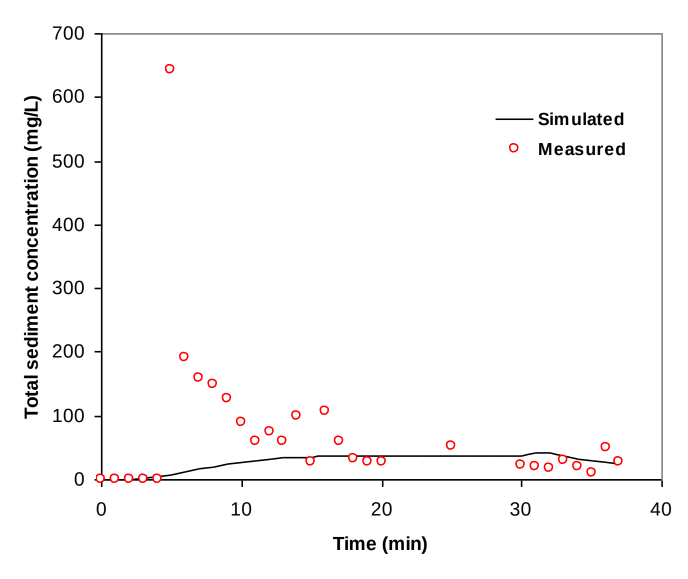
# Experimental Testing of CTT&F - Results

TSS

Unvegetated



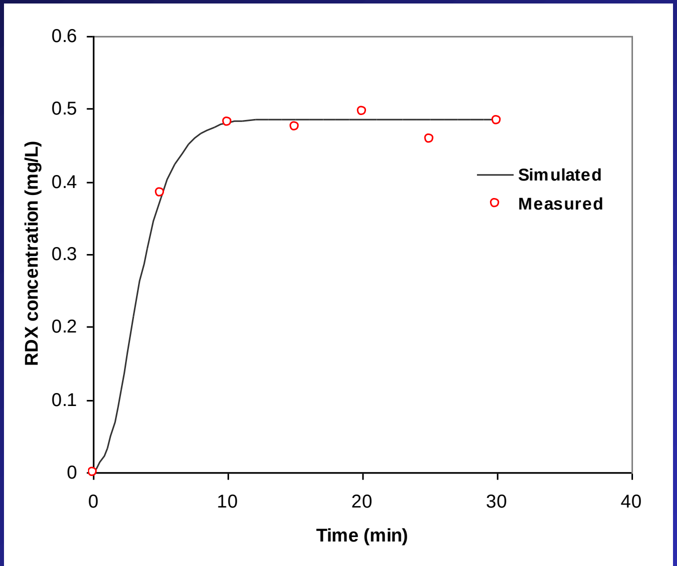

Vegetated



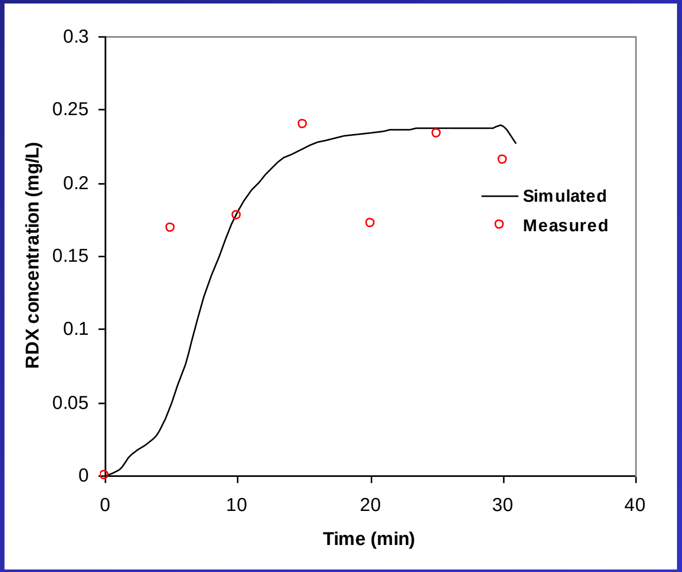
# Experimental Testing of CTT&F - Results

TNT

## Unvegetated




## Vegetated

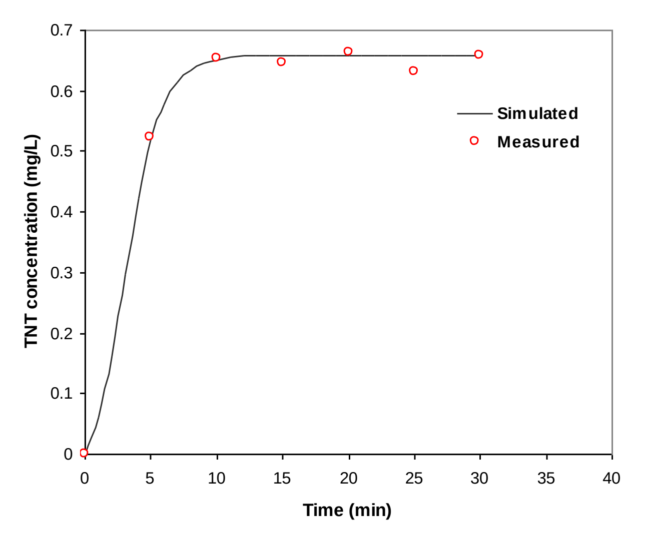


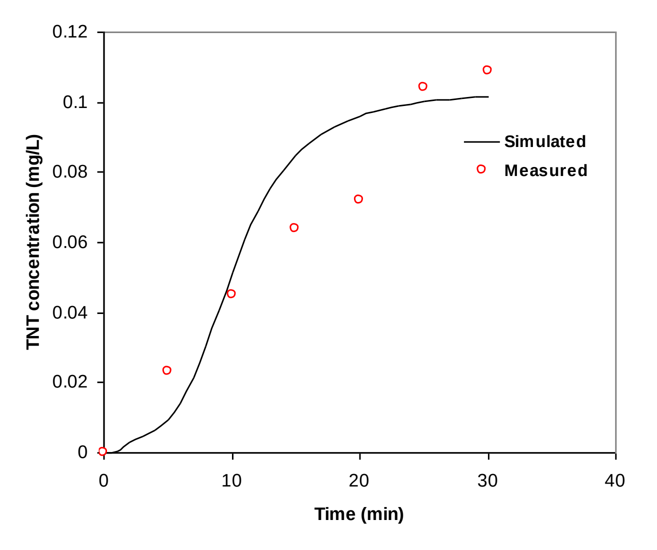
# Experimental Testing of CTT&F - Results

Unvegetated

Vegetated

RDX




US Army Corps of Engineers

# CTT&F Conclusions

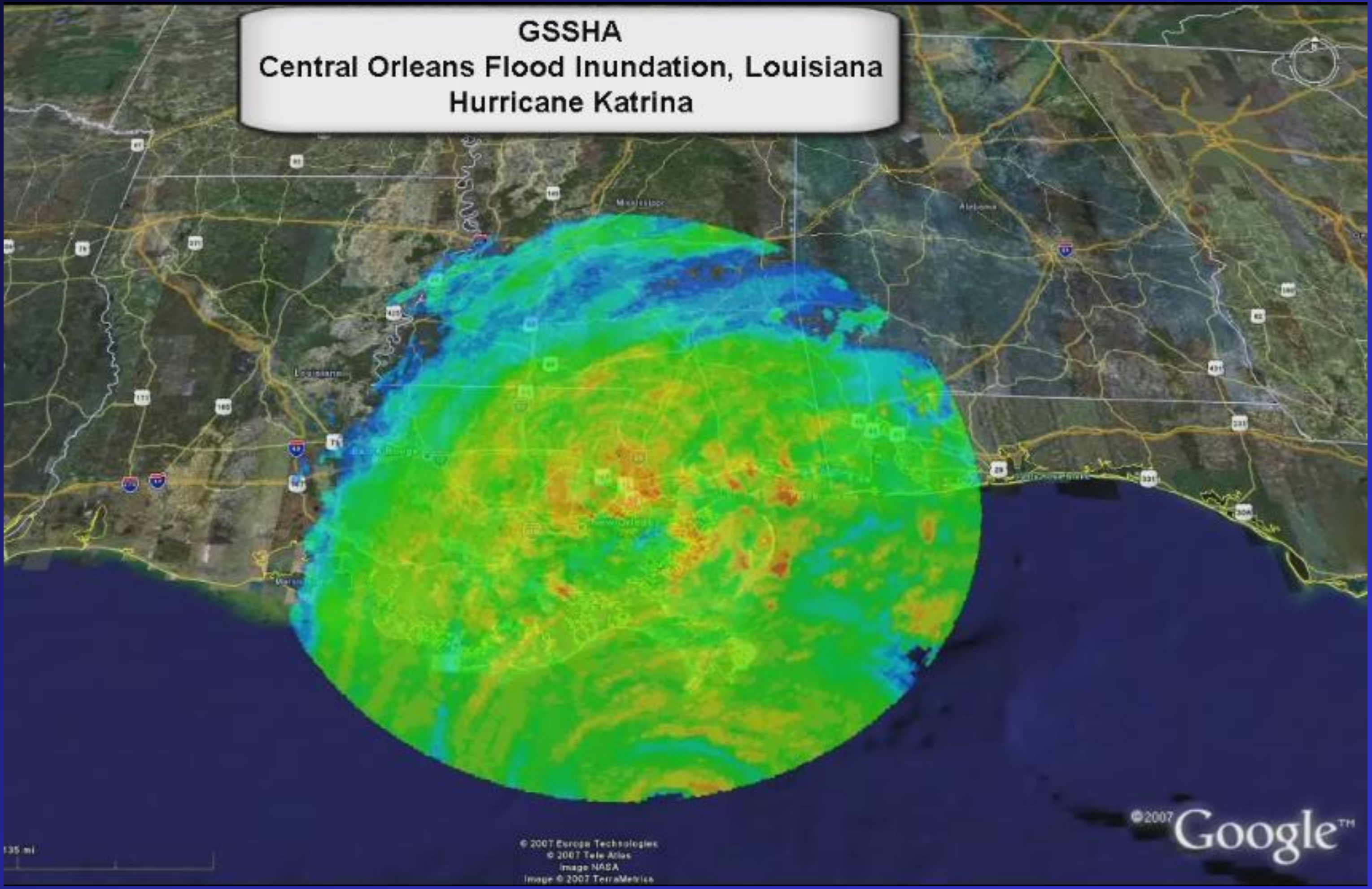
- A constituent transport, transformation and fate sub-model, CTT&F, has been developed for simulating a distributed source.

- The CTT&F equations, which were developed, are comprehensive, self consistent, and fully compatible with the physically based, distributed watershed hydrologic models which provides the required hydrological and sediment variables.

- CTT&F generates time series outputs of model state variables at specified points in space over time. The sub-model also provides the temporal variation and spatial distribution of contaminant sources in different phases.

- Some CTT&F processes were validated from an experimental test plot.

# Example GSSHA Animation



# Questions