Developing an ArcGIS Extension for Estimating Nitrate Fate and Transport

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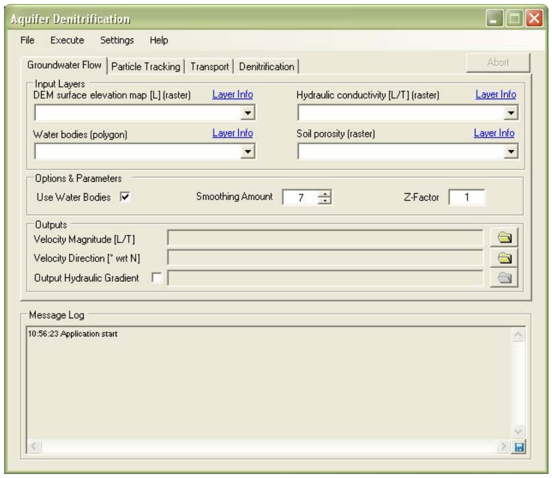
Project

- 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



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Flow Model

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

- 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.

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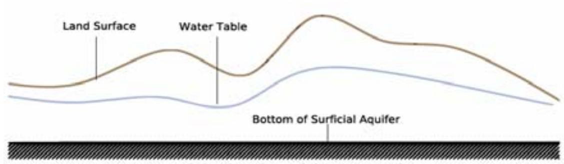
Flow Model

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



$$v_s = -\frac{K}{\theta}\nabla h$$

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

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

$$\frac{\partial h}{\partial x} \approx G_x * A, \quad G_x = \frac{1}{8\Delta x}\begin{bmatrix} 1 & 0 & -1 \\ 2 & 0 & -2 \\ 1 & 0 & -1 \end{bmatrix}$$

$*$ is the convolution operator.

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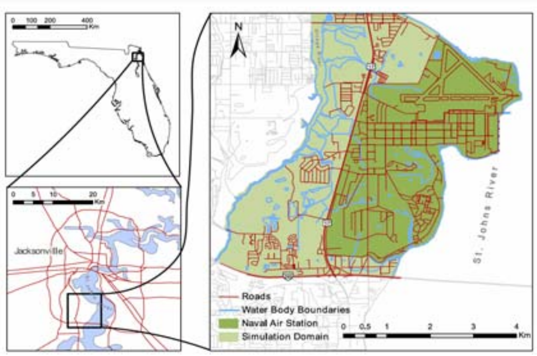
Test Site

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



- 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

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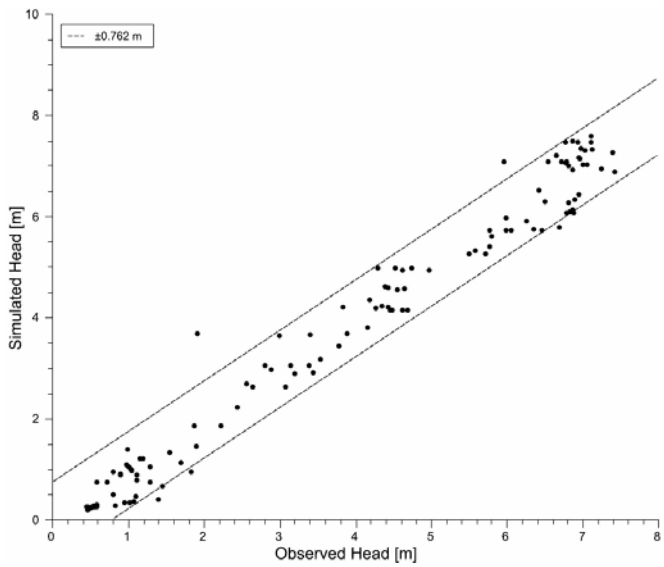
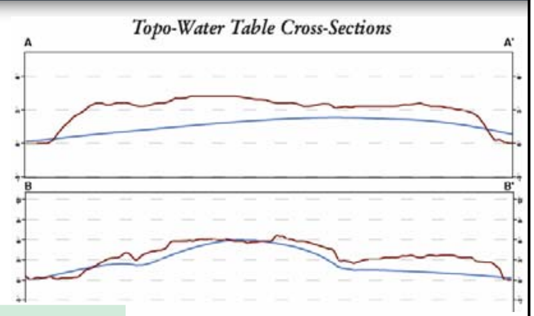
Test Site

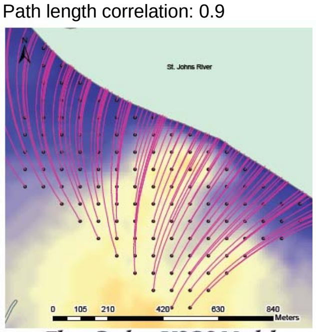


Analysis of the Water Table-Topography Relationship

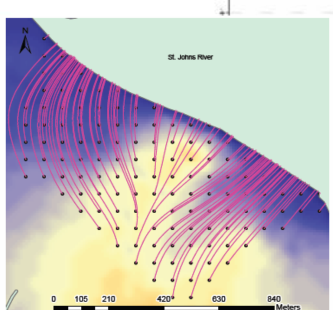
- Important to determine whether the water table is reasonably approximated by the topography
  - Model applicability



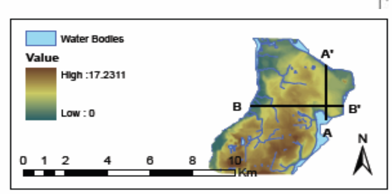
Path length correlation: 0.9



Flow Paths - USGS Model



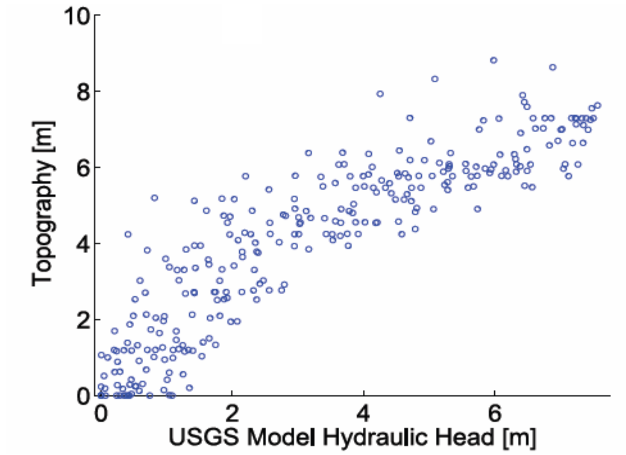
Flow Paths



Land Elevation
Water Table Elevation

Analysis of the Water Table-Topography Relationship

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



- Rank correlation: 0.9

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Transport

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

- 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 1st order decay.

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Transport Model

- Simulating contaminant transport requires solving the advection-dispersion equation

$$\frac{\partial C}{\partial t} = \underbrace{\alpha_{\ell} v \frac{\partial^2 C}{\partial x^2} + \alpha_{T_h} v \frac{\partial^2 C}{\partial y^2} + \alpha_{T_v} v \frac{\partial^2 C}{\partial z^2}}_{\text{Dispersion}} \underbrace{- v \frac{\partial C}{\partial x}}_{\text{Advection}} \underbrace{- kC}_{\text{Decay}}$$

Dispersion Advection Decay

Transport Model

- 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)

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

$$\begin{aligned} F_1 \;=\; & exp\left[\frac{x}{2\alpha_x}\left(1 - \sqrt{1 + \frac{4k\alpha_x}{v}}\right)\right] \times erfc\left[\frac{x - vt\sqrt{1 + \frac{4k\alpha_x}{v}}}{2\sqrt{\alpha_x v t}}\right] + \\ & exp\left[\frac{x}{2\alpha_x}\left(1 + \sqrt{1 + \frac{4k\alpha_x}{v}}\right)\right] \times erfc\left[\frac{x + vt\sqrt{1 + \frac{4k\alpha_x}{v}}}{2\sqrt{\alpha_x v t}}\right] \end{aligned}$$

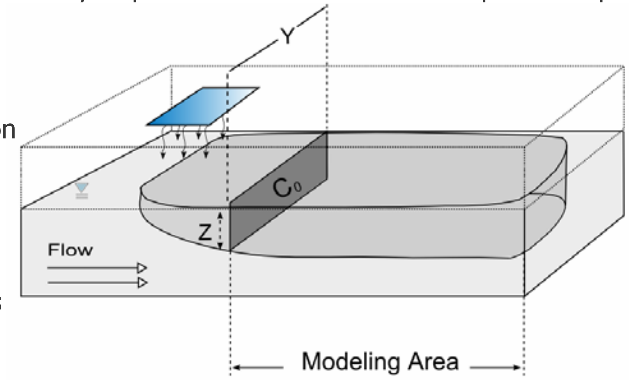
$$F_2 = erf\left(\frac{y + Y/2}{2\sqrt{\alpha_y x}}\right) - erf\left(\frac{y - Y/2}{2\sqrt{\alpha_y x}}\right)$$

$$F_3 = erf\left(\frac{z + Z/2}{2\sqrt{\alpha_z x}}\right) - erf\left(\frac{z - Z/2}{2\sqrt{\alpha_z x}}\right)$$

Transport

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

- 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



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

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

$$F_2 = erf\left(\frac{y+Y/2}{2\sqrt{\alpha_y x}}\right) - erf\left(\frac{y-Y/2}{2\sqrt{\alpha_y x}}\right)$$

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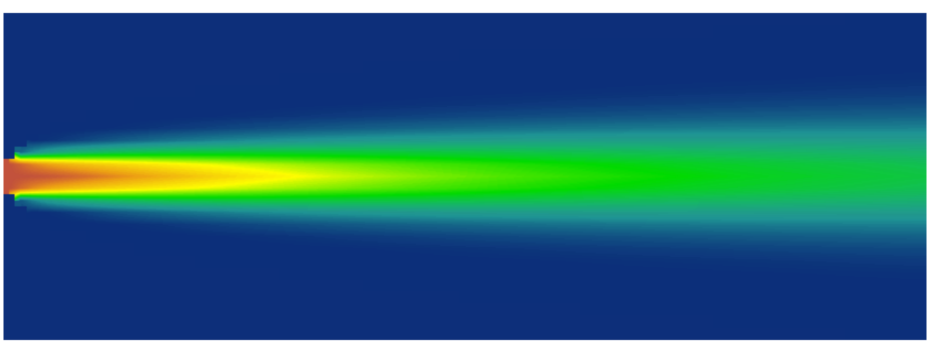
Transport – Domenico Solution

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

- Domenico solution visualization



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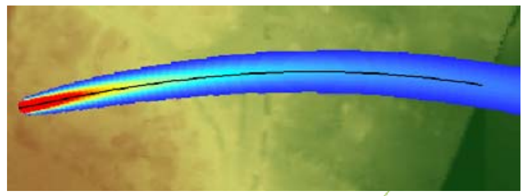
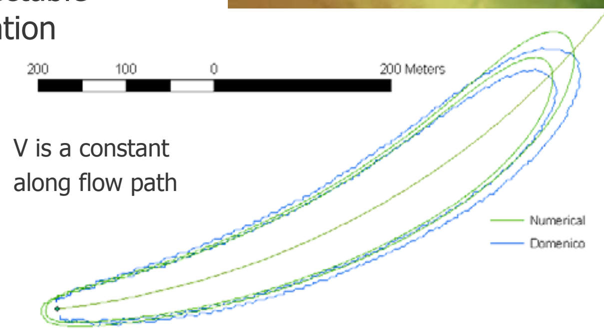
Synthetic Tests

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

- Domenico solution considers only a single plume with a straight flow path
- Plumes are mapped to curved flow paths using a user-selectable transformation





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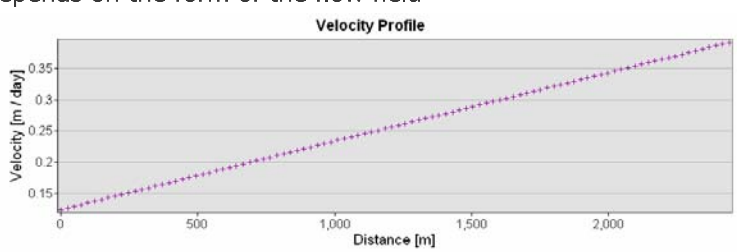
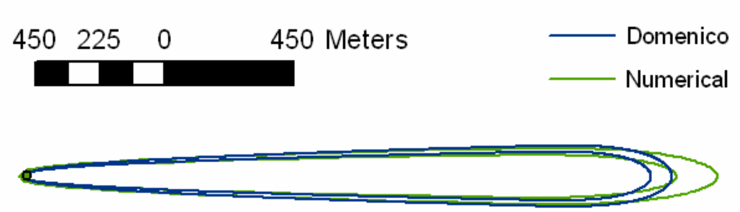
Synthetic Tests

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

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





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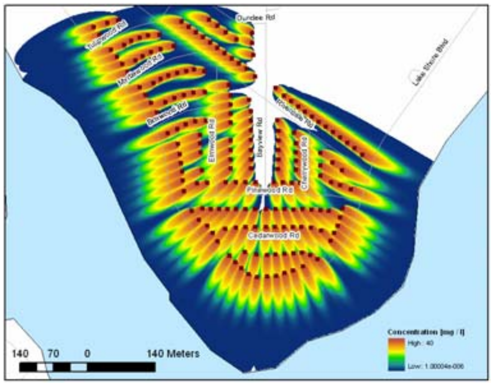
Transport

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

- 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.

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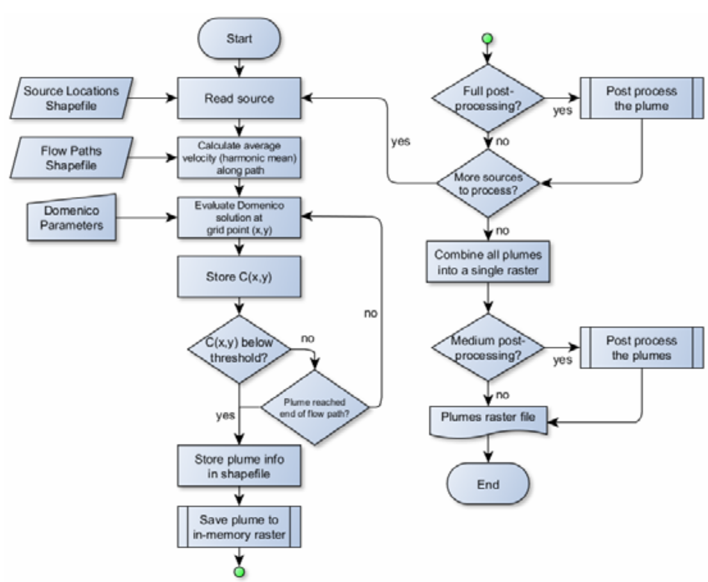
Transport

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



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Test Site

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

- 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

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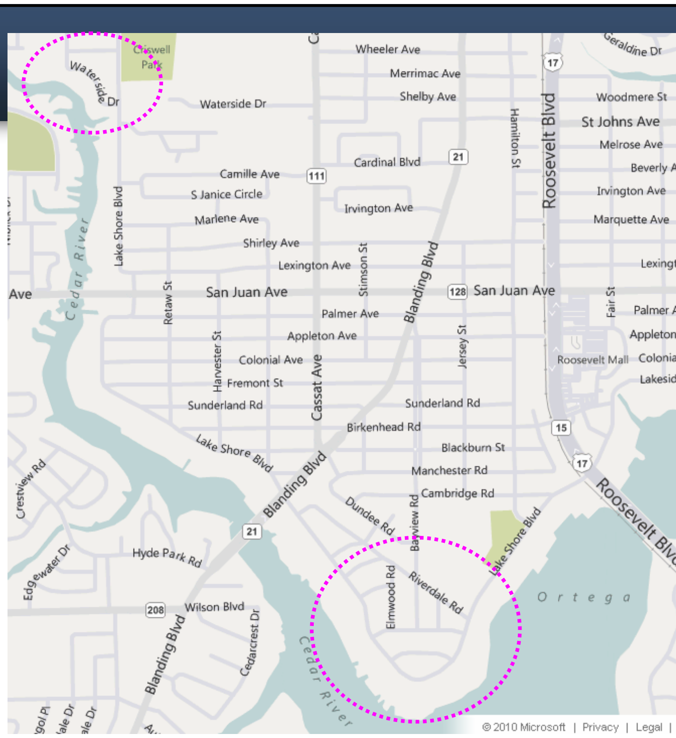

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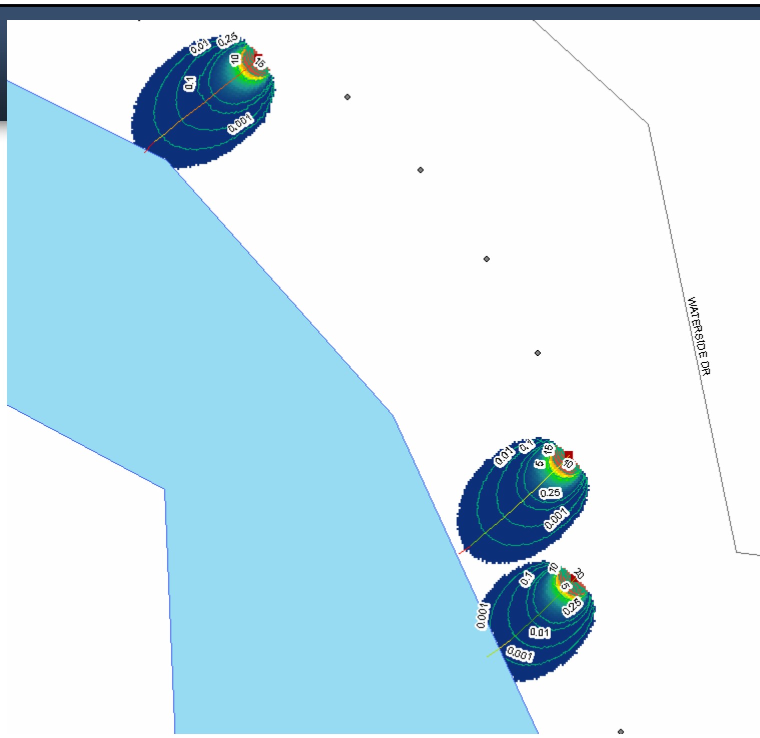
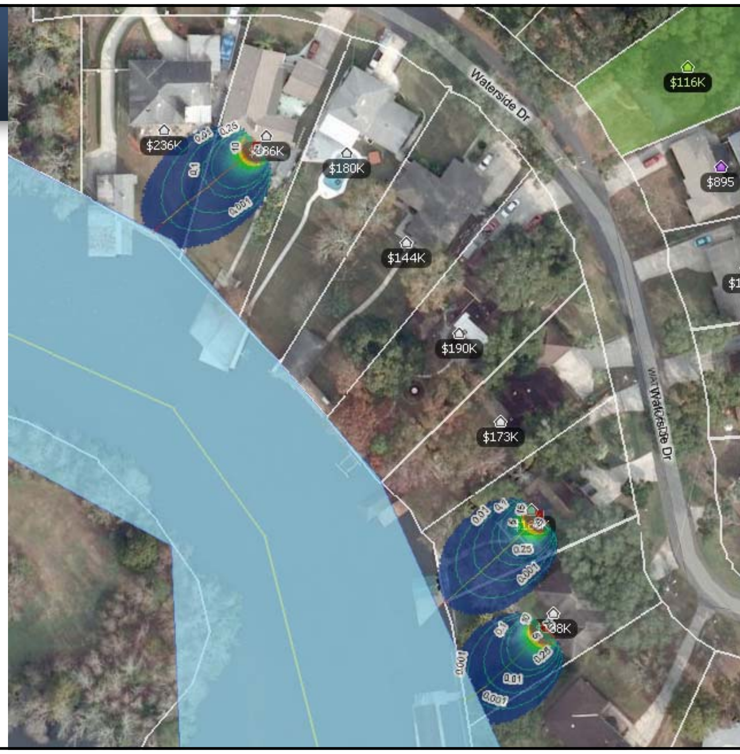
Test Site

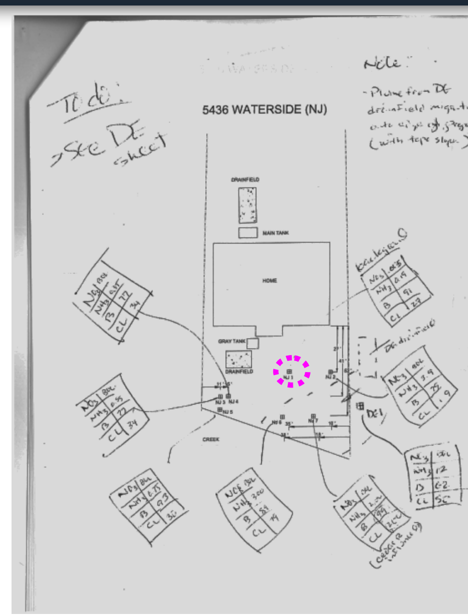
- Flow model: Using a USGS DEM as input
  - Smoothing amount=40
  - Porosity: 0.25
- Transport:
  - Initial concentration: 40 mg/l (McCray 2005)
  - Source dimensions (estimated from provided data) Y=6m (20 ft), Z=1.5m (5 ft)
  - Cutoff threshold 0.0001 mg/l
  - Decay constant: 0.2 per day, a medium-high 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

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

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

Test Site

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

- 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

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Load Calculation

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

- Denitrification is incorporated in the transport module using a first-order reaction.
- The load is determined by mass balance.
- In the steady state:

  Nitrate Load = Mass Rate In – Mass Rate Out

  $M_l = M_{in} - M_{dn}$

Load Calculation

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

- 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

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

- 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-infinte 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.

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Conclusions

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

- 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.

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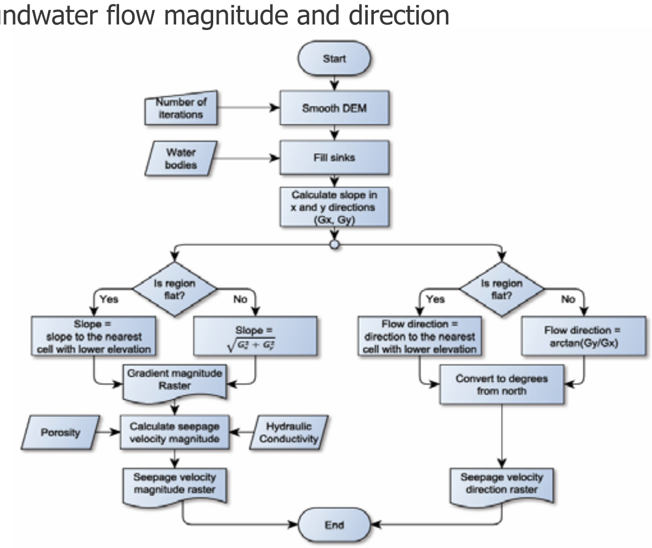
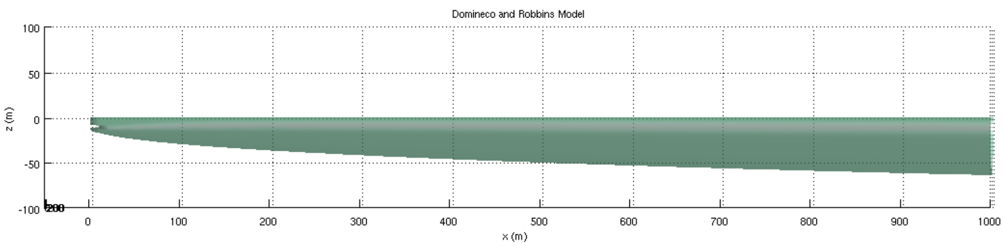
Questions?

Flow Model

- The purpose of the flow module is to generate two rasters, representing the groundwater flow magnitude and direction




Domineco and Robbins Model
z (m)
x (m)
100
50
0
-50
-100
0
100
200
300
400
500
600
700
800
900
1000

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