Advances in the modeling of Watershed and Riverine Fate and Transport of Contaminants

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**Kinetic Processes**: Biodegradation, Hydrolysis, Oxidation, Transformations

**Mass Transfer**: Air-Water, Water-Sediment, Water Column

**Contaminant Partitioning**: Dissolved Contaminant, DOC Sorbed Contaminant, POC Sorbed Contaminant, Solid Sorbed Contaminant

**External Loading**: Deposition, Resuspension, Deposition, Resuspension, Burial, Volatilization
Discussion Items

- Landscape Contaminant Model Development
  - Model Conceptualization
  - Nutrient Simulation Module (NSM)
  - Contaminant Simulation Module (CSM)
- Riverine Contaminant Model Development
  - HEC-RAS (River Analysis System)
- Source Zone Loading Estimation
  - ATTIC (Advanced Tool for Tracking Industrial Chemicals)
- Demonstration Site
  - Calleguas Creek Watershed
EQT - Surface Water Quality Characterization in Remote Sparse Data Environments

Objective
The objective of this work is to develop a landscape contaminant modeling system capable of modeling the fate and transport of constituent parent and daughter products (chemicals and metals) over large spatial and temporal scales in a computationally efficient manner.

Benefits
Model results will be used to characterize the water quality condition of streams and rivers based upon the intended use of the withdrawn water in addition to tracking the movement of contaminants across diverse landscapes.
Landscape Contaminant Modeling

- **SWAT** – Grid and Lumped (Overland and Small Streams)
- **HEC-RAS** (Large Rivers)
- **ATTIC** (Source Zone)
- **GSSHA** (Overland and Small Streams)

**Integrated Model Approach**

Linkage of common WQ kinetics between watershed and river – NSM and CSM

**USACE** – EL, CHL, and HEC
**USDA-ARS / Texas A&M ENSCO Inc.**
Large Basin (Landscape) Hydrology

Large Spatial and Temporal Domains

CONUS and OCONUS Applications
Hydrologic Processes

- Evaporation and Transpiration
- Precipitation
- Infiltration/plant uptake/Soil moisture redistribution
- Lateral Flow
- Surface Runoff
- Return Flow
- Revap from shallow aquifer
- Percolation to shallow aquifer
- Flow out of watershed
- Recharge to deep aquifer

Encompasses the FULL Hydrologic Cycle
Nutrient Simulation Module (NSM-I)

Provides necessary information for the Contaminant Simulation Module

Currently integrated with HEC-RAS.
SWAT and GSSHA nutrients will be upgraded.

Carbon Cycle
NSM-II explicitly models Bed Sediments
Contaminant Simulation Module (CSM)

- **Air-Water**: Contaminant Partitioning
  - **Dissolved Contaminant**
  - **DOC Sorbed Contaminant**
  - **POC Sorbed Contaminant**
  - **Solid Sorbed Contaminant**

- **Volatilization**

- **External Loading**

- **Water Column**
  - Mass Transfer
  - Mass Transfer
  - Deposition
  - Deposition
  - Resuspension
  - Resuspension

- **Benthic Sediment Layer**
  - Mass Transfer
  - Mass Transfer
  - Deposition
  - Deposition
  - Resuspension
  - Resuspension

**Kinetic Processes**:
- Biodegradation
- Hydrolysis
- Oxidation
- Transformations

Work currently underway to integrate with HEC-RAS, SWAT, and GSSHA

Innovative solutions for a safer, better world

BUILDING STRONG®
Contaminant Simulation Module (CSM)

- Multi-media physical transport processes
  - Water column
  - Bed sediments
- Multiple (4) phase partitioning of contaminants
  - Dissolved in water, Sorbed to Organic Carbon (DOC, POC), Sorbed to sediment particles
- Six (6) biochemical transformation processes
  - Ionization
  - First order biodegradation
  - Hydrolysis
  - Photolysis (Photodegradation)
  - Volatilization
  - Reaction and Transformations
Other Processes and Factors

- Sediment settling and resuspension
- Sediment-water transfer
- Air deposition
- Environmental factors
  - Water temperature
  - Inorganic sediments
  - Organic carbon (DOC, POC)
  - pH
  - Light attenuation
Riverine Hydraulics
Base Model - HEC-RAS (River Analysis Systems)

- One-Dimensional (1D) hydraulics program
- Computes river velocities, stages, profiles, and inundated areas (with GeoRAS) given streamflow and geometry
- Steady, Unsteady Flow, and Quasi-Unsteady (for Sediment analysis)
- HEC-RAS simulates sediment transport/movable beds resulting from scour and deposition
- Graphical User Interface
- Data storage/management
- Graphics, Tabular Output & Reporting
- GeoRAS – GIS pre and postprocessor
- Nationally accepted by state and local agencies, academia and Federal agencies.
Riverine Hydraulics

- Steady flow
- Unsteady flow

Momentum Equation:
\[ \frac{\partial Q}{\partial t} + \frac{\partial (\alpha Q^2/A)}{\partial x} + g A (\frac{\partial h}{\partial x} - S_o + S_f) = 0 \]

Continuity Equation:
\[ \frac{\partial Q}{\partial x} + \frac{\partial A}{\partial t} = 0 \]

Energy (momentum) Equation:
\[ \frac{\partial (\alpha Q^2/A)}{\partial x} + g A (\frac{\partial h}{\partial x} - S_o + S_f) = 0 \]
Riverine Sediment Transport

Fluvial sediment schematic

Suspended load – sand, silt & clay
Bed load – sand, gravel, cobbles & boulders
Wash load – silt & clay
Bed material load – sand, gravel, cobbles & boulders
Landscape Contaminant Modeling System

SWAT Soil & Water Assessment Tool

GSSHA

HEC-DSS

NSMI

CSM

HEC-RAS

Graphical Editor

Selected Data Set: MINNESOTA - LOWER/2337.0 DS BOUNDARY/DISSOLVED OXYGEN/01JA...

Date/Time   Original (mg/l)   Estimate/Entry (mg/l)   Revised (mg/l)
            30Sep2000, 24:00   3.93            3.93
            07Oct2000, 24:00   11.35           11.35
            14Oct2000, 24:00   23.65           23.65
            21Oct2000, 24:00   10.00           10.00
            28Oct2000, 24:00   8.70            8.70
            04Nov2000, 24:00   8.06            8.06
            11Nov2000, 24:00   8.06            8.06
            18Nov2000, 24:00   6.99            6.99
            02Dec2000, 24:00   5.65            5.65
            09Dec2000, 24:00   5.65            5.65
            16Dec2000, 24:00   6.36            6.36
            23Dec2000, 24:00   7.78            7.78

Innovative solutions for a safer, better world
Advanced Tool for Tracking Industrial Chemicals

• ATTIC is a semi-structured data mining and semantic processing tool that has been custom designed for navigation of chemical and industry data.

• The software framework provides users with unique graphical user interfaces (GUI) focused on each data type.

• Users may use keyword querying, meta data filters, and geographical screening to locate the data of interest.

• Designed by subject matter experts (SME) to assist and retain manual SME reviews, for eventual use in non-SME evaluations.

Used to help estimate Source Zone Loadings!
ATTIC Purpose and Uses

• Assists identification of commercial activities and products associated with specific chemicals of interest (COIs)

• Allows user to locate chemical, industrial, and medical facilities with activities or products associated with specific COIs within a target geographic region of interest (ROI)

• Contains data that allows user to manually evaluate facilities for the likelihood of being a source COI to the environment

• Allow SMEs to enhance data and create reviews for future rapid automated and/or non-SME analyses
Integrate ATTIC with Basin Hydrology

- Ability to choose a basin of interest in ATTIC
- Use GIS flow direction to pre-screen sources
- Filter ATTIC facilities and ag. sources using hydrology to provide source loading at +
- Export max and min source loading estimates to table

a#: agricultural sources
x#: industrial facility sources
+ : possible site of interest
### Agricultural Zone Loadings

<table>
<thead>
<tr>
<th>Zone</th>
<th>Fertilizers (N-P-K) (kg/acre)</th>
<th>Inorganic Pesticides (kg/acre)</th>
<th>Organic Pesticides (kg/acre)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>100 - 30 - 60</td>
<td>2</td>
<td>12.5</td>
</tr>
<tr>
<td>B</td>
<td>200 - 10 - 20</td>
<td>1</td>
<td>20</td>
</tr>
<tr>
<td>C</td>
<td>80 - 80 - 80</td>
<td>1</td>
<td>4</td>
</tr>
<tr>
<td>D</td>
<td>0 - 0 - 0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>E</td>
<td>40 - 0 - 10</td>
<td>0</td>
<td>5</td>
</tr>
<tr>
<td>F</td>
<td>100 - 30 - 60</td>
<td>5</td>
<td>30</td>
</tr>
<tr>
<td>G</td>
<td>0 - 0 - 0</td>
<td>3</td>
<td>10</td>
</tr>
<tr>
<td>H</td>
<td>200 - 30 - 60</td>
<td>7</td>
<td>15</td>
</tr>
</tbody>
</table>

### Industrial Facilities Loadings

<table>
<thead>
<tr>
<th>Company</th>
<th>Organics (kg/day)</th>
<th>Inorganic Solubles (kg/day)</th>
<th>Insoluble Particulate</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kapital-Prok-Chernozemeye</td>
<td>10-100</td>
<td>0-1</td>
<td>1-10</td>
</tr>
<tr>
<td>Russkoye_pole</td>
<td>1-10</td>
<td>0-1</td>
<td>0-1</td>
</tr>
<tr>
<td>Nils-Povyolzhye</td>
<td>1-10</td>
<td>0-1</td>
<td>0-1</td>
</tr>
<tr>
<td>Reyting_Plus</td>
<td>0-1</td>
<td>10-100</td>
<td>0-1</td>
</tr>
<tr>
<td>Rusinvest</td>
<td>1-10</td>
<td>10-100</td>
<td>0-1</td>
</tr>
<tr>
<td>Lovin-Ognezaschita_Firm</td>
<td>100-1000</td>
<td>1-10</td>
<td>10-100</td>
</tr>
<tr>
<td>Nauka_i_teknologii</td>
<td>0-1</td>
<td>1-10</td>
<td>0-1</td>
</tr>
<tr>
<td>Shelkovo_Agrokhim</td>
<td>100-1000</td>
<td>0-1</td>
<td>10-100</td>
</tr>
<tr>
<td>Korpas_Veterinary_Firm</td>
<td>0-1</td>
<td>0-1</td>
<td>0-1</td>
</tr>
<tr>
<td>TIL</td>
<td>10-100</td>
<td>1-10</td>
<td>0-1</td>
</tr>
</tbody>
</table>

- Based upon facility and agricultural zone evaluations, SMEs develop estimates for basin loadings of various classes of compounds.
- Speciation of most toxic chemicals of interest may be given higher scrutiny and more detailed estimates.
Agricultural Loading Estimation

- **Data**
  - Open Source Regional Crop Data
  - Imagery-Driven Crop Identification where Needed/Possible

- **Methodology**
  - Crop → Common Pests → Req’d Pesticide → Application Rate
  - Crop → Soil Type → Fertilizer Requirements → Application Rate
NICB uses 100% recycled fiber. The mill receives over 100 truckloads of Old Corrugated Containers a day. Material is reduced to a slurry and re-formed to create new brown paper. We have our own waste-water treatment plant to clean and recycle waste-water.
Demonstration Site
Calleguas Creek Watershed, Ventura County, California

- Drainage Area is 343 mi² (888.4 km²)
- 20 flow gages
- 20 precipitation gages (daily and hourly)
- For multiple sites, datasets (flow, sediment concentration, nutrient concentration, and contaminant concentration) spanning 20+ years (1993 to present) is available at disparate locations.
- Ranges from steep to mild slopes, urban (civil and military) to agriculture, and main stem river connects to the ocean.
- Data is being gathered and models are being set up to start flow and sediment calibration.
- Contaminant calibration will be done in Fiscal Year 2016.
Questions???