Developing an ArcGIS Extention for Estimating Groundwater Environmental Impacts of Nitrate Contamination from Energy Biomass Resources Development

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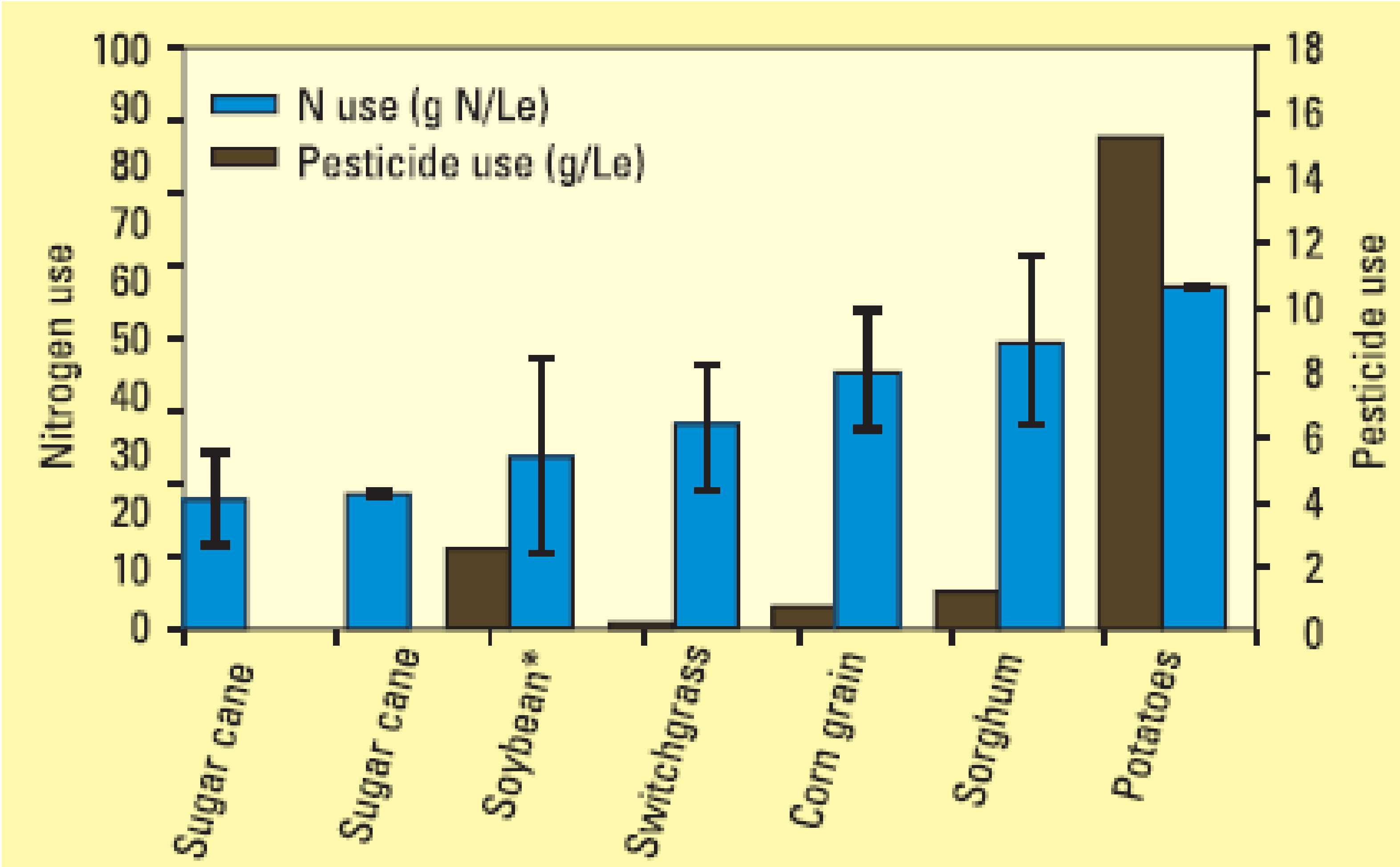
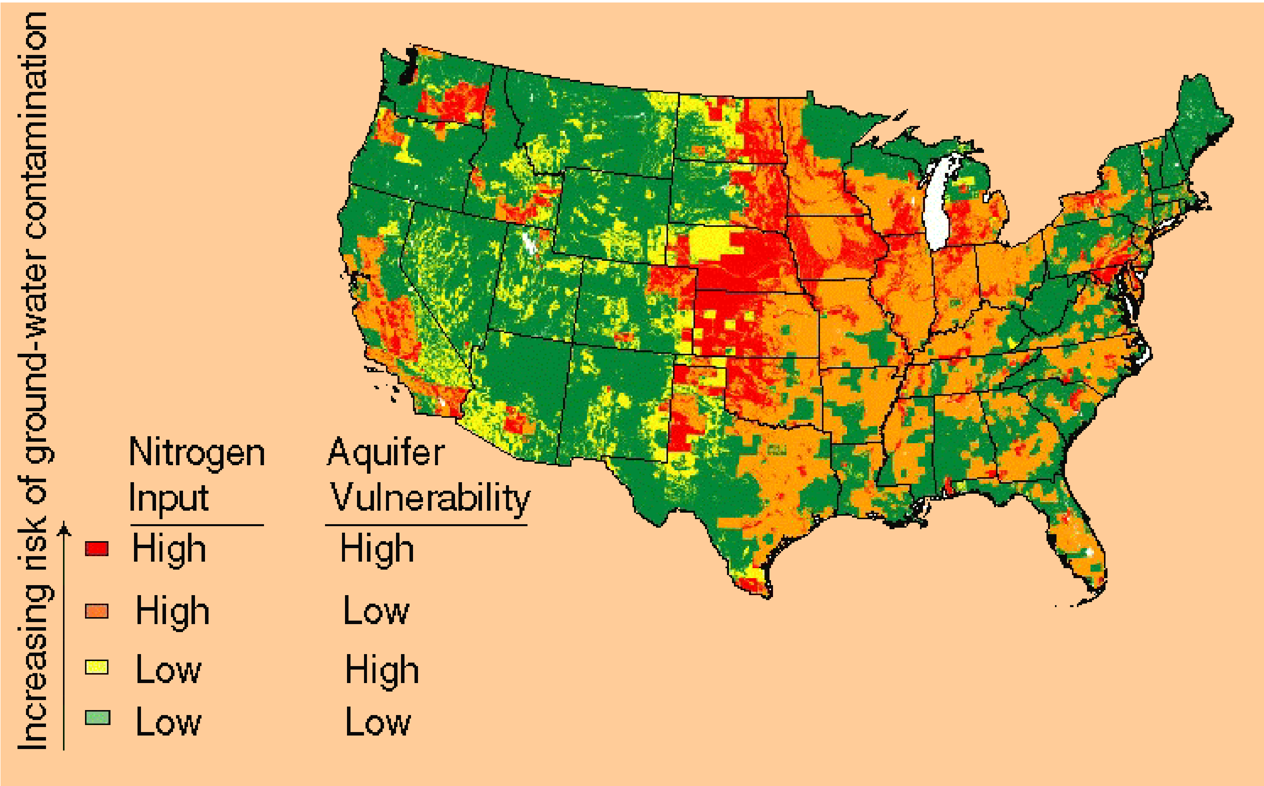


Nitrogen and pesticide requirements for producing 1 L of ethanol (if fertilized) from different crops. (Adapted from Dominguez-Faus et al., 2009)

Risk of Groundwater Contamination by Nitrate

Although nitrate generally is not an adult public-health threat, ingestion in drinking water by infants can cause low oxygen levels in the blood, a potentially fatal condition (Spalding and Exner, 1993).



Areas in the United States with the highest risk of nitrate contamination of shallow ground water

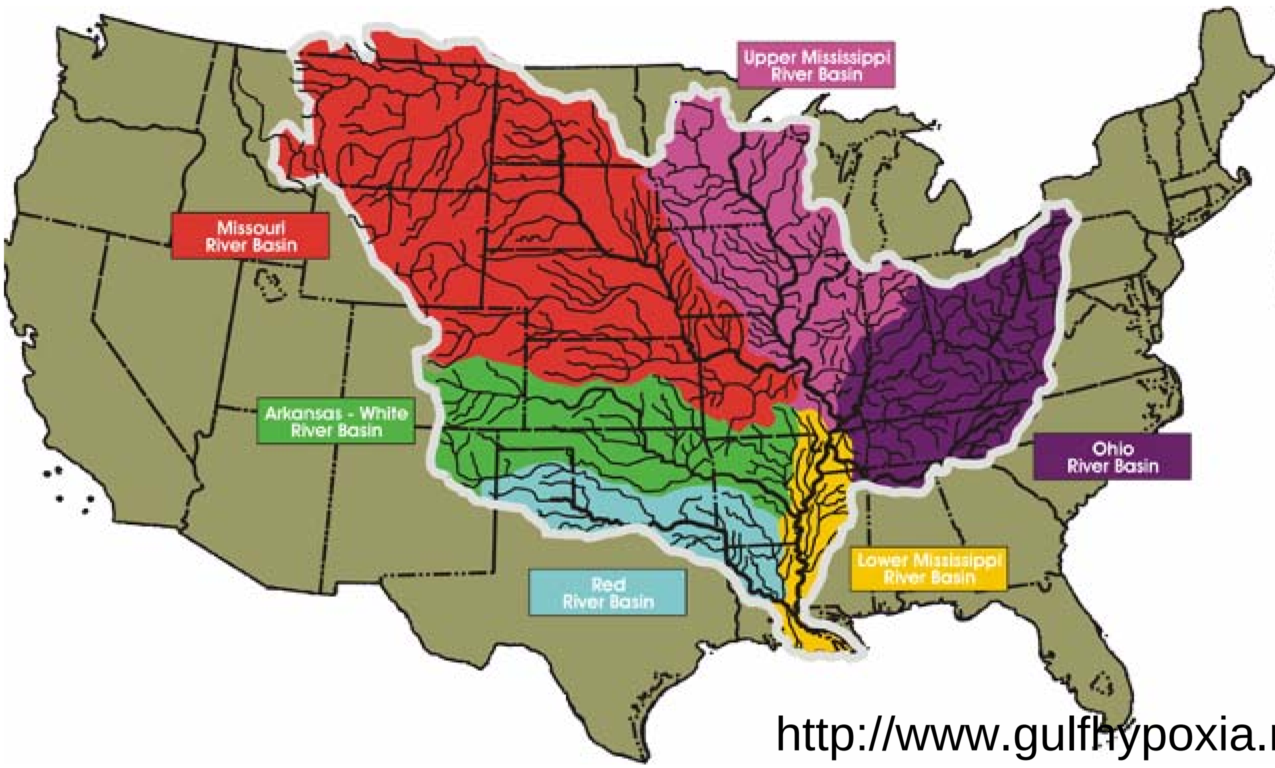
EPA drinking-water standard of 10 mg/L nitrate as nitrogen (NO_3-N)

Natural ground waters usually less than 2 mg/L

http://water.usgs.gov/nawqa/wcp/

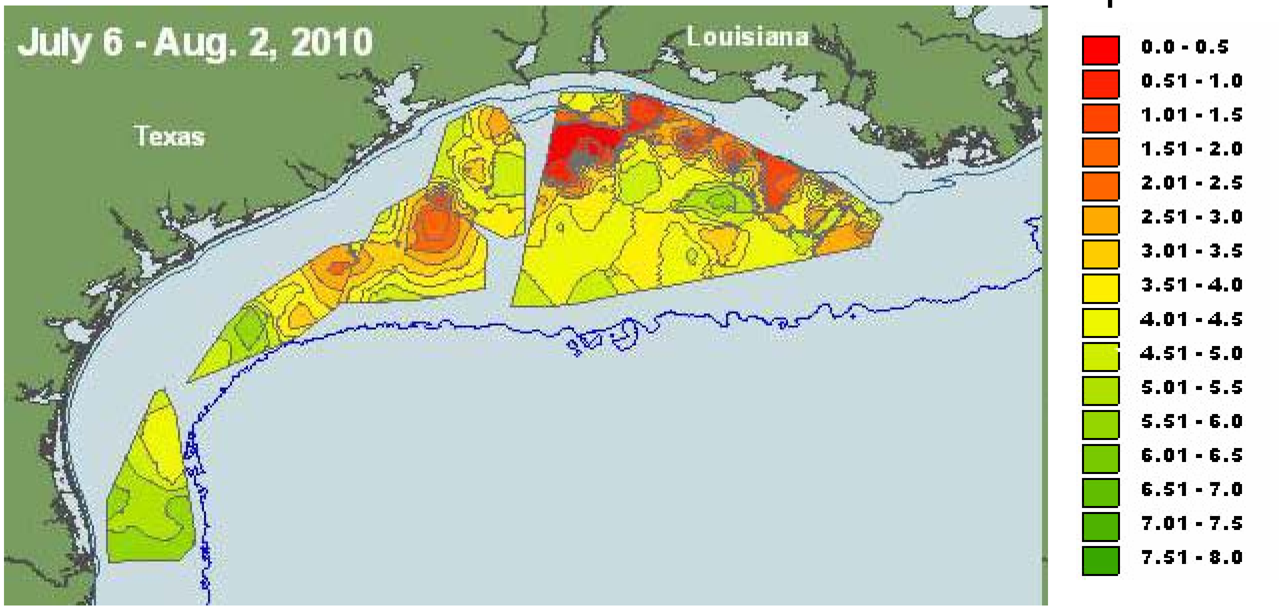
Hypoxic Zone in Gulf of Mexico

The high fertilizer application rates provide the greatest fluxes of N and P to local waterways and Mississippi River basin and are therefore considered as one of the primary contributors to the growing hypoxic zone in the Gulf of Mexico.

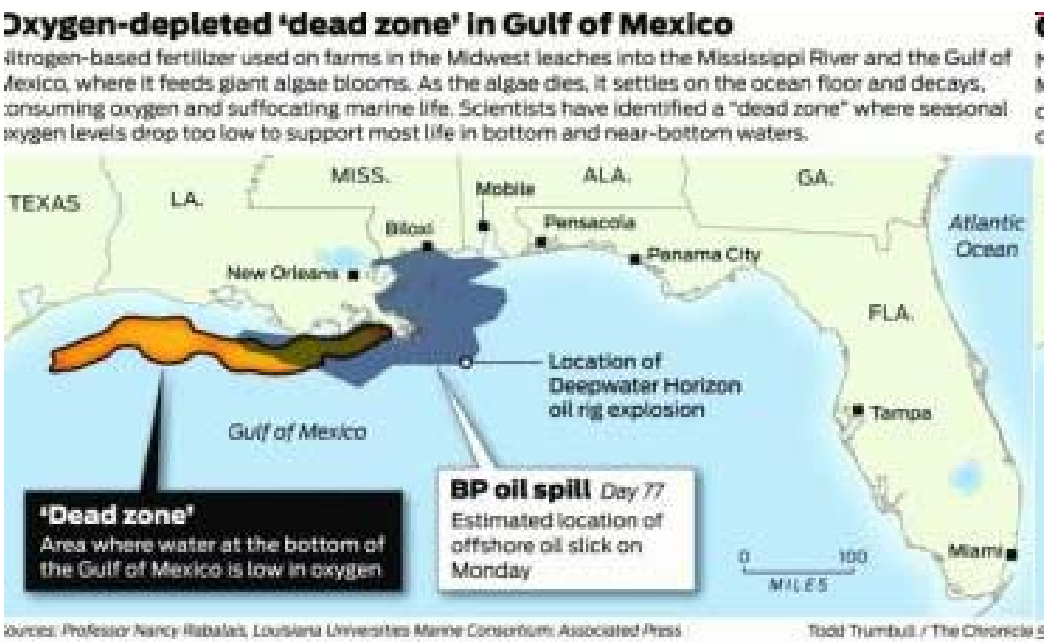


http://www.gulfhypoxia.net/Overview/

http://ecowatch.ncddc.noaa.gov/hypoxia



- Contours of dissolved oxygen
- The size is > 20,700 Km^2 in 2008.



"While the BP oil spill has been labeled the worst environmental catastrophe in recent U.S. history, a biofuel is contributing to a Gulf of Mexico "dead zone" the size of New Jersey that scientists say could be every bit as harmful to the gulf."

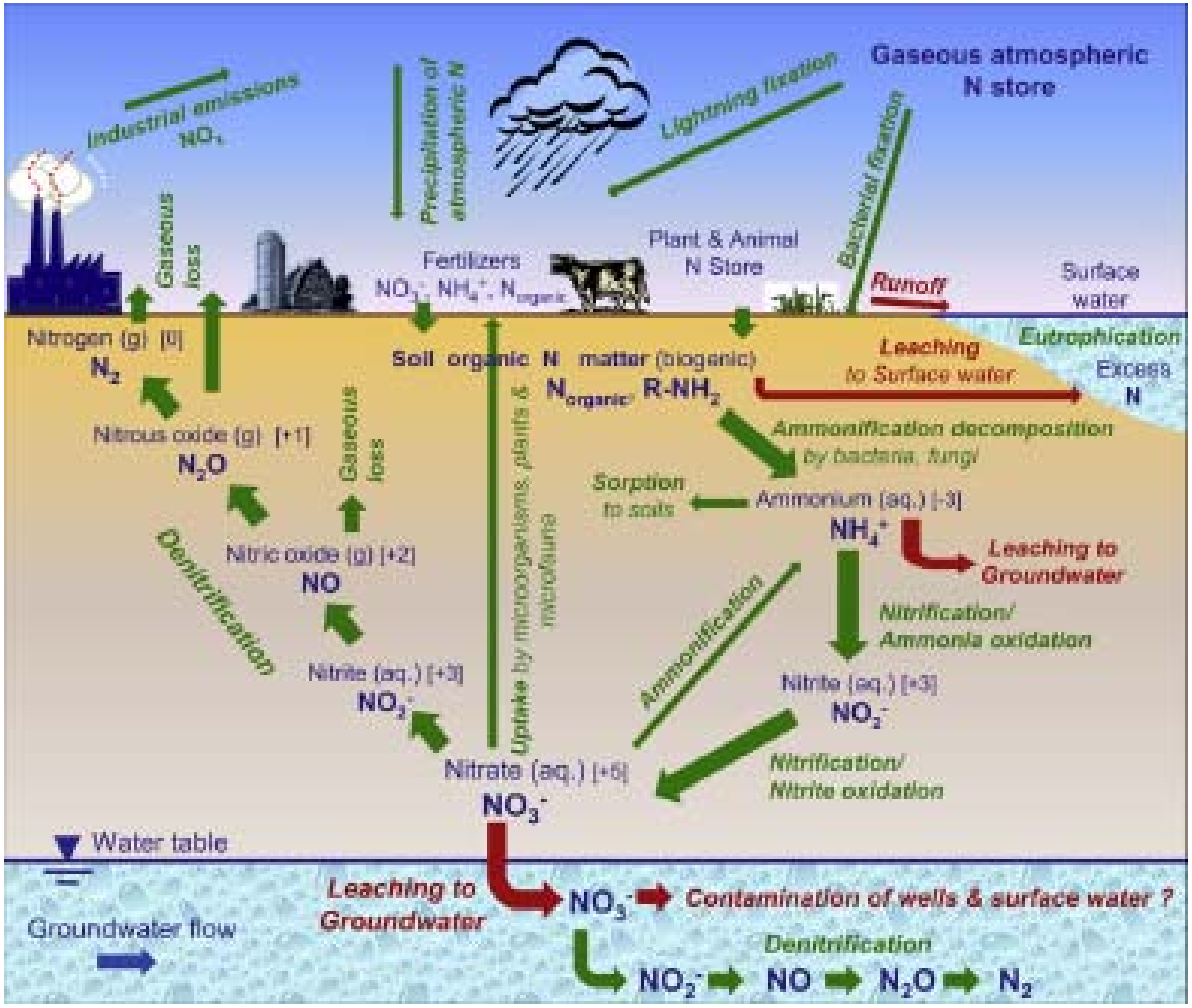
Dead zone in gulf linked to ethanol production, San Francisco Chronicle, July 6

Sustainability of Biofuel Production

- Sustainable biofuel production requires careful assessment of the threats to water quality (and quantity) on local and national scales.
- Water footprint of biofuels
- Twomey et al. (2010) ("The unintended energy impacts of increase nitrate contamination from biofuel production") are concerned about energy costs for treating contaminated water.
- Nitrate (and phosphorus) contamination in
  – Surface water resources
  – Groundwater resources

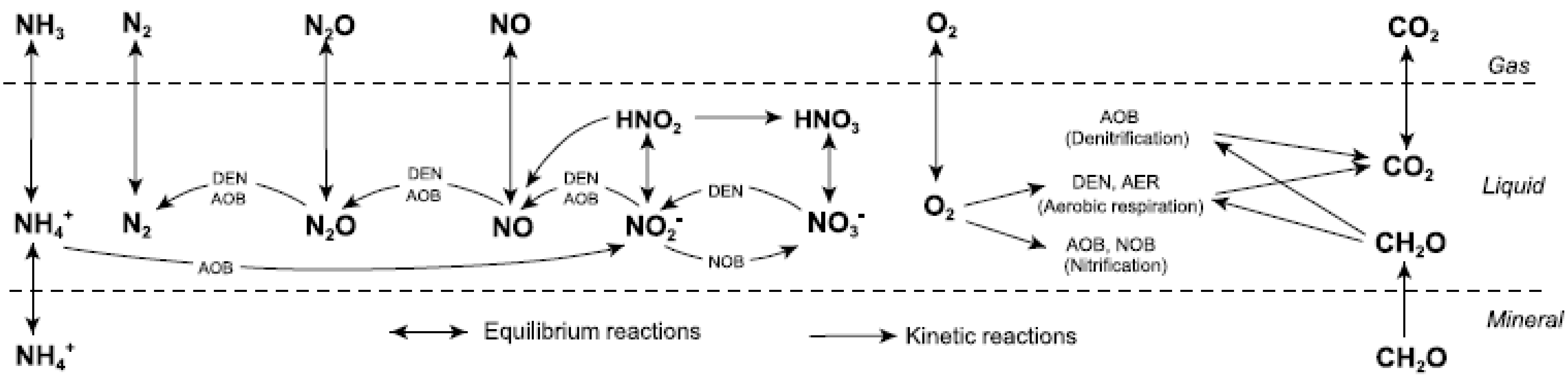
Assessment of Environmental Impacts

The study is focused on groundwater environment. The impact is invisible but can last long.



Impacts on Groundwater Environment

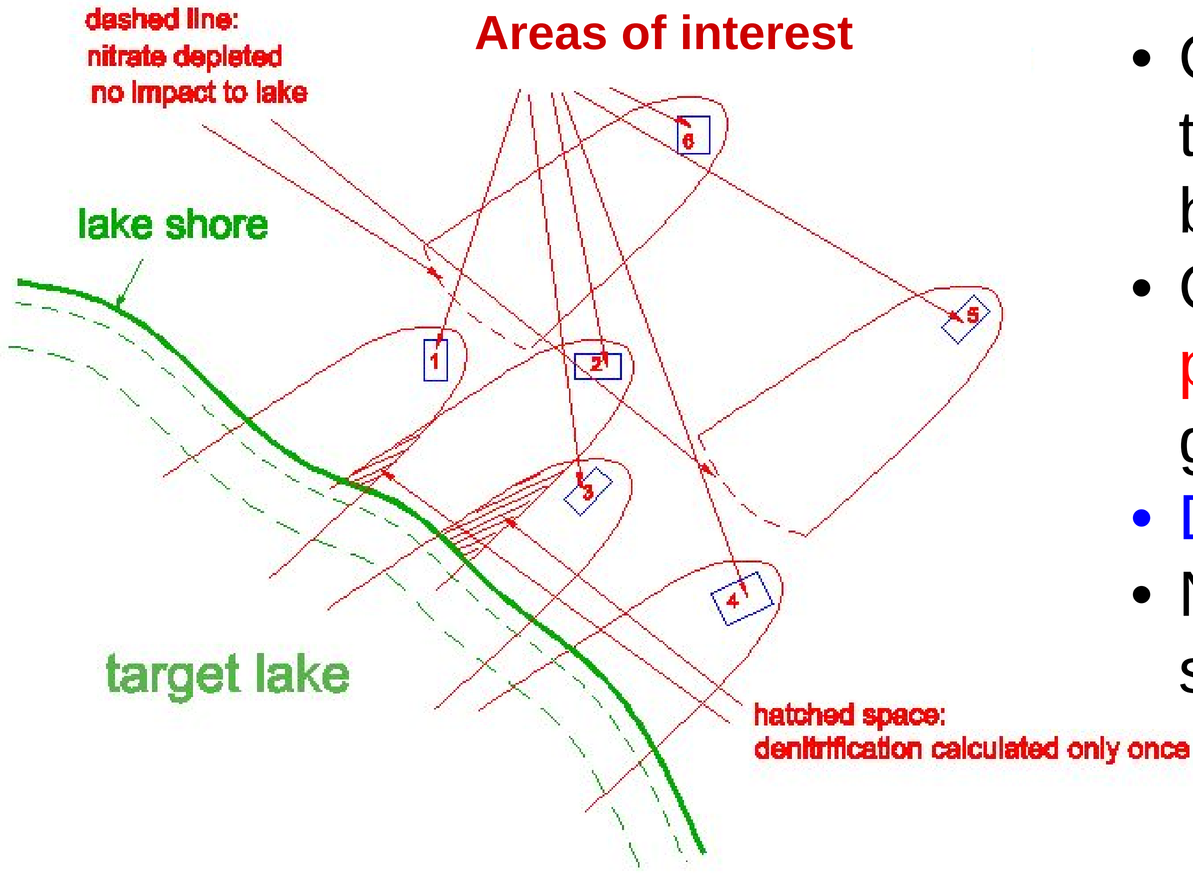
- This study is focused on
  - Nitrate concentration in groundwater
  - Nitrate load to surface water bodies
- Groundwater modeling is needed to simulate nitrate fate and transport in subsurface.
- A full-scale modeling is possible with existing computational codes (e.g., MODFLOW and MT3DMS), but may not be necessary.



Maggi et al. (2008)

Simplified Model

A simplified model for screening and planning study.



- Groundwater flow to surface water bodies
- Groundwater plume in groundwater
- Denitrification
- Nitrate load to surface water

Denitrification

Denitrification … has been identified as basic factor contributing to the generally low levels of nitrate found in the groundwater of the Southeastern United States. (Fedkiw, 1991)

Denitrification refers to the biological reduction of nitrate to nitrogen gas.

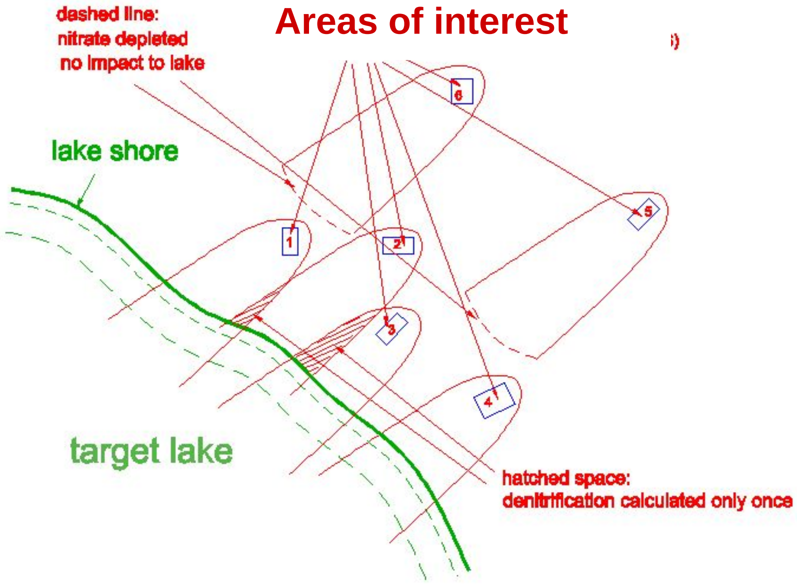
A fairly broad range of heterotrophic anaerobic bacteria are involved in the process, requiring an organic carbon source for energy as follows

$$NO_3^- + \text{Organic carbon} \rightarrow NO_2^- + \text{Organic carbon} \rightarrow N_2 + CO_2 + H_2O$$

$$NO_3^- \rightarrow NO_2^- \rightarrow NO \rightarrow N_2O \rightarrow N_2$$

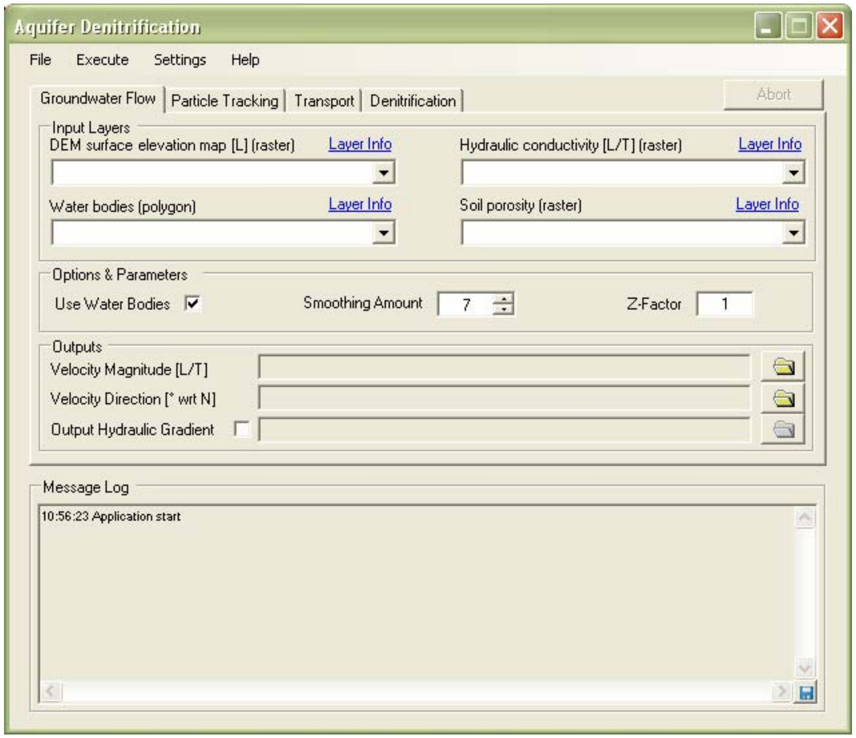
Combine with GIS

Geographic information systems (GIS) or **geospatial information systems** is a set of tools that captures, stores, analyzes, manages, and presents data that are linked to location(s).



Incorporate spatial variability of areas of interest

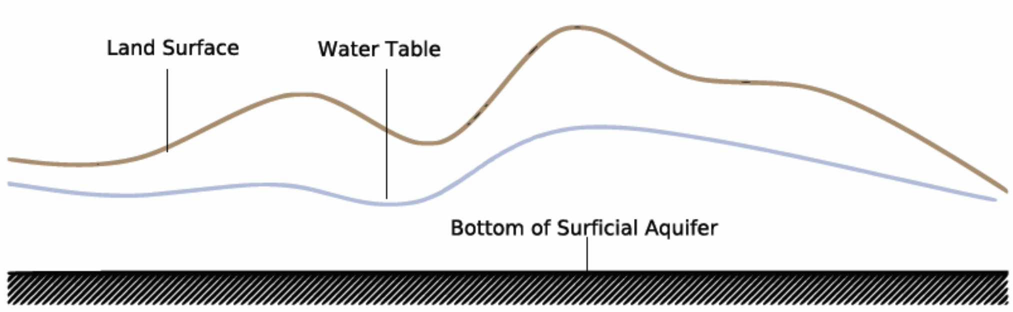
Provide a framework of developing user friendly graphic interface and visualization



Flow Model

- Estimate groundwater flow velocity and travel time to a target water body based on the following approximations
  - Steady state flow
  - Dupuit Approximation (3D->2D)
    - 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



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

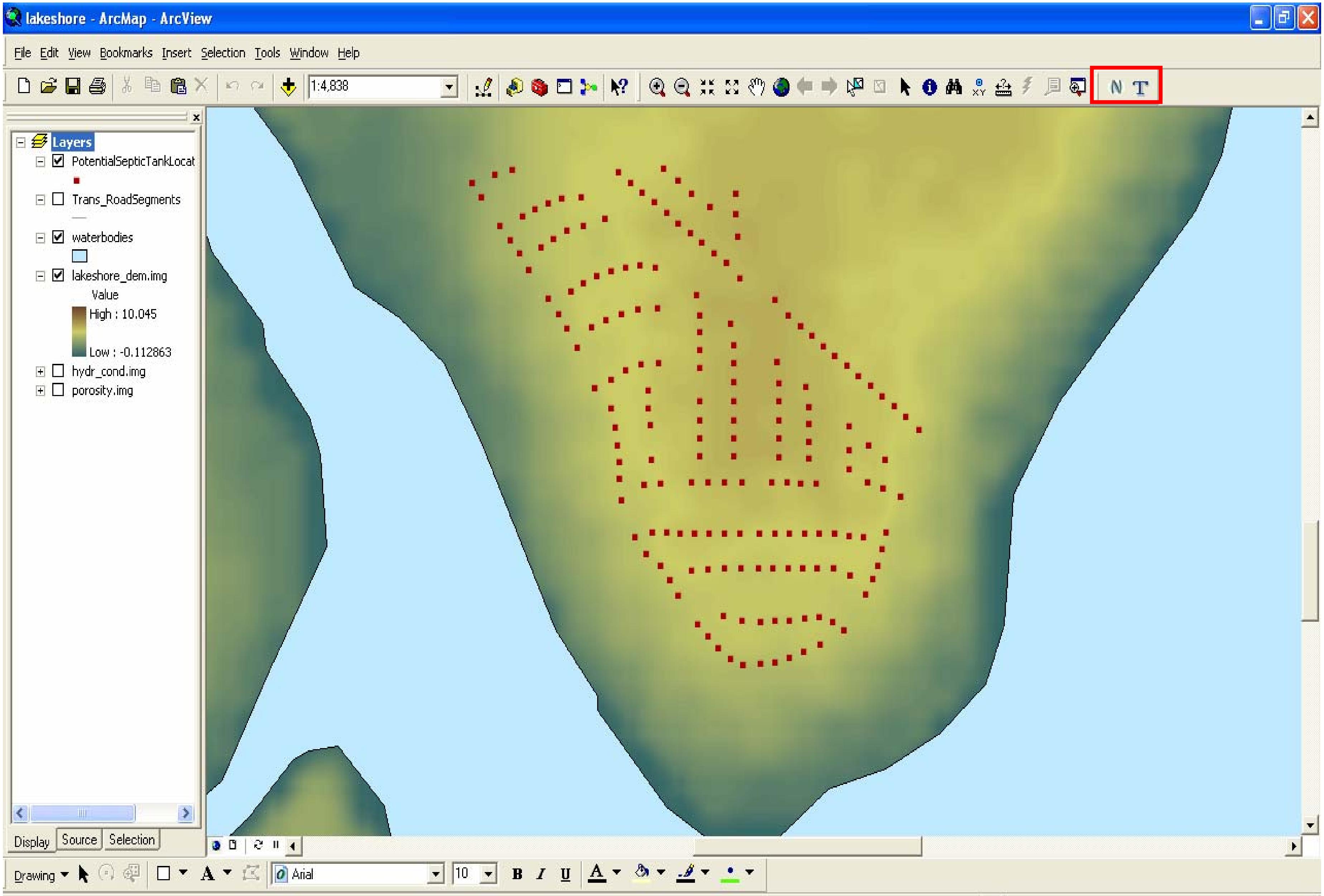
- Apply a smoothing algorithm (an averaging filter) to the DEM to obtain hydraulic head gradient

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

$*$ is the convolution operator.

- 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: $tan^{-1}\left(\frac{{}^{\partial h}/_{\partial x}}{{}^{\partial h}/_{\partial y}}\right)$

ArcGIS-N


lakeshore - ArcMap - ArcView
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waterbodies
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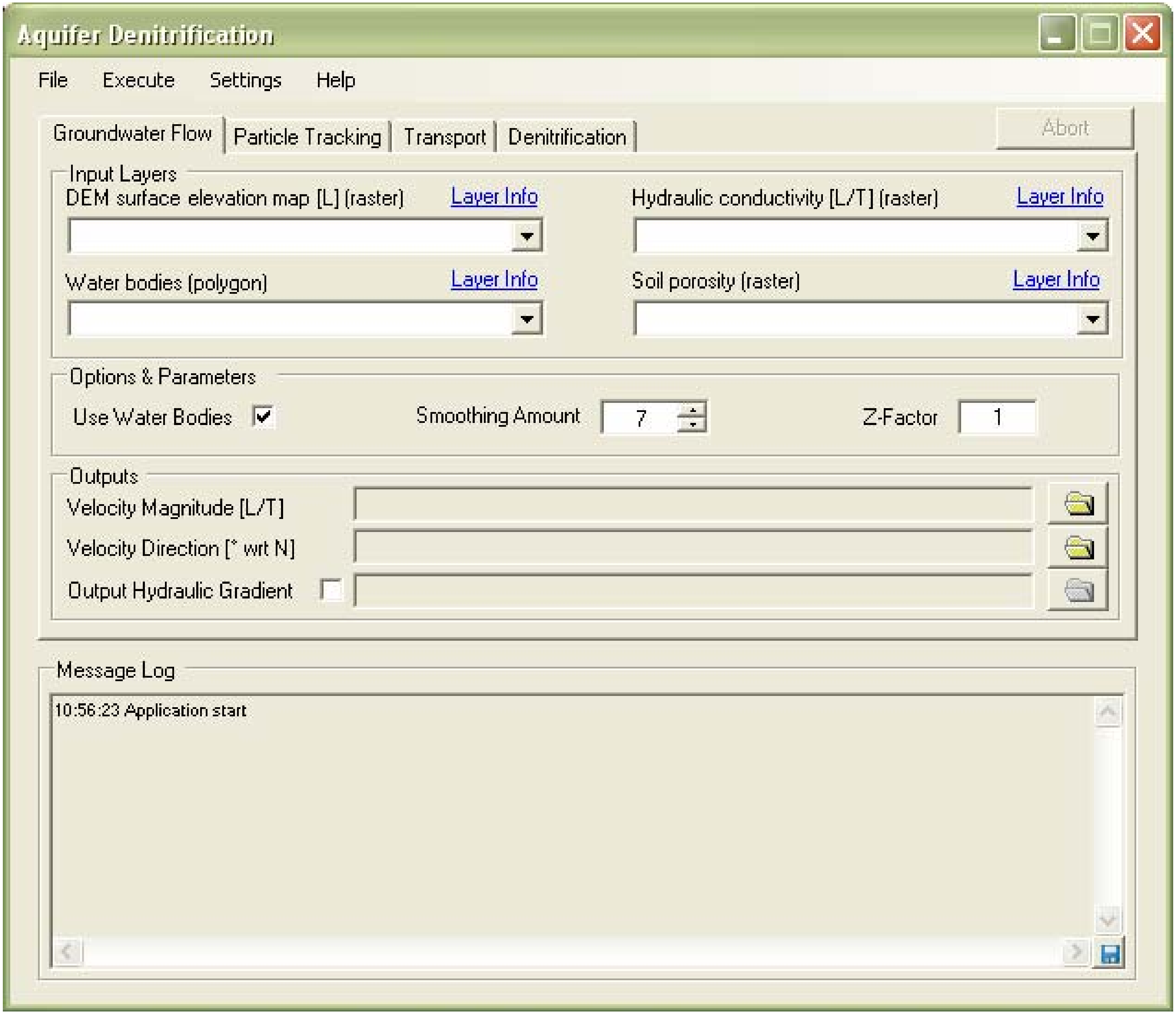
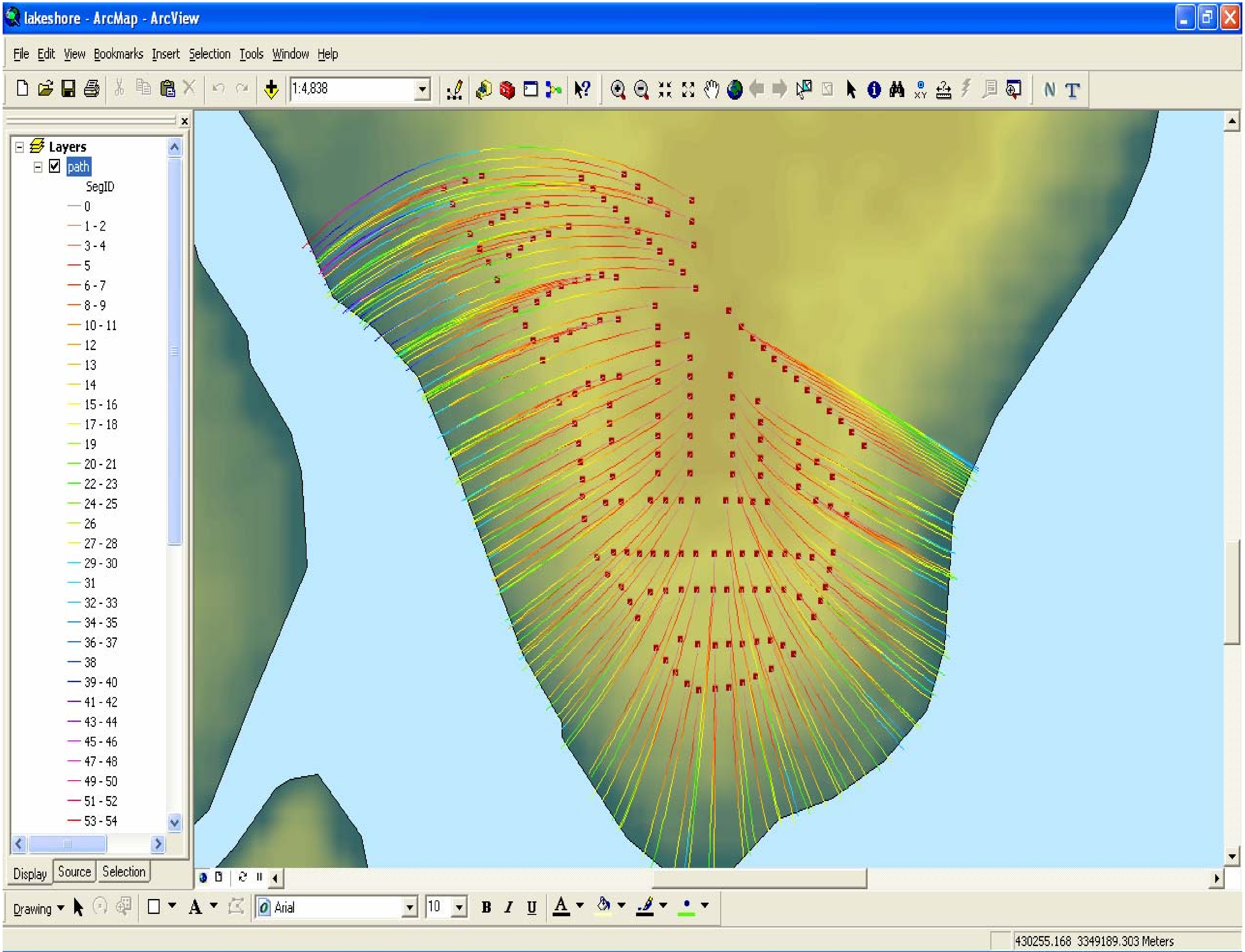

Aquifer Denitrification
File
Execute
Settings
Help
Groundwater Flow
Particle Tracking
Transport
Denitrification
Abort
Input Layers
DEM surface elevation map [L] (raster)
Layer Info
Hydraulic conductivity [L/T] (raster)
Layer Info
Water bodies (polygon)
Layer Info
Soil porosity (raster)
Layer Info
Options & Parameters
Use Water Bodies
Smoothing Amount
7
Z-Factor
1
Outputs
Velocity Magnitude [L/T]
Velocity Direction [° wrt N]
Output Hydraulic Gradient
Message Log
10:56:23 Application start


lakeshore - ArcMap - ArcView
File Edit View Bookmarks Insert Selection Tools Window Help
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Layers
path
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53 - 54
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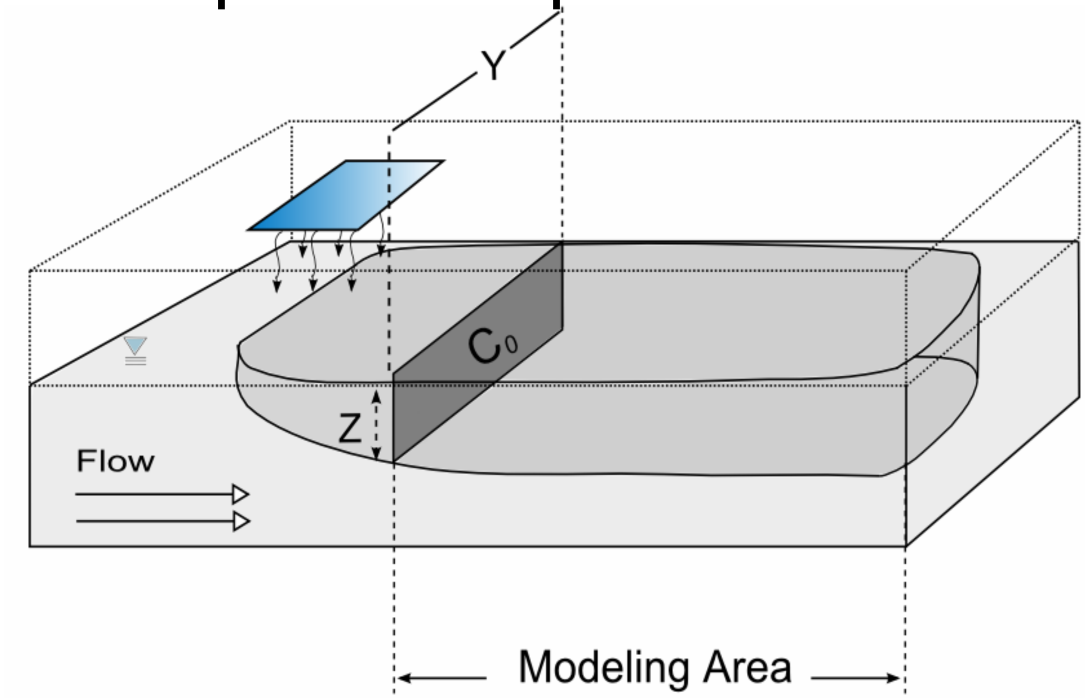
Transport

Use a steady-state, 2-D version of the Domenico solution to reduce memory requirements and increases computation speed



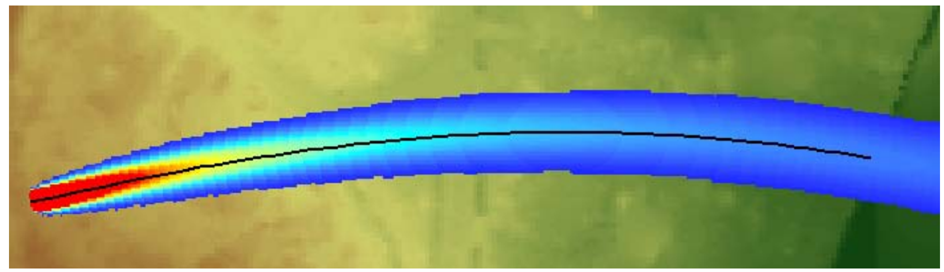
$$C(x,y,t=\infty) = \frac{C_0}{2} F_1(x,t=\infty) F_2(y,x)$$

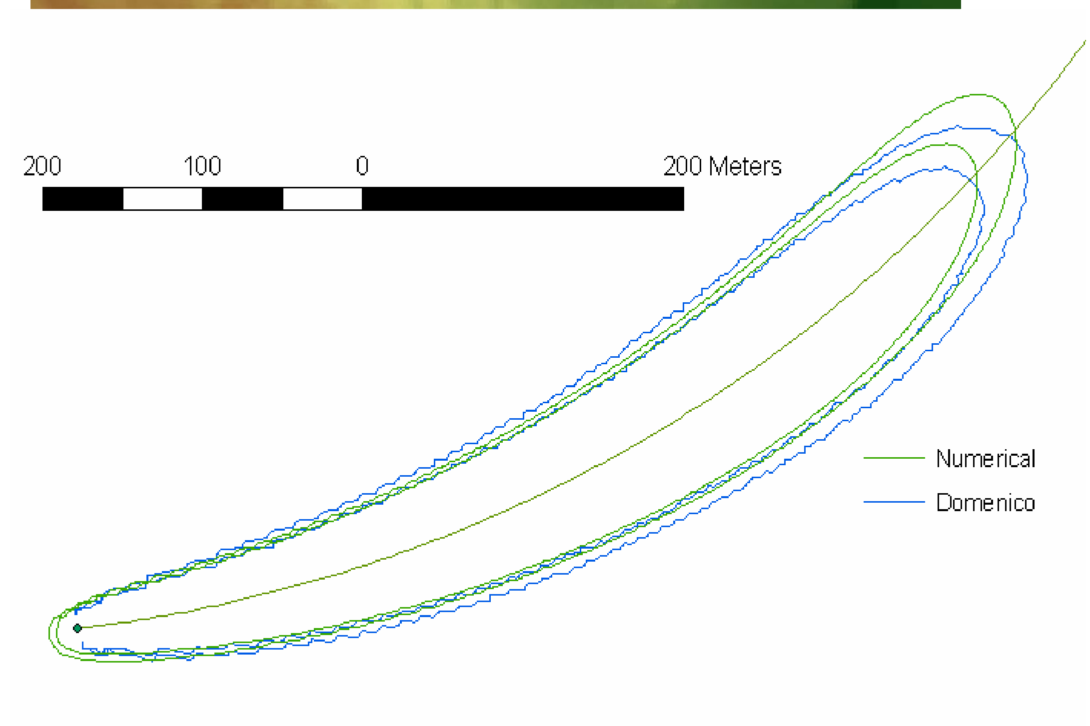
$$F_1(x,\infty) = exp\left[\frac{x}{2\alpha_x}\left(1-\sqrt{1+\frac{4k\alpha_x}{v}}\right)\right]$$

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

Transport

- Domenico solution considers uniform flow, i.e., straight flow paths

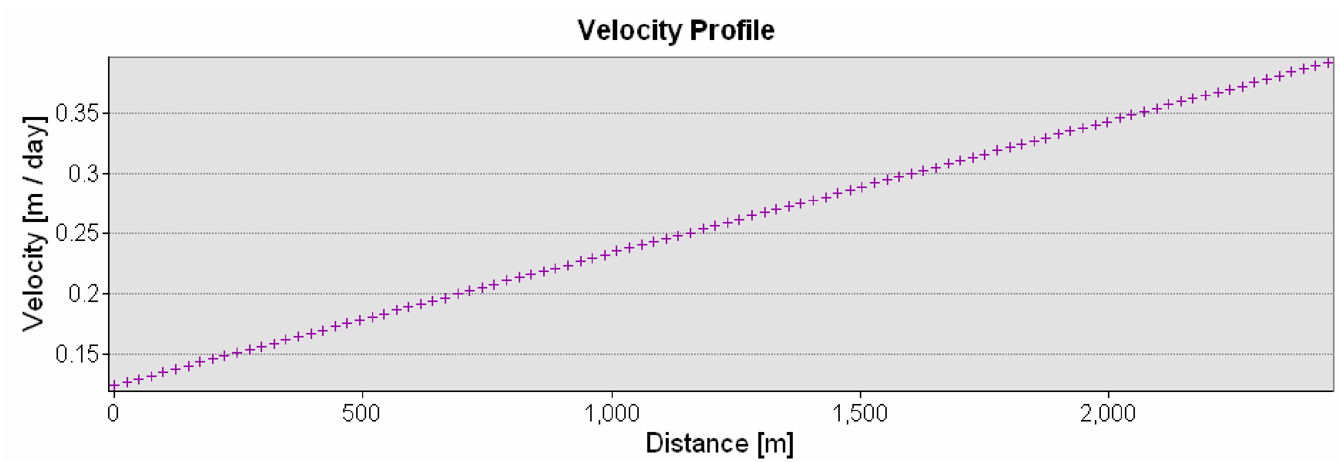


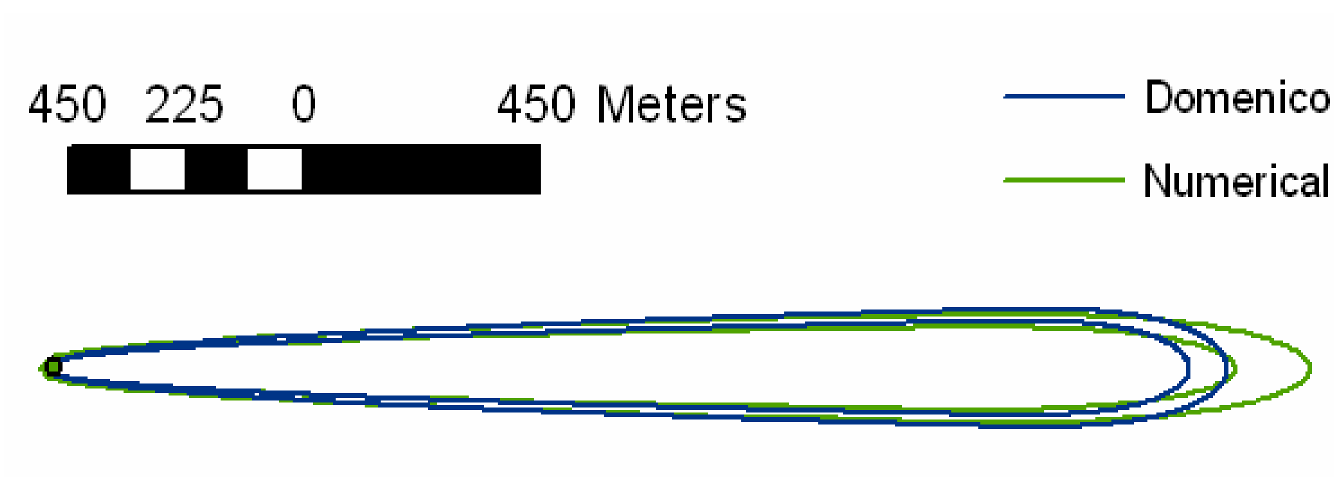


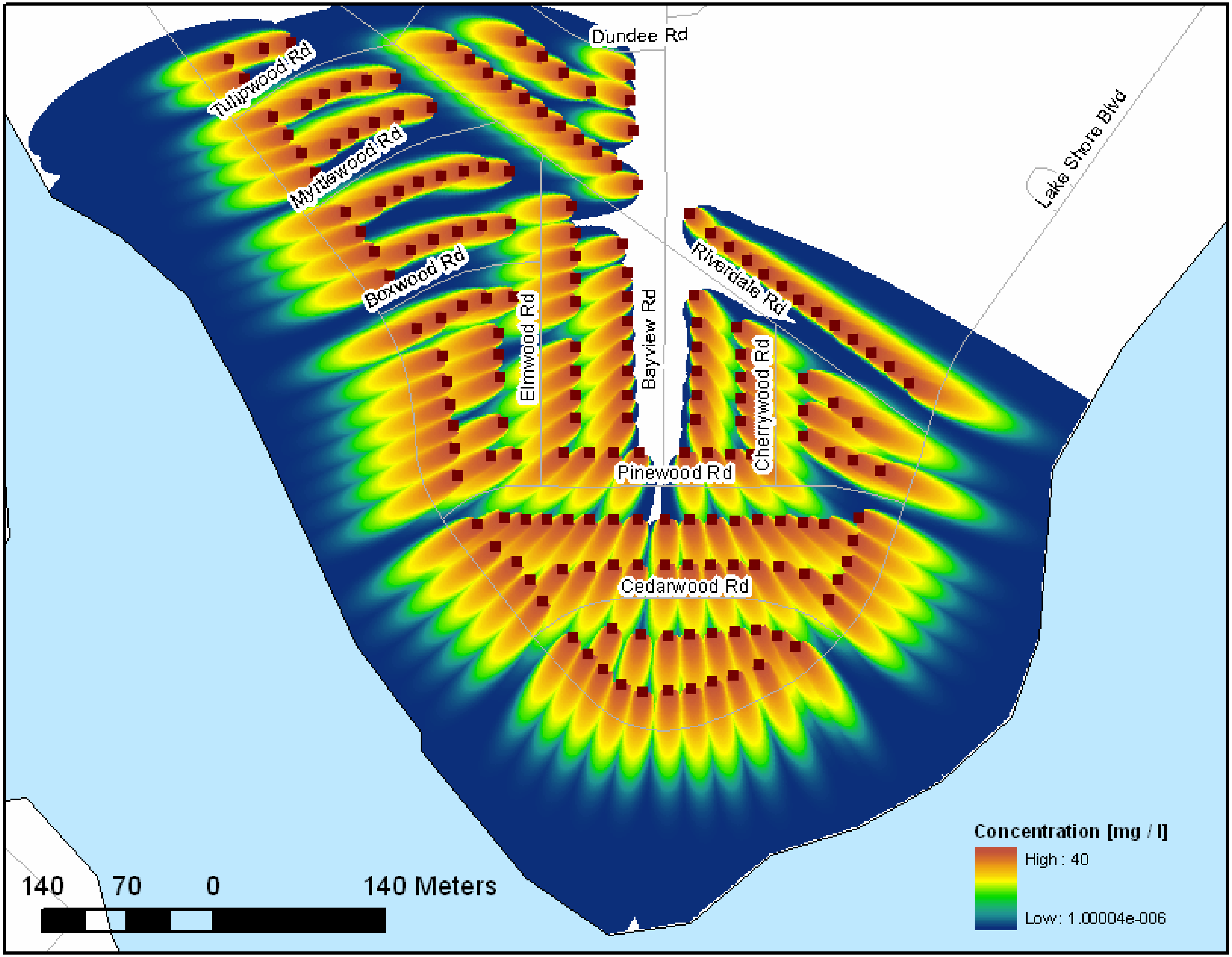
- Plumes are mapped to curved flow paths using a user-selectable transformation
- Velocity is a constant along flow path

Synthetic Tests

Effect of velocity averaging





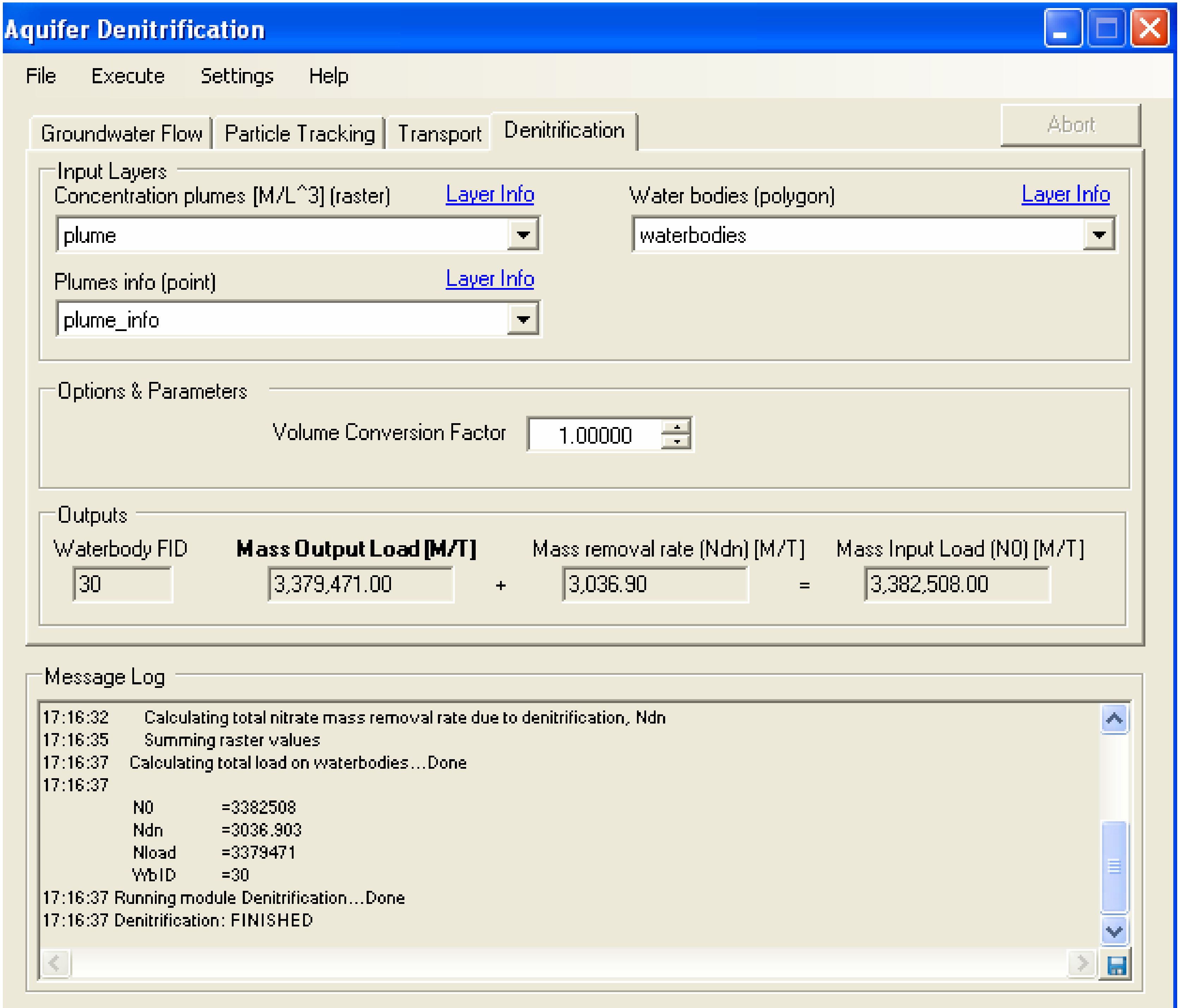

Dundee Rd
Tulipwood Rd
Myrtlewood Rd
Boxwood Rd
Elmwood Rd
Bayview Rd
Riverdale Rd
Cherrywood Rd
Lake Shore Blvd
Pinewood Rd
Cedarwood Rd
140 70 0 140 Meters
Concentration [mg / l]
High : 40
Low: 1.00004e-006

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:

Nitrate Load = Mass Rate In – Mass Rate Out

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



Aquifer Denitrification
File
Execute
Settings
Help
Groundwater Flow
Particle Tracking
Transport
Denitrification
Abort
Input Layers
Concentration plumes [M/L^3] (raster)
Layer Info
plume
Water bodies (polygon)
Layer Info
waterbodies
Plumes info (point)
Layer Info
plume_info
Options & Parameters
Volume Conversion Factor
1.00000
Outputs
Waterbody FID
30
Mass Output Load [M/T]
3,379,471.00
+
Mass removal rate (Ndn) [M/T]
3,036.90
=
Mass Input Load (N0) [M/T]
3,382,508.00
Message Log
17:16:32 Calculating total nitrate mass removal rate due to denitrification, Ndn
17:16:35 Summing raster values
17:16:37 Calculating total load on waterbodies…Done
17:16:37
N0 =3382508
Ndn =3036.903
Nload =3379471
WbID =30
17:16:37 Running module Denitrification…Done
17:16:37 Denitrification: FINISHED

Model Limitations

- Steady-state models
- Only consider surficial aquifer
- No recharge: mounding due to irrigation not considered.
- 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

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.

- This software can be applied to any contaminants, not limited to nitrate.