Developing an ArcGIS Extension for Estimating Nitrate Fate and Transport

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Project

- Modules
  - Flow
  - Transport
  - Denitrification

- Flow, transport and denitrification modules have been developed.

- Flow module has been tested with data provided by Hal Davis.

- Transport and denitrification modules are being tested using data provided by FDEP. Preliminary results are presented.
• Demo
  – Flow transport and denitrification

Flow Model

Flow model estimates groundwater flow velocity and travel time to a target water body using various approximations
  – Steady state flow
  – Dupuit Approximation
    • Flow is horizontal
    • Hydraulic gradient is assumed to be the slope of the water table
  – Water table is a subdued replica of the topography

• Process an input DEM and use it to approximate water table.

• Use Darcy’s Law to calculate the flow velocity.
Flow Model

- Apply a smoothing algorithm (an averaging filter) to the DEM to get water table.

- Calculate the hydraulic gradient
  - Apply a Sobel filter (similarly for $\frac{\partial h}{\partial y}$)
  - Magnitude of the gradient is: $\sqrt{\left(\frac{\partial h}{\partial x}\right)^2 + \left(\frac{\partial h}{\partial y}\right)^2}$
  - Direction is: $\tan^{-1}\left(\frac{\partial h/\partial x}{\partial h/\partial y}\right)$

\[ v_s = -\frac{K}{\theta} \nabla h \]

Test Site

- U.S. Naval Air Station (NAS) Jacksonville
  - 4 mi south-east of Lakeshore neighborhood
- Quite flat
- Shallow water table
  - 0 – 1.5 m
- Surficial Aquifer
  - 12 – 30 m thick
  - Medium to fine grain unconsolidated sands

- A MODFLOW model was constructed by the USGS (Davis et al 1996, Davis 1998)
  - Steady state, single layer model
  - Calibrated with 128 well measurements
Analysis of the Water Table-Topography Relationship

- Important to determine whether the water table is reasonably approximated by the topography
  - Model applicability

Path length correlation: 0.9
Analysis of the Water Table-Topography Relationship

Introduction • Background • Conceptual Model • Implementation • Test Case • Conclusions • Future Work

• Rank correlation: 0.9

Transport

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• General idea:
  – Given a set of septic tank locations, track groundwater flow to water body
  – Use analytical solution for a given nitrate concentration at a septic tank to calculate concentration at point \((x,y)\).

• The effect of denitrification on plume size is taken care of by 1\textsuperscript{st} order decay.
Simulating contaminant transport requires solving the advection-dispersion equation:

$$\frac{\partial C}{\partial t} = \alpha_f v \frac{\partial^2 C}{\partial x^2} + \alpha_{fh} v \frac{\partial^2 C}{\partial y^2} + \alpha_{hv} v \frac{\partial^2 C}{\partial z^2} - \nu \frac{\partial C}{\partial x} - kC$$

Dispersion  Advection  Decay

To simplify, use an analytical solution (Domenico & Robbins (1985), Domenico (1987), Martyn-Hayden & Robbins (1997)).

- Used in other models e.g. BIOSCREEN, BIOCHLOR, FOOTPRINT, REMChlor (EPA), SWLOAD.xls (Pennsylvania DEP)

\[
C(x, y, z, t) = \frac{C_0}{8} F_1(x, t) F_2(y, x) F_3(z, x)
\]

\[
F_1 = \exp \left[ \frac{x}{2\alpha_x} \left( 1 - \frac{1 + 4k\alpha_x}{v} \right) \right] \times \exp \left[ \frac{x}{2\alpha_x} \left( 1 + \frac{4k\alpha_x}{v} \right) \right] \times \exp \left[ \frac{x}{2\alpha_x} \right] + \frac{x-vt+1+4k\alpha_x}{2\sqrt{\alpha_x vt}}
\]

\[
F_2 = \exp \left[ \frac{y + Y/2}{2\sqrt{\alpha_y}} \right] - \exp \left[ \frac{y - Y/2}{2\sqrt{\alpha_y}} \right]
\]

\[
F_3 = \exp \left[ \frac{z + Z/2}{2\sqrt{\alpha_z}} \right] - \exp \left[ \frac{z - Z/2}{2\sqrt{\alpha_z}} \right]
\]
• Use a steady-state, 2-D version of the Domenico solution
  – Greatly reduces memory requirements and increases computation speed

• BIOCHLOR uses a similar approximation for computing mass loads

• Is reasonable if vertical dispersion is small

\[ C(x, y, t - \infty) = \frac{C_0}{2} F_1(x, t - \infty) F_2(y, x) \]

\[ F_1(x, \infty) = \exp \left[ \frac{x}{2\alpha x} \left( 1 - \sqrt{1 + \frac{4\alpha x z}{v}} \right) \right] \]

\[ F_2 = c r f \left( \frac{y}{2\sqrt{\alpha y^2}}, \frac{Y}{2} \right) c r f \left( \frac{y}{2\sqrt{\alpha y^2}}, \frac{Y}{2} \right) \]

Transport – Domenico Solution

• Domenico solution visualization
- Domenico solution considers only a single plume with a straight flow path

- Plumes are mapped to curved flow paths using a user-selectable transformation

\[ V \text{ is a constant along flow path} \]

- Effect of velocity averaging
  - Depends on the form of the flow field

\[ \text{Velocity Profile} \]

450 225 0 450 Meters

\[ \text{Domenico} \]

\[ \text{Numerical} \]
Domenico solution considers only a single plume in isolation
- Our tool can handle many plumes

Plume overlap will affect how much nitrate is removed due to denitrification
- Use Max.
- During the last presentation in April, used the Lakeshore neighborhood as an example to demonstrate the flow model.

- Use data from a nearby location (Waterside Dr.) and compare with measurements provided by the FDEP.

- Model parameter values are not site-specific and were taken from the literature.
Test Site

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- Flow model: Using a USGS DEM as input
  - Smoothing amount=40
  - Porosity: 0.25

- Transport:
  - Initial concentration: 40 mg/l (McCray 2005)
  - Source dimensions (estimated from provided data) Y=6m (20 ft), Z=1.5m (5 ft)
  - Cutoff threshold 0.0001 mg/l
  - Decay constant: 0.2 per day, a medium-high value (McCray2005)
  - Dispersivity: longitudinal=2.113 m (~7 ft), transverse = longitudinal x 10% = 0.234 m (~0.7 ft)

- DEP data assumes septic tanks to be in the middle of the property.
  - Model allows for exact locations to be specified if available.
Test Site

- 5436 Waterside Dr.

- Model produces a value close to the measured (0.05 mg/l)
  - 0.01 mg/l

- Comparison difficult without knowing exact coordinates of drain field and values of site-specific parameters (conductivity, dispersivity, rate constant)
  - Calibration required
Test Site

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- 5476 Waterside Dr.
- Comparison difficult without further understanding of plume behavior.
- 1.9 mg/l while adjacent measurements are BDL

Test Site

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- Modeling several sites with the same set of parameters may introduce error in the results at each individual location
- Modeling results should be taken as a bulk estimate
Load Calculation

- Denitrification is incorporated in the transport module using a first-order reaction.
- The load is determined by mass balance.
- In the steady state:
  \[ \text{Nitrate Load} = \text{Mass Rate In} - \text{Mass Rate Out} \]
  \[ M_l = M_{in} - M_{dn} \]

Load Calculation

- \( M_{in} \) is calculated based on the mass flowing into the system from the constant concentration boundary
  - Advection and dispersion are taken into account
  \[ M_{in} = C_0 \Delta y \Delta z \theta v - \alpha_L \Delta y \Delta z \theta v \frac{C - C_0}{\Delta x} \]
- \( M_{dn} \) is calculated from the definition of a first-order reaction and the volume of the calculation cell. The coefficient \( k \) is a function of OC.
  \[ M_{dn} = kC \theta \Delta x \Delta y \Delta z \]
Model Limitations

- Steady-state models.
- Only surficial aquifer considered
  - Saturated zone only
  - No Karst
- No recharge → mounding due to STE not considered.
- Plume evolves in an isolated, semi-infinite domain
  - $x \rightarrow [0, +\infty)$, $y \rightarrow (-\infty, +\infty)$, $z \rightarrow (-\infty, +\infty)$
  - Influences from other plumes or contaminants cannot be considered directly.
- Only consider uniform flow in the longitudinal direction
  - Flow field should not deviate too much from this assumption or results may be inaccurate.
- Other parameters (e.g., dispersivity and decay rate) are assumed constant in the current model
- Contaminant source is modeled as a constant concentration plane
  - A constant concentration will remain at the source for all time.

Conclusions

- Developed the ArcGIS extension with flow, transport and denitrification modules.
  - Flow module has been validated using real data
  - Transport has been verified using MT3DMS modeling results.
  - In the process of validating transport module.
- In the area of interest, the water table is a subdued replica of the topography.
- Domenico solution with warping and velocity averaging provides a satisfactory approximation of plume size and shape compared with MT3DMS
- Preliminary tests indicate modeling results appear to be comparable to site data.
  - More detailed comparison entails model calibration and the collection of site specific parameters.
The purpose of the flow module is to generate two rasters, representing the groundwater flow magnitude and direction.