An Overview of ArcNLET and Associated Tools for Estimating Nitrogen Load from Septic Systems to Surface Water Bodies

Ming Ye (mye@fsu.edu)
Department of Scientific Computing
Florida State University

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Presentation to FDEP

Outlines

- ArcNLET: ArcGIS-based Nitrogen (Nitrate) Load Estimation Toolkit
- Introduction of ArcNLET
  - Rational of developing ArcNLET
  - Functions of ArcNLET and associated software
  - Simplification and limitations of ArcNLET
  - Data requirements of using ArcNLET
- New development for
  - Ammonium and nitrate transport modeling in vadose zone
  - Ammonium transport modeling in groundwater
- Applications of ArcNLET
- Suggestions and comments

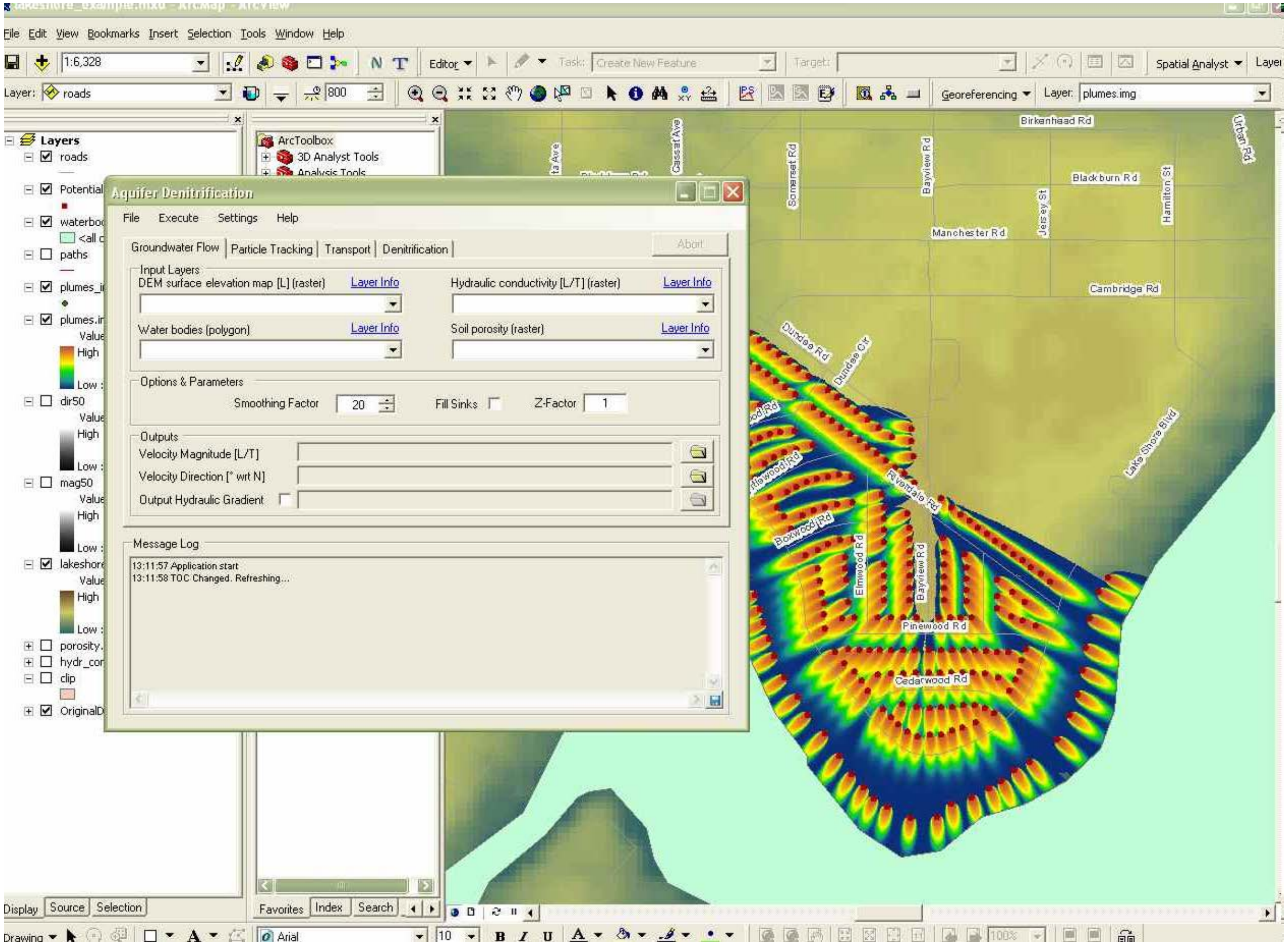
ArcNLET Project Team

- Contract Manager:
  - Rick Hicks (FDEP) (Richard.W.Hicks@dep.state.fl.us)
- Principal Investigator:
  - Ming Ye (FSU) (mye@fsu.edu)
  - Paul Lee (FDEP) (retired in 2012)
- Graduate Students:
  - Fernando Rios (Graduated in 2010)
  - Raoul Fernendes (Graduated in 2011)
  - Nathan Portraz (Left FSU in 2013 due to illness)
- Post-docs:
  - Liying Wang (2011-2012)
  - Huaiwei Sun (2012-2013)
  - Yan Zhu (2014-2015)
  - Mohammad Sayemuzzaman (2014-2015)

What is ArcNLET?

ArcGIS-based Nitrate Load Estimation Toolkit

- A simplified conceptual model of groundwater flow and solute transport
- Implementation as an ArcGIS extension
- Generate plumes of nitrate and ammonium separately
- Estimate loads of nitrate and ammonium separately



Input Layers

- DEM surface elevation map [L] (raster):
- Hydraulic conductivity [L/T] (raster):
- Water bodies (polygon):
- Soil porosity (raster):

Options & Parameters

- Smoothing Factor: 20
- Fill Sinks: ☐
- Z-Factor: 1

Outputs

- Velocity Magnitude [L/T]
- Velocity Direction [° wrt N]
- Output Hydraulic Gradient ☐

Message Log

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13:11:57 Application start
13:11:58 TOC Changed. Refreshing...
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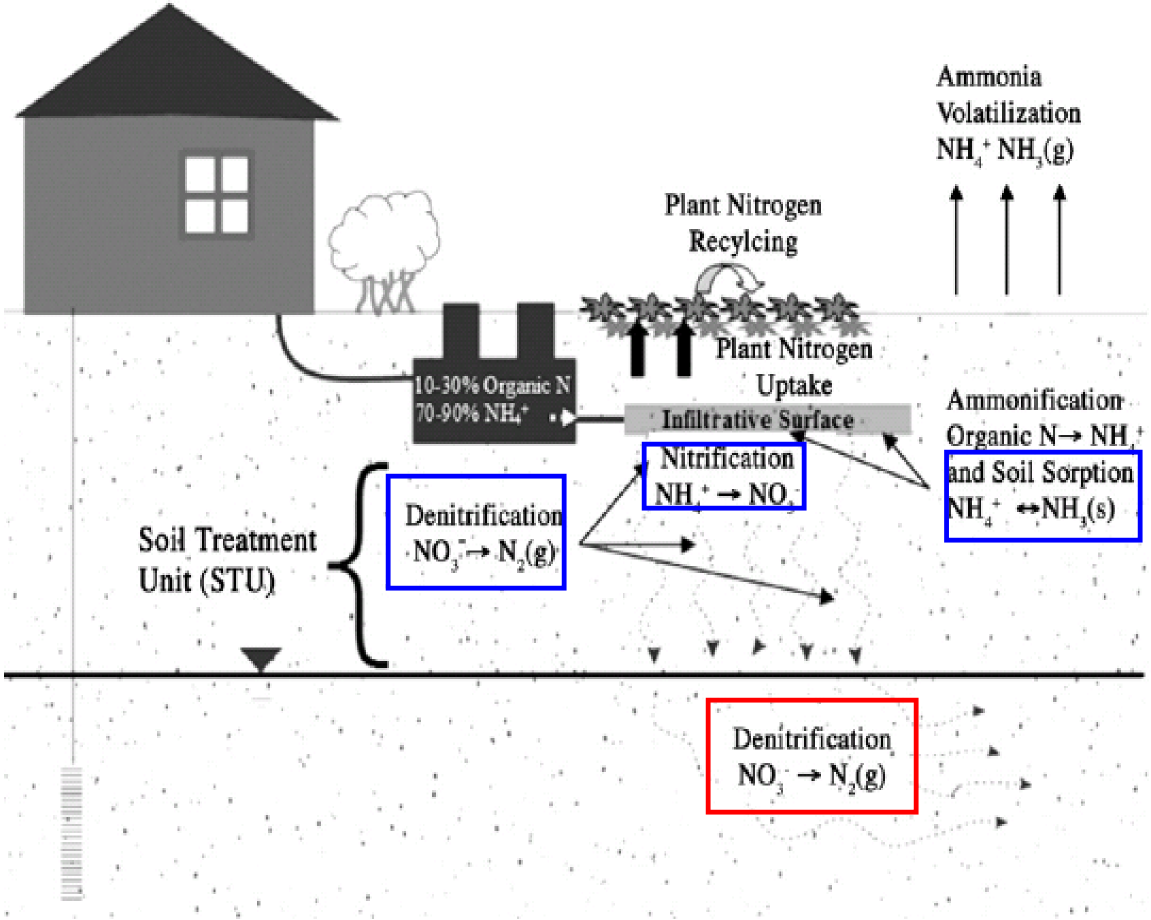
Compatible with ArcGIS 9.3, 10, and 10.1

ArcNLET Functions



From Heatwole and McCray (2007)

Vadose Zone Processes:

- Unsaturated flow (1-D)
- Ammonium and nitrate transport with sorption, nitrification, and denitrification

Groundwater Process:

- Groundwater flow (2-D)
- Ammonium and nitrate transport with sorption, nitrification, and denitrification

Surface processes for failed septic tanks have not been considered.

Why Developing ArcNLET?

- There is no suitable tool for estimating nitrate load to meet TMDL requirements and perform Nitrogen BMAP.
- Existing tools are either too simple or too complex.
- An example of simple model (an empirical model):
  - Nitrogen Load Model (NLM) by Valiela et al. (1997, 2000)
  - nitrogen load is evaluated as nitrogen released per person per year × people/house × number of houses × 60% not lost in septic tanks and leaching fields × 66% not lost in plumes × 65% not lost in aquifer.
  - While the coefficients can be adjusted for different sites based on literature data, field data, and best engineering judgment, NLM does not consider spatial variability of hydrogeological conditions and processes.
- An example of complex model (a mechanical model):
  - TOUGHREACT-N by Maggi et al. (2008): Simulate coupled processes of advective and diffusive nutrient transport, multiple microbial biomass dynamics, and equilibrium and kinetic chemical reactions in soil and groundwater
  - Difficult to set up the model for TMDL due to lack of data
  - Time consuming to run the execute

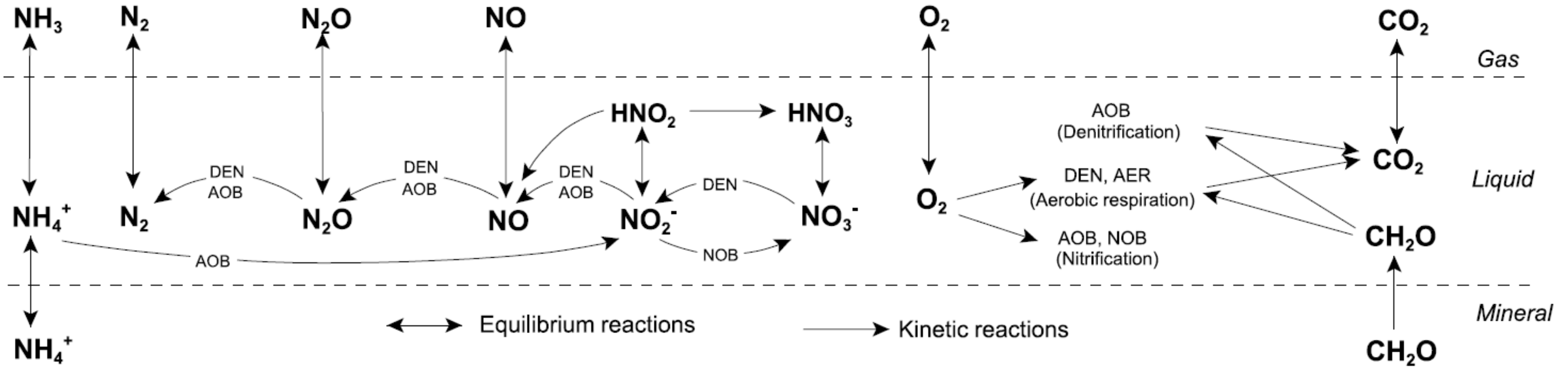


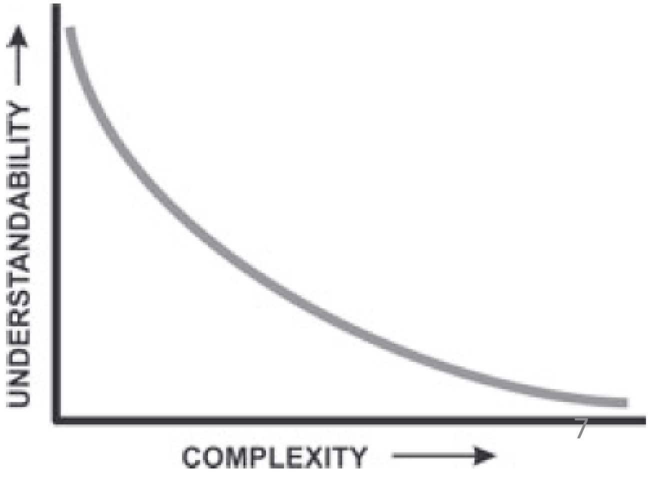
Table 1c. Biological and Nonbiological Reactions of Nitrification and Denitrification[a]

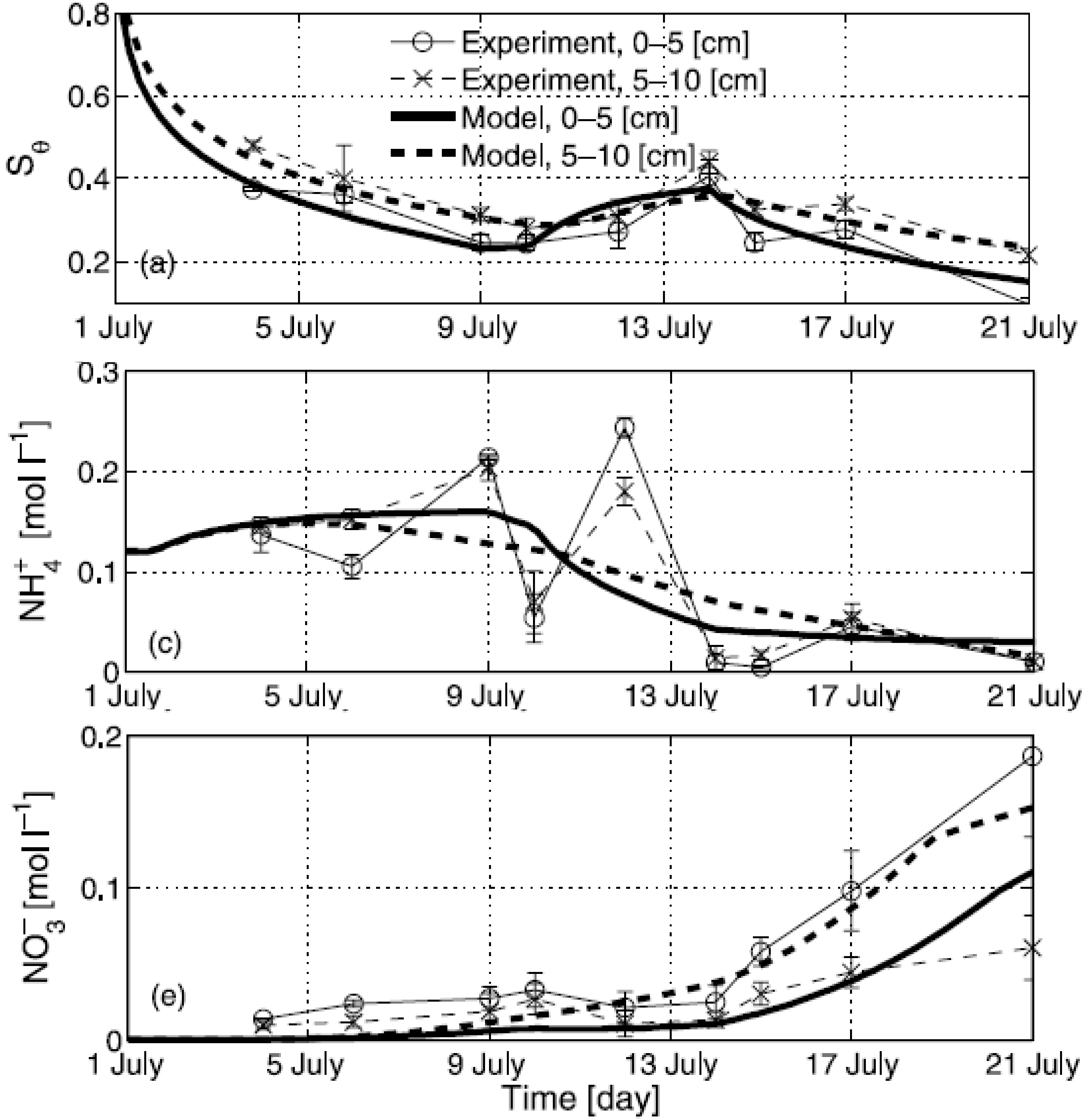
Biological	Mediator	$\widehat{\mu}^*$, s^{-1}	$K_C \cdot 10^{-5}$, mol L^{-1}	$K_e \cdot 10^{-5}$, mol L^{-1}	$K_I \cdot 10^{-5}$, mol L^{-1}	$Y \cdot 10^{-5}$ mg mol^{-1}
$NH_4^+ + 3/2\ O_2(aq) \rightarrow NO_2^- + H_2O + 2\ H^+$	AOB	$9.53 \cdot 10^{-6}$(b)	14,8(c)	2.41	0	20
$NO_2^- + 1/2\ O_2(aq) \rightarrow NO_3^-$	NOB	$1.23 \cdot 10^{-5}$(b)	14.8(c)	2.41	0	25
$2NO_3- + CH_2O \rightarrow + 2NO_2^- + CO_2(aq) + H_2O$	DEN	$2.14 \cdot 10^{-5}$(b)	10	11.3(c)	2.52	6.66
$4NO_2^- + CH_2O + 4H^+ \rightarrow 4NO(aq) + CO_2(aq) + 3H_2O$	DEN	$3.19 \cdot 10^{-6}$(b)	10	11.3(c)	2.52	6.66
	AOB	$9.82 \cdot 10^{-7}$(b)	10	11.3(c)	6.15	6.66
$8NO(aq) + 2CH_2O \rightarrow 4N_2O(aq) + 2CO_2(aq) + 2H_2O$	DEN	$8.97 \cdot 10^{-6}$(b)	10	11.3(c)	2.52	6.66
	AOB	$8.87 \cdot 10^{-5}$(b)	10	11.3(c)	6.15	6.66
$4N_2O(aq) + 2CH_2O \rightarrow 4N_2(aq) + 2CO_2(aq) + 2H_2O$	DEN	$1.23 \cdot 10^{-7}$(b)	10	11.3(c)	2.52	6.66
	AOB	$3.38 \cdot 10^{-8}$(b)	10	11.3(c)	6.15	6.66
$CH_2O + O_2(aq) \rightarrow CO_2(aq) + H_2O$	DEN	$2.66 \cdot 10^{-6}$(b)	10	11.3(c)	0	6.66
	AER	$4.49 \cdot 10^{-6}$(b)				

Nonbiological	$\widehat{\nu}$ mol L^{-1} s^{-1}
$3NO_2^- + H^+ \rightarrow H_2O + NO_3^- + 2NO(aq)$	$4.08 \cdot 10^{-4}$
% CH_2O production	$9.86 \cdot 10^{-6}$ *
% HCO_3^- production	$3.52 \cdot 10^{-8}$ *

$$\left.\frac{\partial C_{wi}}{\partial t}\right|_B = \sum_p \widehat{\mu_{ip}} M_{ip} B_{ip} - \sum_c \widehat{\mu_{ic}} M_{ic} B_{ic}$$

$$M_i = \frac{C_{wi}}{K_{C_{wi}} + C_{wi}} \frac{e_i}{K_{e_i} + e_i} \frac{K_{I_i}}{K_{I_i} + I_i} f(S_\theta) g(\mathrm{pH})$$



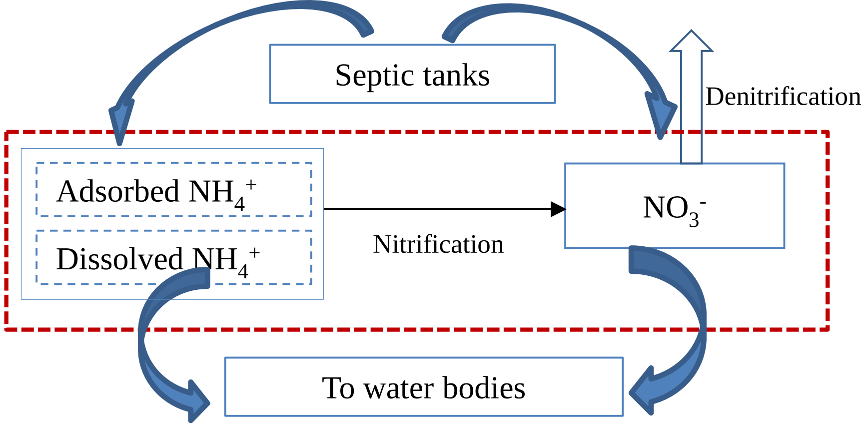


TOUGHREACT-N is still not complicated enough???

Why Developing ArcNLET?

- Develop a simplified model that
  - Considers key hydrogeologic processes of groundwater flow and nitrogen fate and transport
  - Handles spatial variability of hydrogeological parameters and processes
  - Provides estimates of quantities needed for TMDL and BMAP
- Implement the model by developing a user-friendly ArcGIS extension to
  - Use ArcGIS functions to handle spatial variability during pre- and post-processing of ArcNLET modeling
  - Simulate flow and nitrogen fate and transport within the ArcGIS environment but invisible to users
  - Provide a management and planning tool for environmental management and regulation
- Disseminate the software and conduct technical transfer to FDEP staff and other interested parties.

Nitrogen transformation processes considered in ArcNLET for both vadose zone and groundwater



Septic tanks

Denitrification

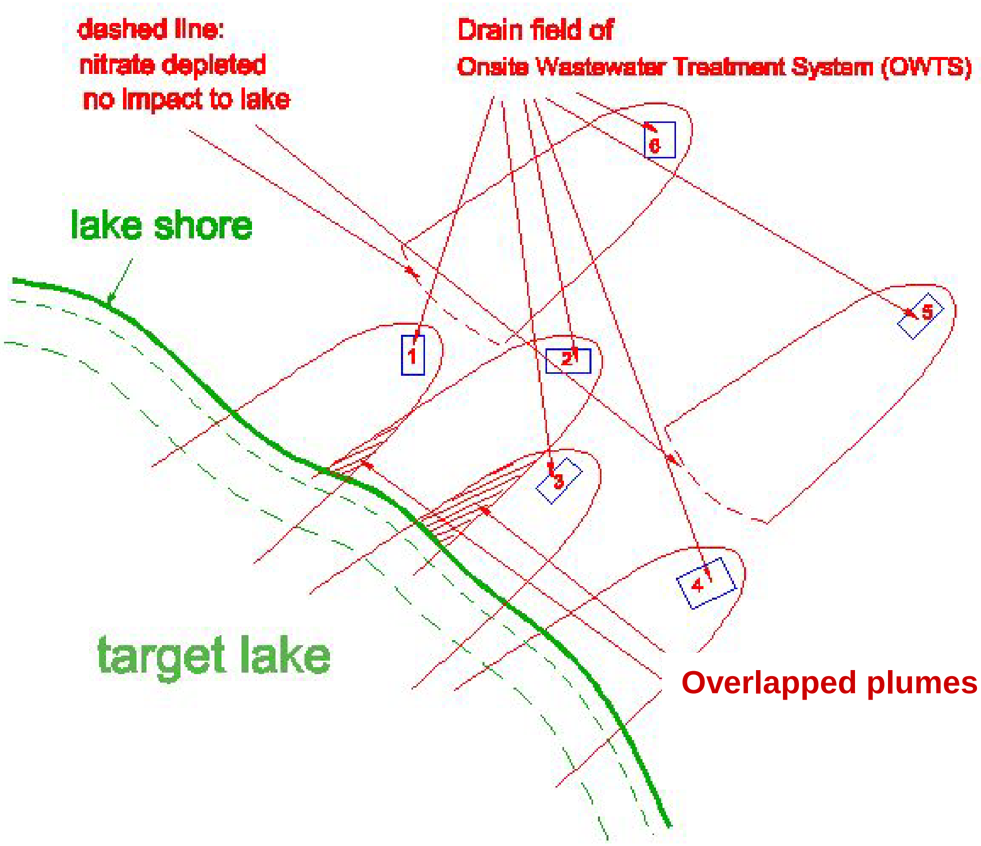
Adsorbed NH_4^+

Dissolved NH_4^+

Nitrification

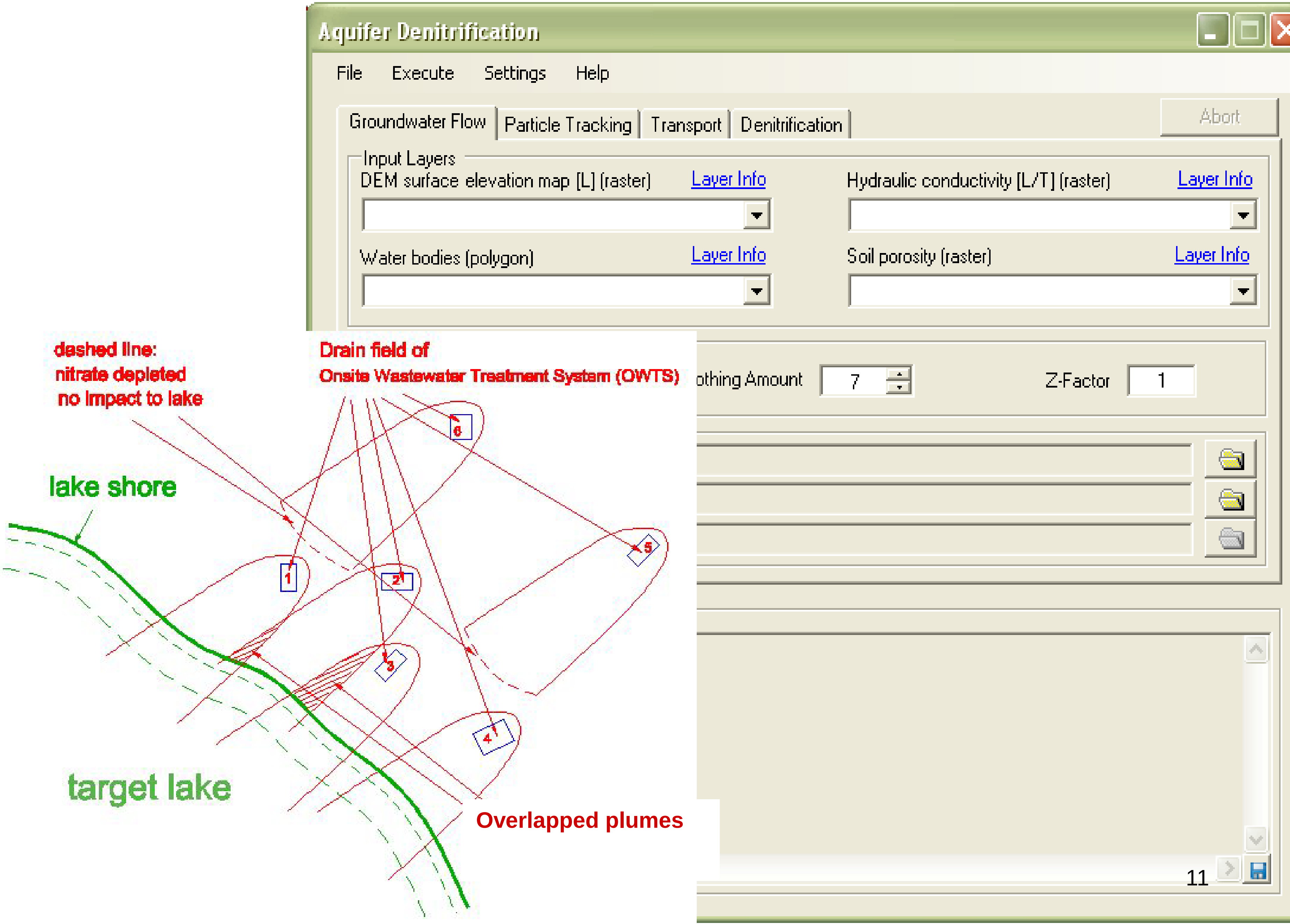
NO_3^-

To water bodies



- ***Groundwater flow model*** to estimate
  - flow path
  - flow velocity
  - travel time
- ***Nitrate transport model*** to consider
  - Advection
  - Dispersion
  - Denitrification
- ***Load estimation model*** to estimate nitrate load

ArcNLET Functions: Graphic User Interface

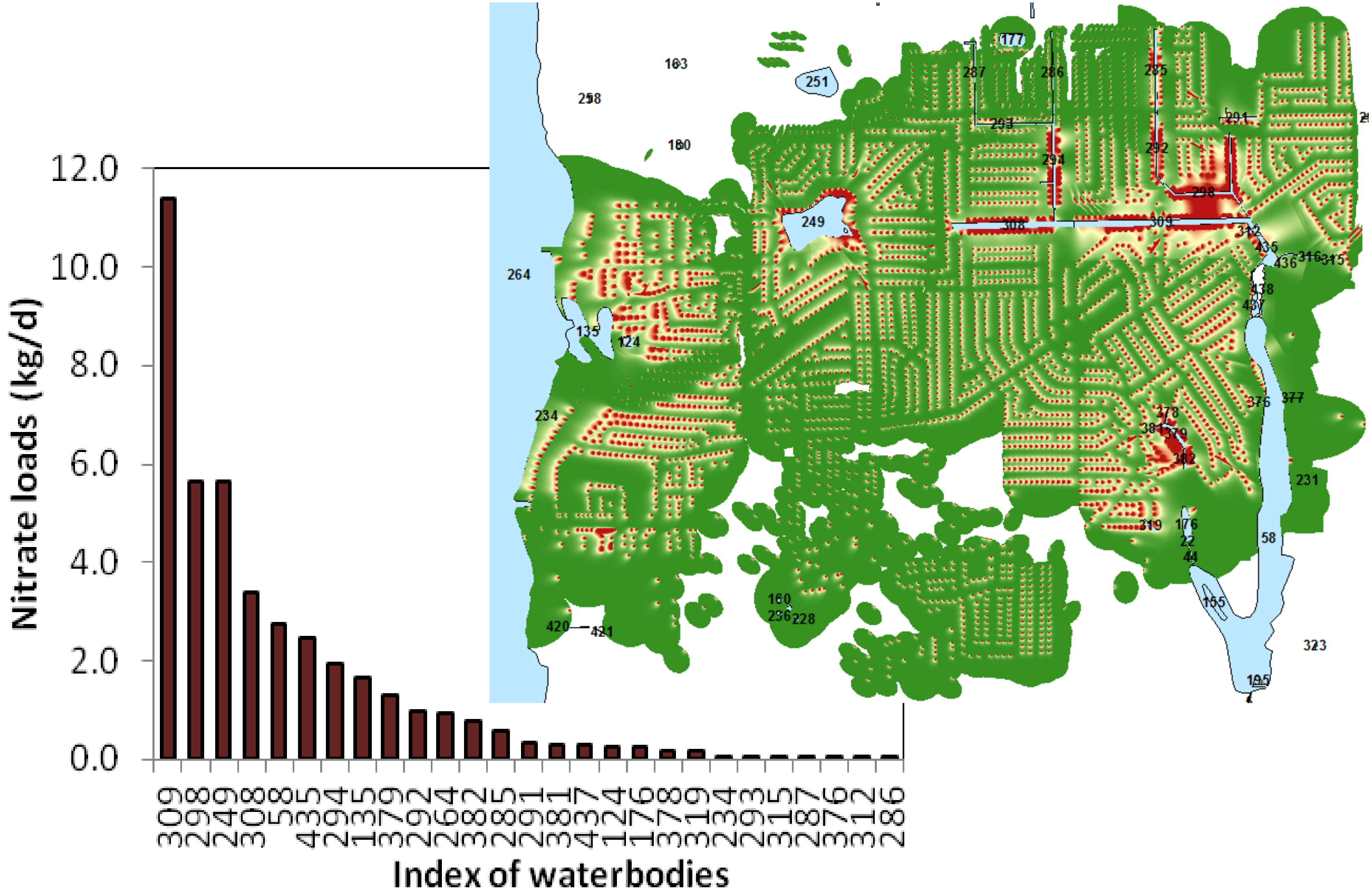


othing Amount 7

Z-Factor 1

Overlapped plumes

Illustration of simulated nitrate plumes and nitrate load



Software Download and Reference

- ArcNLET: http://people.sc.fsu.edu/~mye/ArcNLET
- Peer-reviewed journal articles:
  - Rios, J.F. (*student*), M. Ye, L. Wang, P.Z. Lee, H. Davis, and R.W. Hicks (2013), ArcNLET: A GIS-based software to simulate groundwater nitrate load from septic systems to surface water bodies, *Computers and Geosciences*, 52, 108-116, 10.1016/j.cageo.2012.10.003.
  - Wang, L. (*post-doc*), M. Ye, J.F. Rios, R. Fernandes, P.Z. Lee, and R.W. Hicks (2013), Estimation of nitrate load from septic systems to surface water bodies using an ArcGIS-based software, *Environmental Earth Sciences*, DOI 10.1007/s12665-013-2283-5.
  - Wang, L. (*post-doc*), M. Ye, P.Z. Lee, and R.W. Hicks (2013), Support of sustainable management of nitrogen contamination due to septic systems using numerical modeling methods, *Environment Systems and Decisions*, 33, 237-250, doi:10.1007/s10669-013-9445-6.
  - **Ye, M.**, H. Sun, and K. Hallas, Numerical Estimation of Nitrogen Load from Septic Systems to Surface Water Bodies for Nutrient Pollution Management in the St. Lucie River and Estuary Basin, Florida, *Environmental Earth Sciences*, Under Revision.
  - Zhu, Y. (*post-doc*), **M. Ye**, E. Roeder, R.W. Hicks, L. Shi, and J. Yang, Simulating Ammonium and Nitrate Reactive Transport from Septic Systems to Surface Water Bodies within ArcGIS Environments, Environmental Modelling & Software, Under Review.

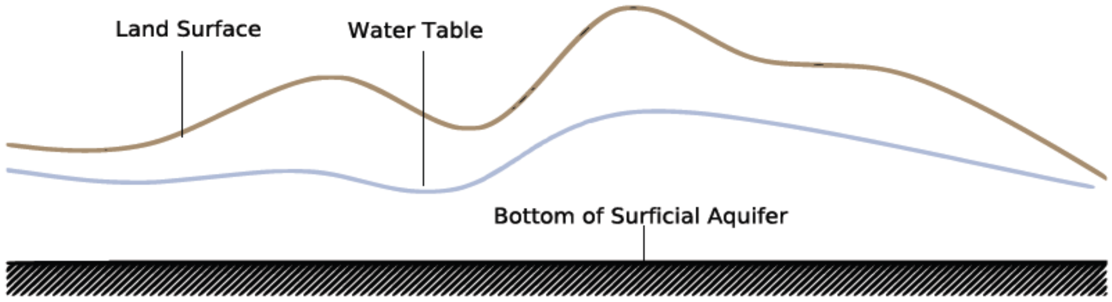
Simplifications and Limitations in Groundwater Flow Modeling

Simplifications:

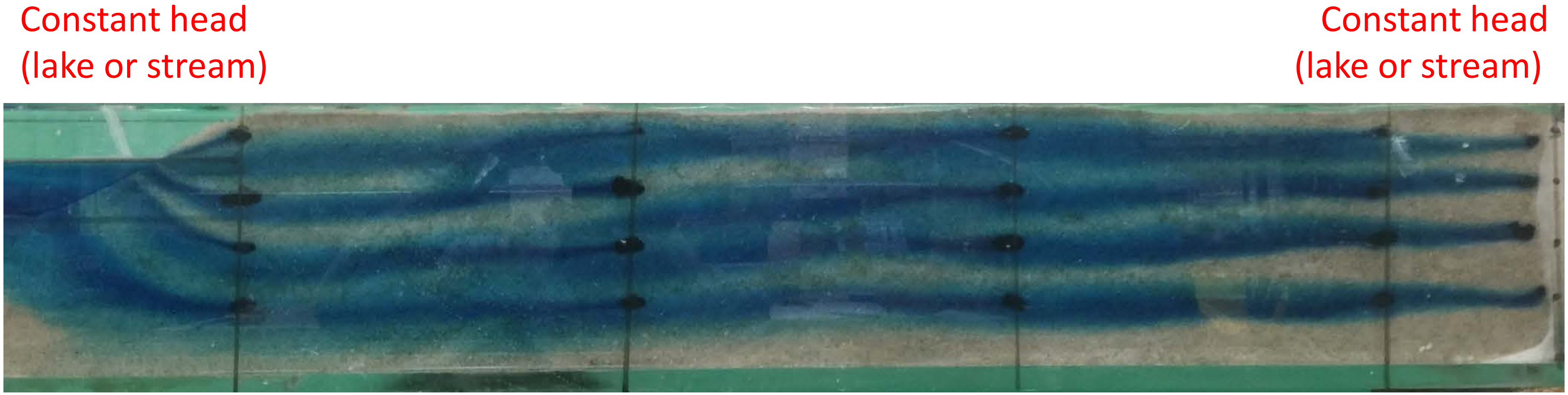
- Treat water table as subdued replica of topography (Process topographic to approximate shape of water table)
- Use Dupuit assumption to simulate 2-D, horizontal groundwater flow

Limitations:

- Steady-state flow
- 2-D flow instead of fully 3-D flow



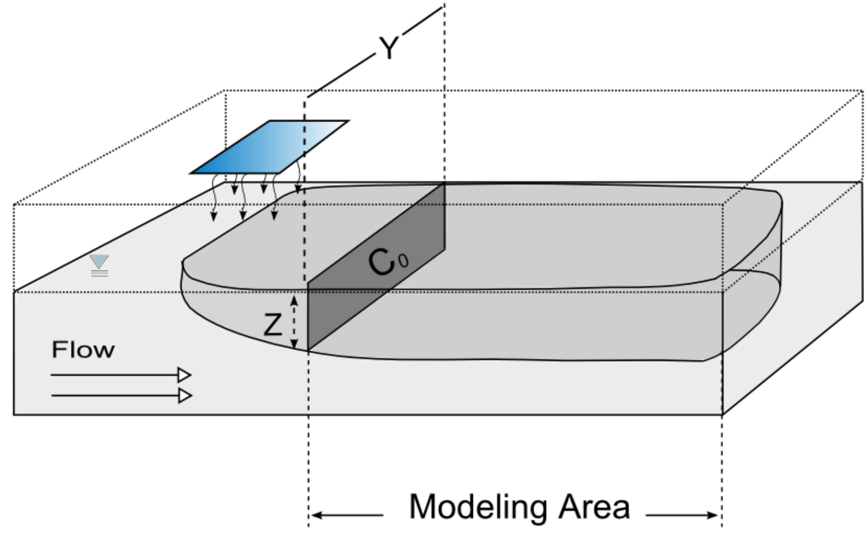
Laboratory Experiment to Illustrate Dupuit Assumption



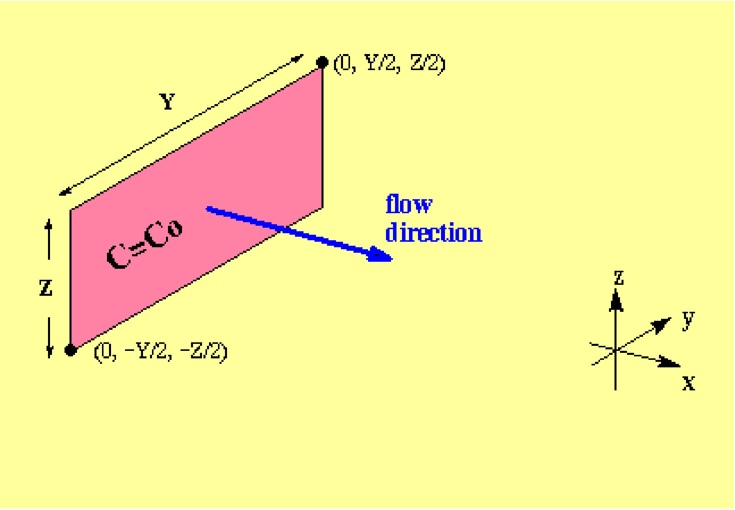
- Horizontal flow except near the lake
- Hydraulic head is constant along a vertical line except near the lake
- No need to simulate 3-D flow except near the lake
- Special treatment is needed near the lake.

Simplifications and Limitations in Nitrate Transport Modeling

EPA BIOCHLOR model



Domenico analytical solution



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

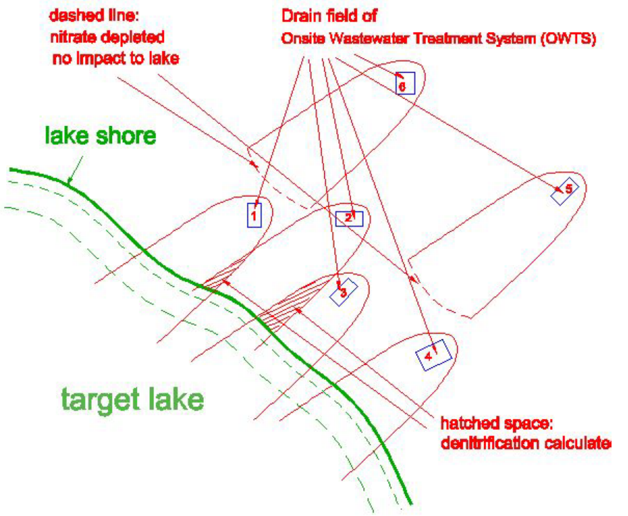
Denitrification

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

Simplifications and Limitations in Nitrate Transport Modeling

- Simplifications:
  - Analytical solution of transport model with uniform flow
  - Linear kinetic reaction for denitrification process
- Limitations:
  - Steady state model
  - Pseudo-3D model
  - Need a fudge factor near surface water bodies
  - Use of empirical or calibrated value of decay coefficient

Input Data for Running ArcNLET



All input data files are in ArcGIS format.

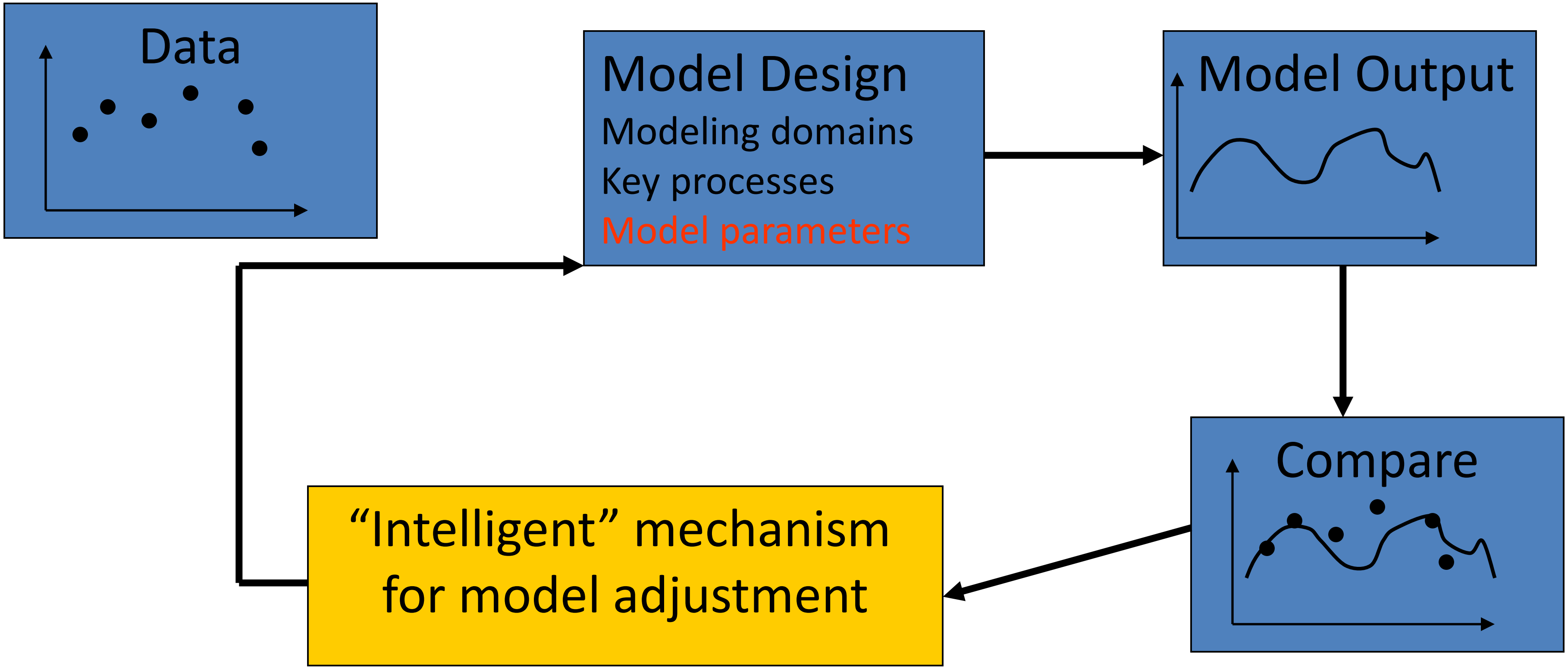
- Locations of water bodies
- Locations of septic tanks
- Topography (DEM: Digital Elevation Model): Process it to obtain water table
- Hydrogeological and transport parameters
  - Smoothing factor (used to process topography)
  - Hydraulic conductivity (from SSURGO)
  - Porosity (from SSURGO)
  - Dispersivity
  - Decay coefficient of denitrification
  - Source load and concentration

Input Data for ArcNLET
Site-Specific Modeling

- The ArcNLET model requires several model parameters that are largely unknown.
- The parameter values may be obtained from literature, but the values are not site-specific.
- A better way to determine the parameter values is model calibration to adjust the parameter values to match model simulations to site observations of system state variables such as hydraulic head and nitrate concentration.

Hydraulic heads
Ammonium concentrations
Nitrate concentrations

Manual Model Calibration: Trial and Error



Data

Model Design
Modeling domains
Key processes
Model parameters

Model Output

Compare

“Intelligent” mechanism for model adjustment

ArcNLET Modeling Procedure

For each site, whenever site-specific data are available,

- Compile historical data to understand groundwater flow and nitrogen transport at the modeling sites.
- Select/collect calibration data of hydraulic head and nitrogen concentration to estimate ArcNLET flow and transport model parameters.
- Calibrate the ArcNLET model.
- Simulate nitrogen transport at the modeling site, using the calibrated model.
- Estimate the nitrogen load.
- Conduct Monte Carlo simulation to quantify uncertainty in the load estimates due to uncertainty in model parameters.

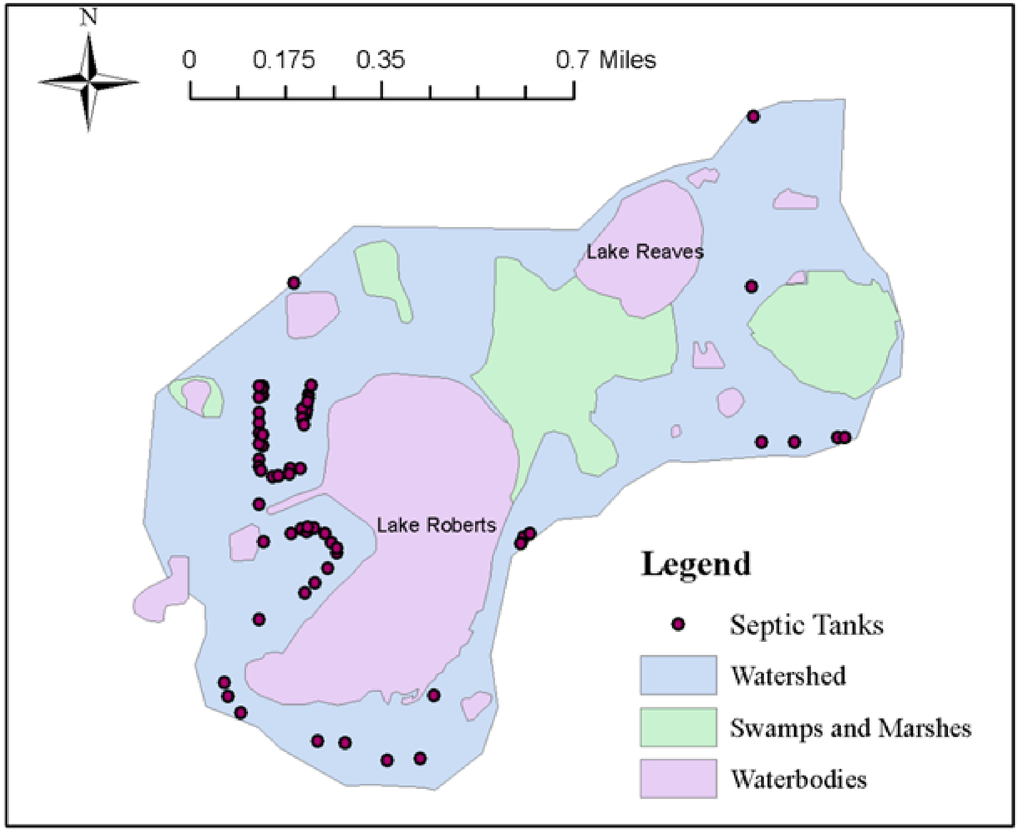
Requirements on Potential Users

- The GUI make it relatively easy for people with little experience in analyzing groundwater transport problems to apply a solute-transport model to a field problem.
- **Users of ArcNLET need to have**
  - Basic knowledge of hydrogeology such as concepts of groundwater flow and solute transport
  - Intermediate level of ArcGIS skills for preparing input files and visualizing software output files
- The model (simple or complex) is not an end in itself, but a tool to organize one’s thinking and engineering judgment.
- **Interpretation and improvement of ArcNLET results require**
  - Fundamental understanding of groundwater flow and solute transport
  - Familiarity with site-specific information such as geology and hydrogeology
- A model or a software is not a magic box, and it cannot tell what we do not know.

ArcNLET Application

- ArcNLET for nitrate only
  - Jacksonville
  - St. Lucie River and Estuary Basin (Port St. Lucie, City of Stuart, and Martin County)
  - Lakes Marshall, Roberts, Weir, and Denham
- ArcNLET for both ammonium and nitrate
  - Jacksonville
  - Indian River County (on-going)

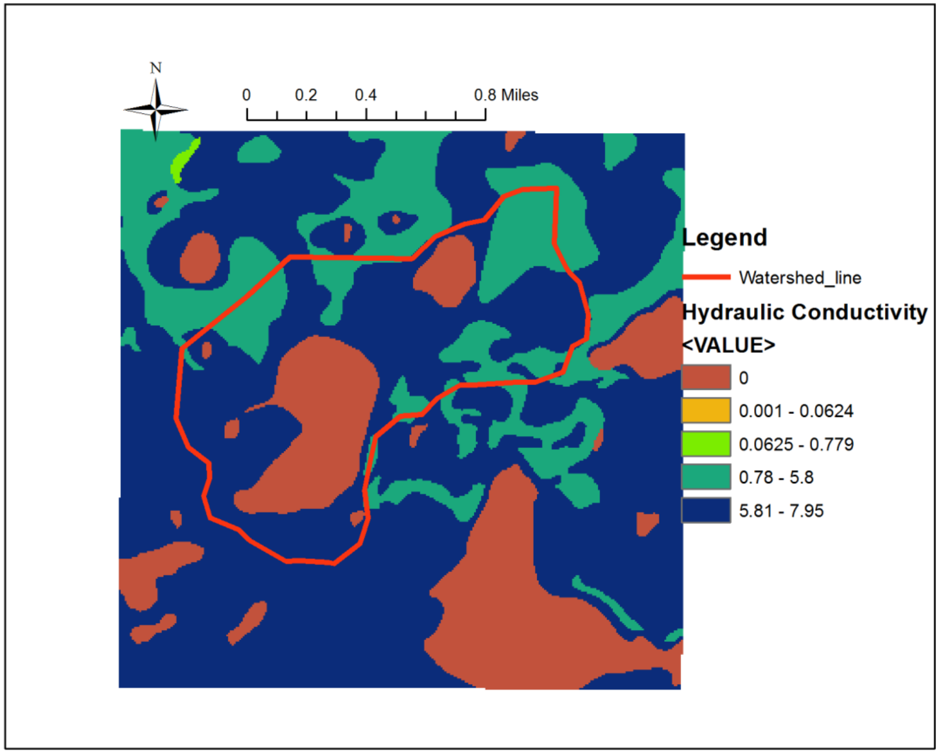
ArcNLET Modeling for Lake Roberts

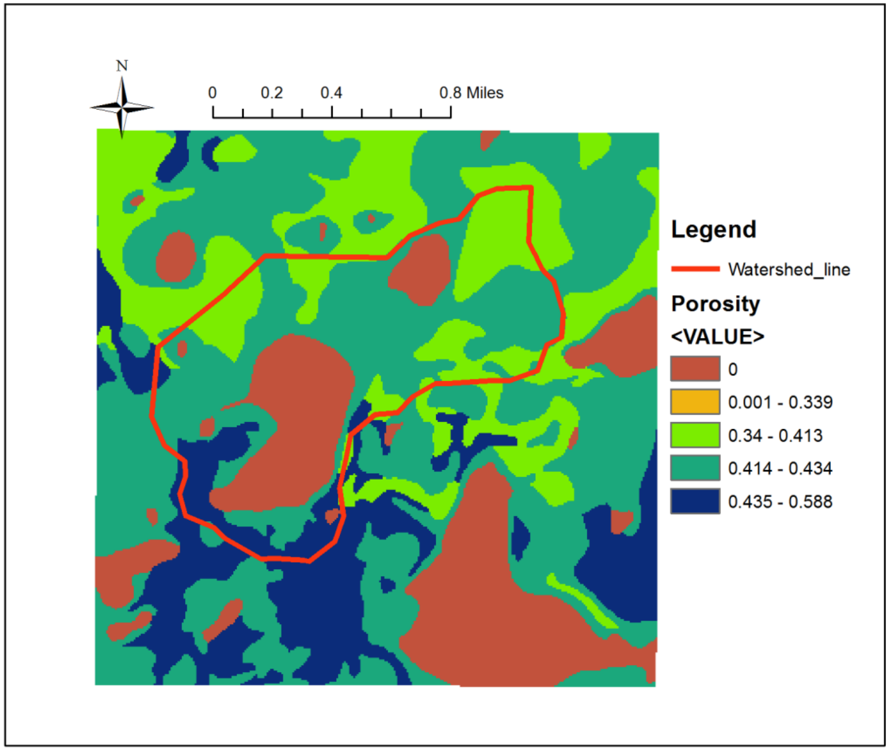


- Boundary of the watershed
- Locations of septic tanks, water bodies, and swamps and marshes
- Swamps and marshes are merged into water bodies later on for calculation of nitrogen load.

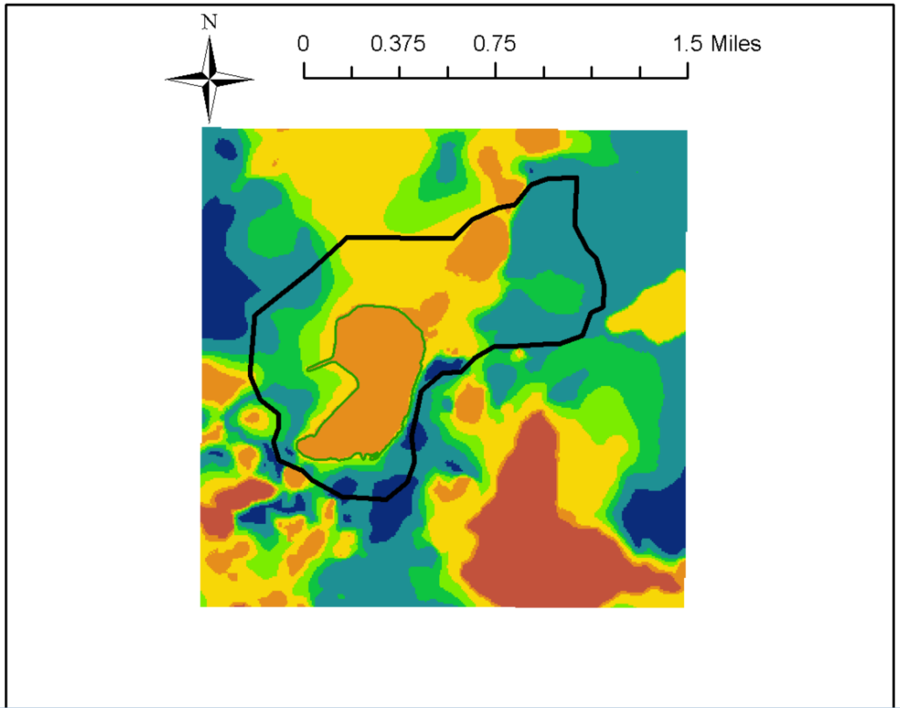
Hydraulic Conductivity and Porosity

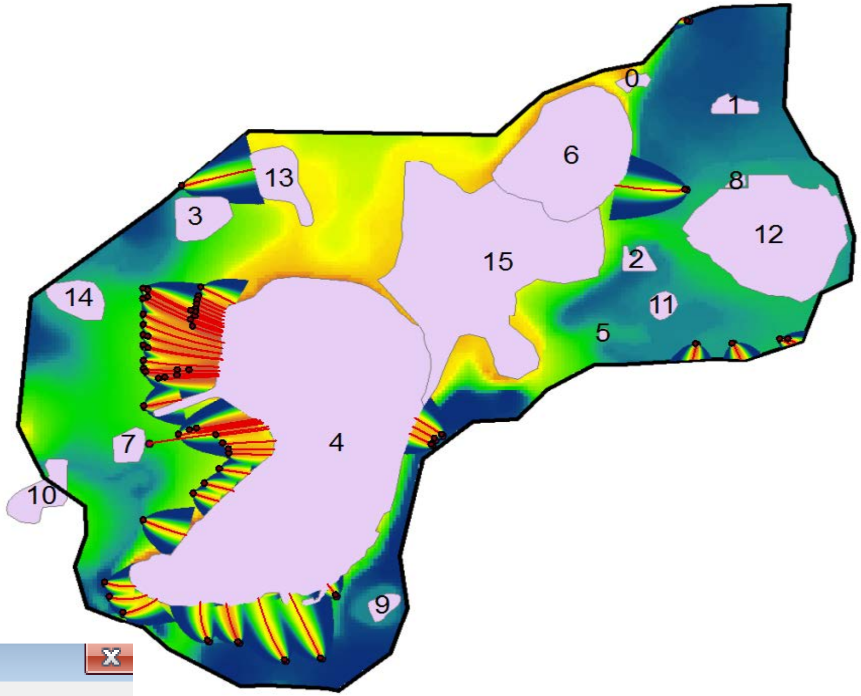
The spatial data are processes from the SSURGO database of USDA.

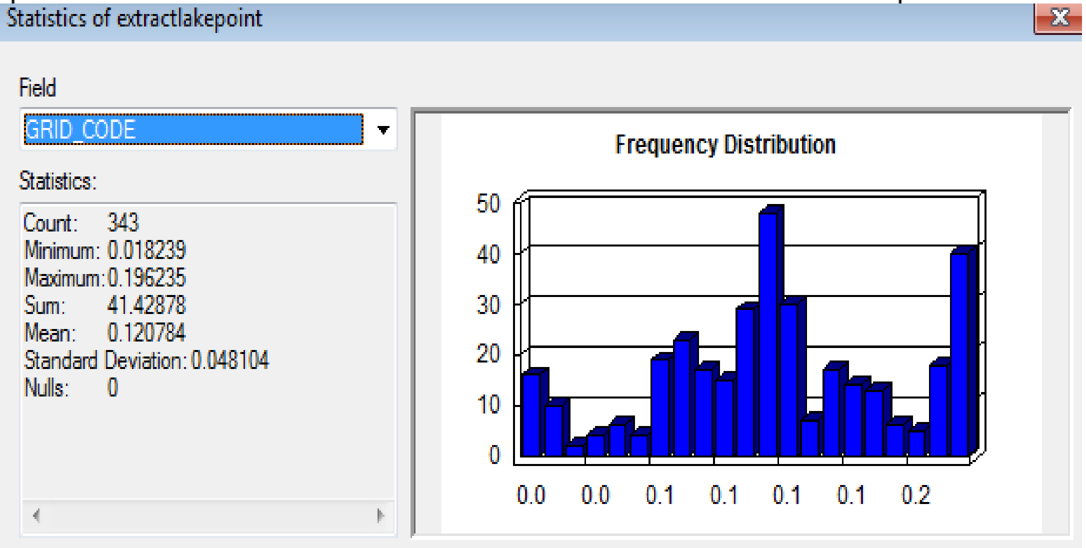




DEM and Smoothing







Statistics:

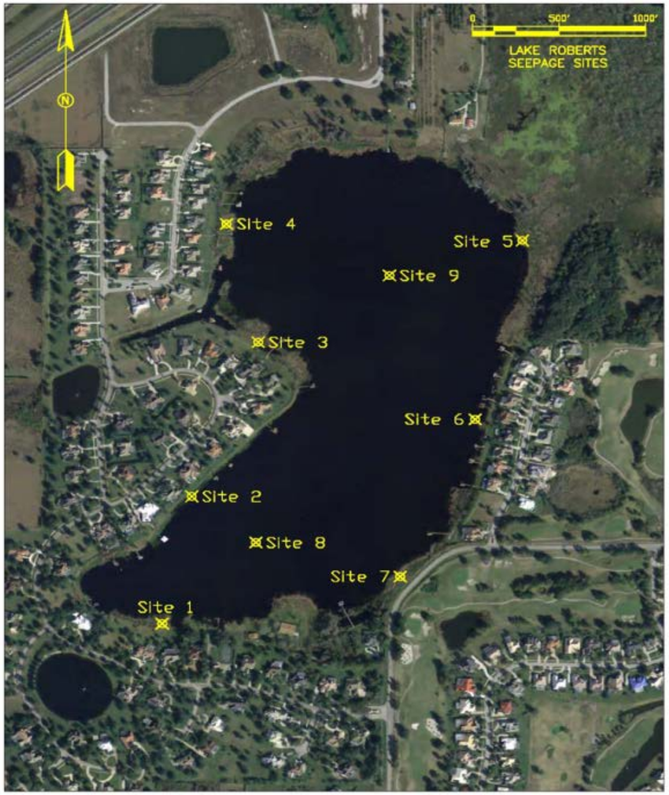
Count: 343
Minimum: 0.018239
Maximum: 0.196235
Sum: 41.42878
Mean: 0.120784
Standard Deviation: 0.048104
Nulls: 0

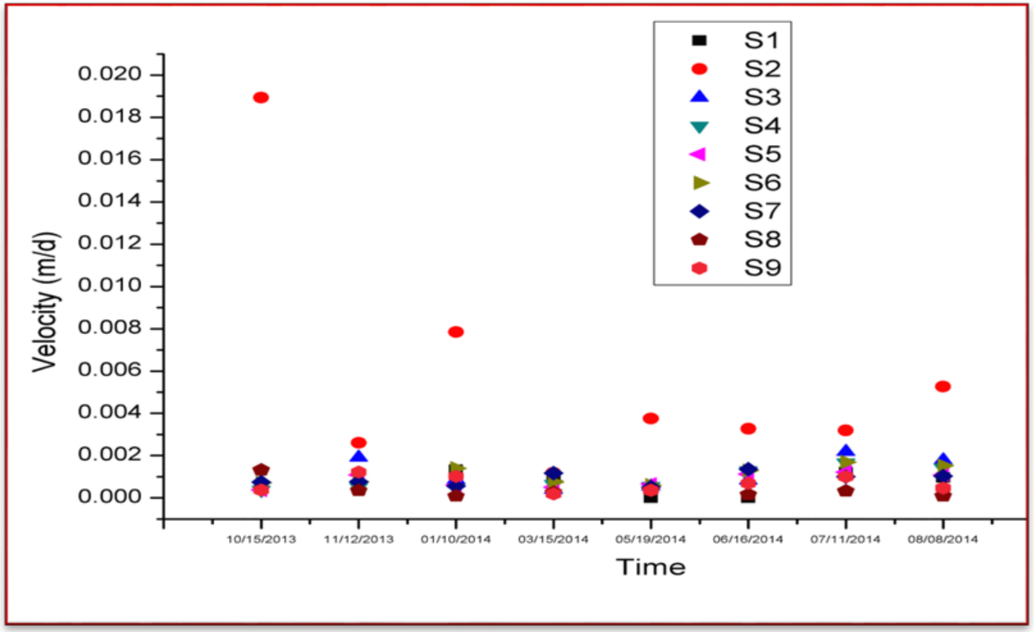
Statistics of simulated groundwater flow (m/d) to the lake using

- Smoothing factor of 50
- Hydraulic conductivity and porosity from SSURGO

Seepage Measurements

Calibration is needed!





Measured seepage rate: 0.00~0.019 m/d. Most are in the order of magnitude of 0.001 m/d.

Seepage velocities at the 9 measurement sites

Model Calibration: Hydraulic Conductivity

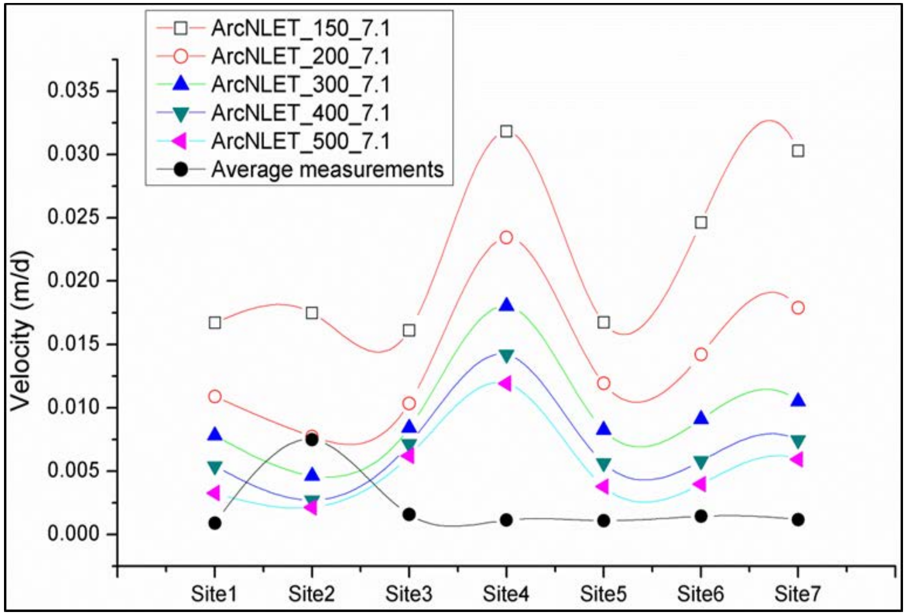
Model calibration to decrease

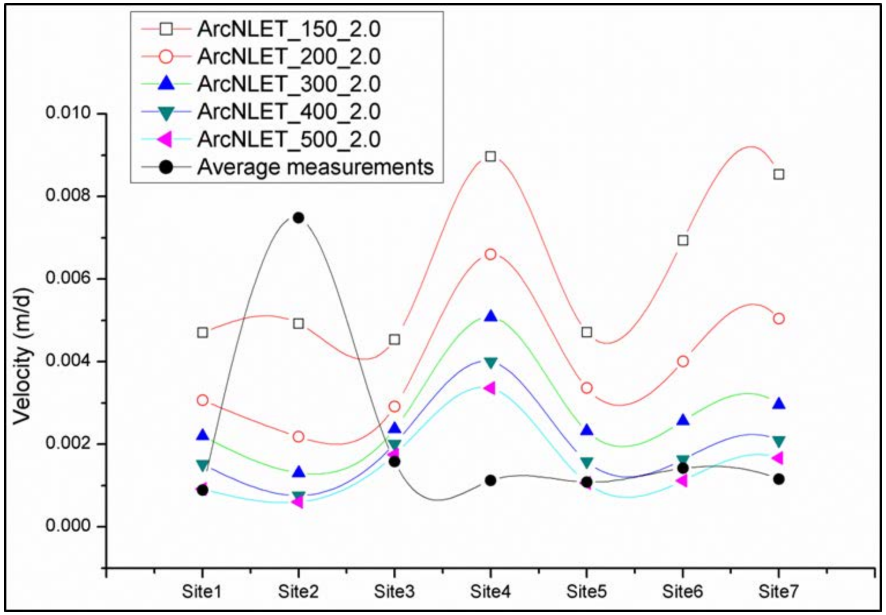
- **Hydraulic gradient and**
- **Hydraulic conductivity**

Darcy's law

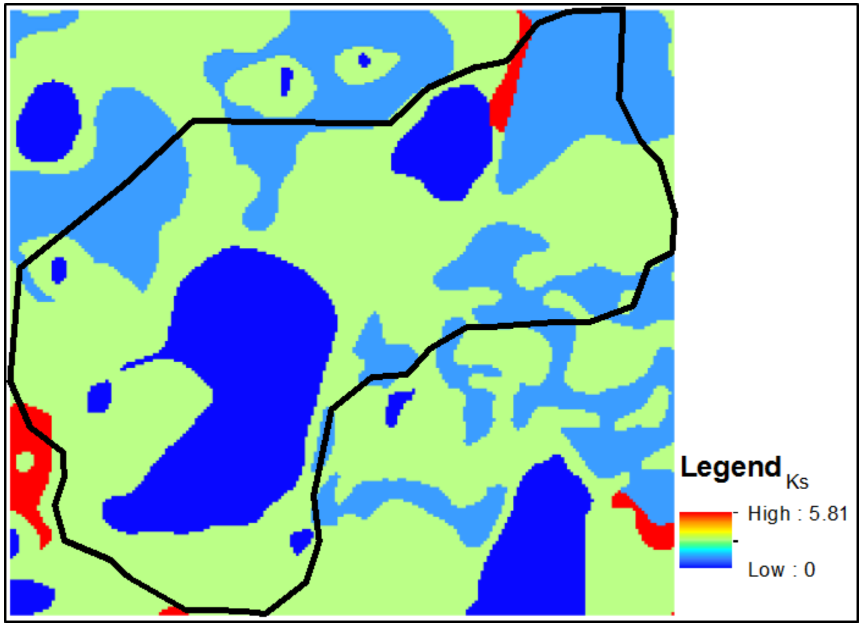
$$q_x = -K\frac{\partial h}{\partial x} \approx -K\frac{\partial z}{\partial x}$$

$$q_y = -K\frac{\partial h}{\partial y} \approx -K\frac{\partial z}{\partial y}$$

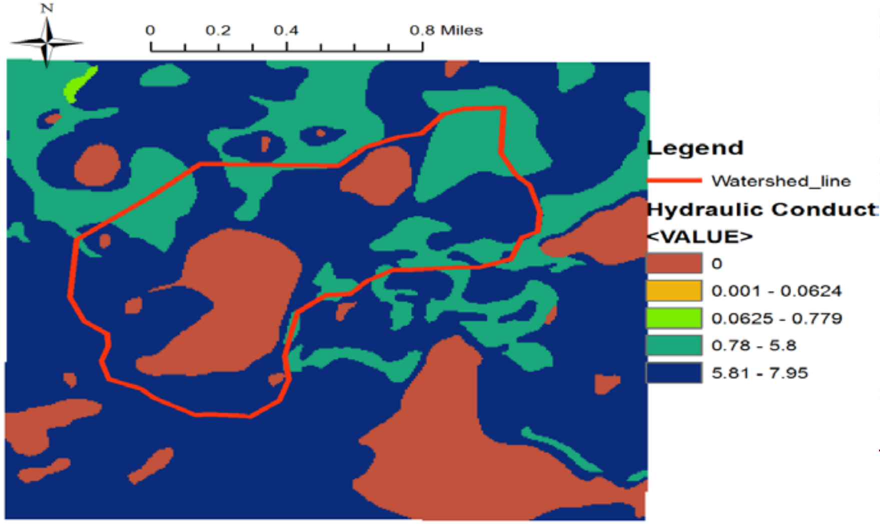


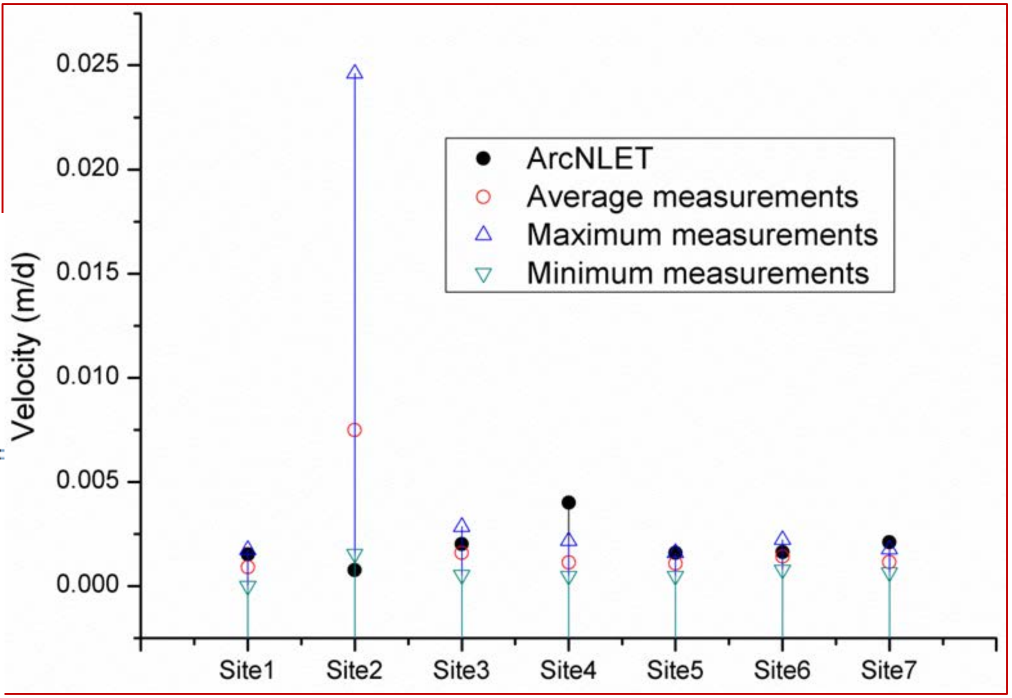


Calibration Results



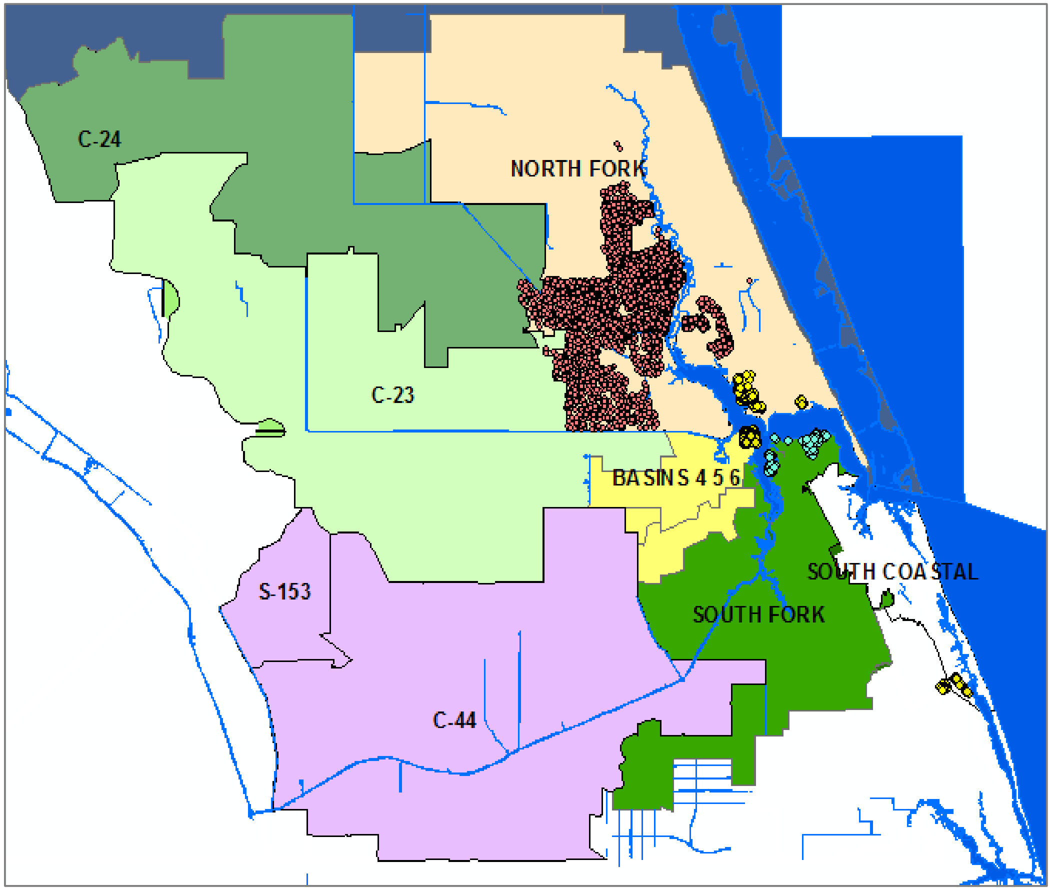
- Smoothing factor = 400
- For the sand zone, use K=2.0 m/d.
- Simulations can reasonably match the observations.





ArcNLET Modeling for St. Lucie

- Estimate nitrogen loads from removed septic systems to surface water bodies in the City of Port St. Lucie, City of Stuart, and Martin County located in the St. Lucie River and Estuary Basin
- The load estimates can be used to calculate credit for septic tank phase out projects in support of the on-going Basin Management Action Plan (BMAP).



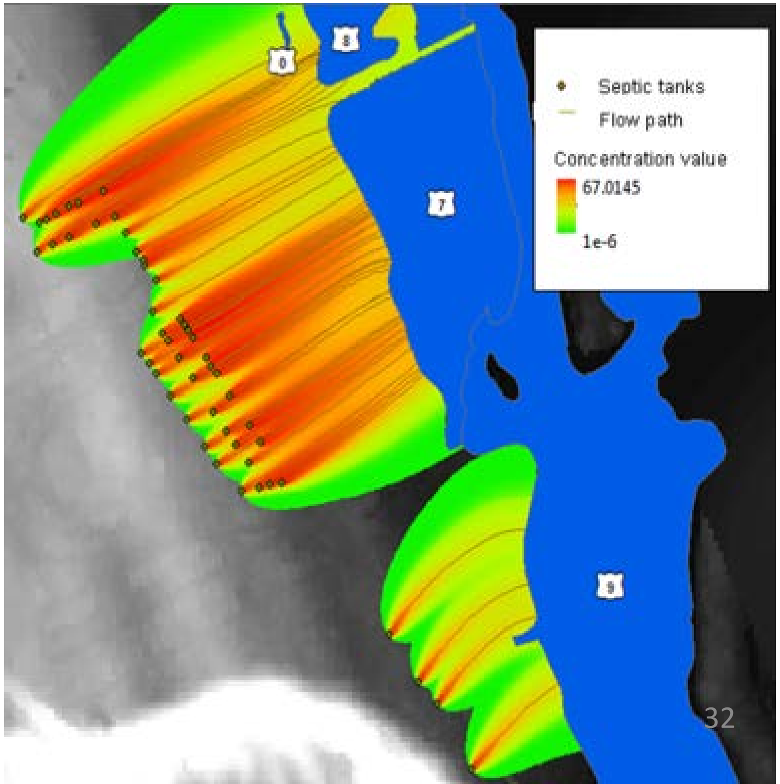
Spatial Variability of Reduction Ratio

The nitrogen reduction ratios in this study have a large range but are comparable with the literature data, especially with that of Roeder (2008) obtained in the Wekiva Study.

Reference	Site Location	Daily nitrogen loads per septic system (g/d)	Daily nitrogen loadings to surface water per septic system (g/d)	Nitrogen reduction ratio
Roeder (2008)	Wekiva Study Area, FL	21.7		**70.0%** [a]
Valiela et al. (1997)	Waquoit Bay, MA	23	9.87 [b]	**57.1%**
Meile et al. (2010)	McIntosh County, GA			**65-85 %** [c]
This study	Port St. Lucie, FL	23	7.60	67.0%
	Stuart, FL	23	11.4	50.4%
	North River Shores, FL	23	20.3	11.7%
	Seagate Harbor, FL	23	20.5	10.8%
	Banner Lake, FL	23	8.15	64.6%
	Rio, FL	23	4.80	79.1%
	Hobe Sound, FL	23	6.78	70.5%

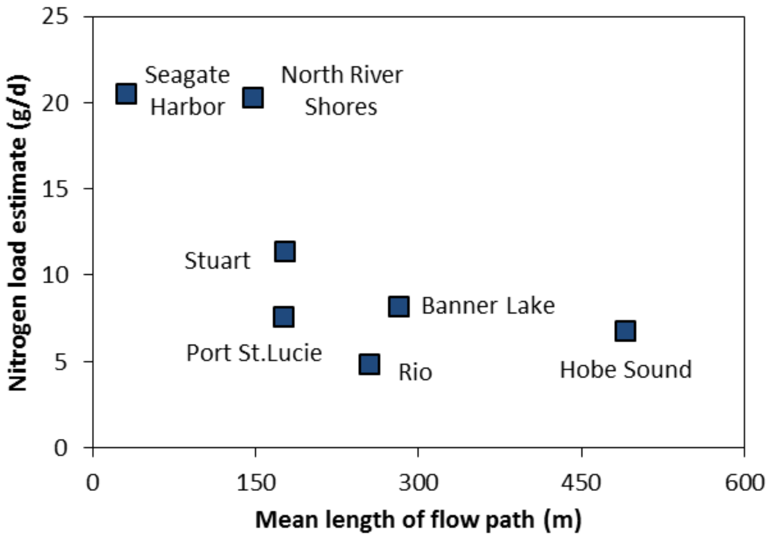
Simulated Nitrogen Plumes

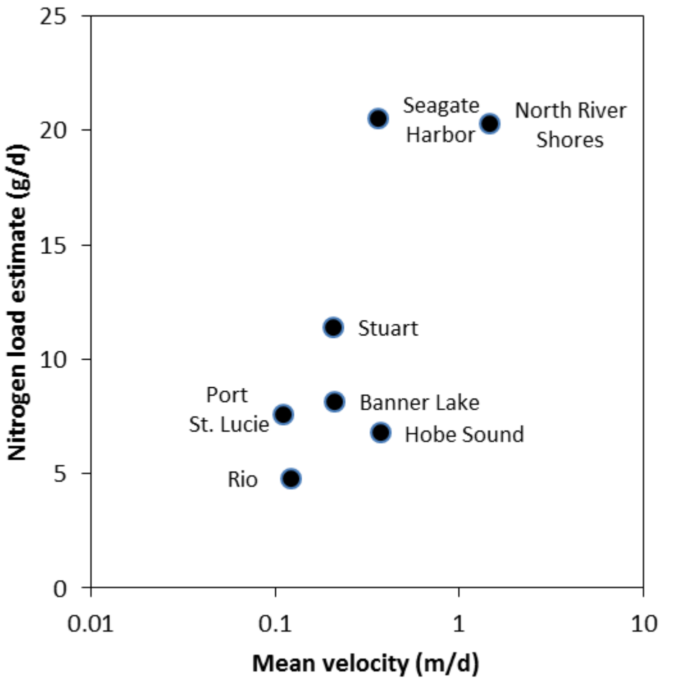
Spatial variability is obvious at different modeling sites, e.g., Seagate Harbor (left) (reduction ratio of 10.8%) and Hobe sound (right) (reduction ration of 70.5%) in the Martin County.



Factors Controlling Load Estimate

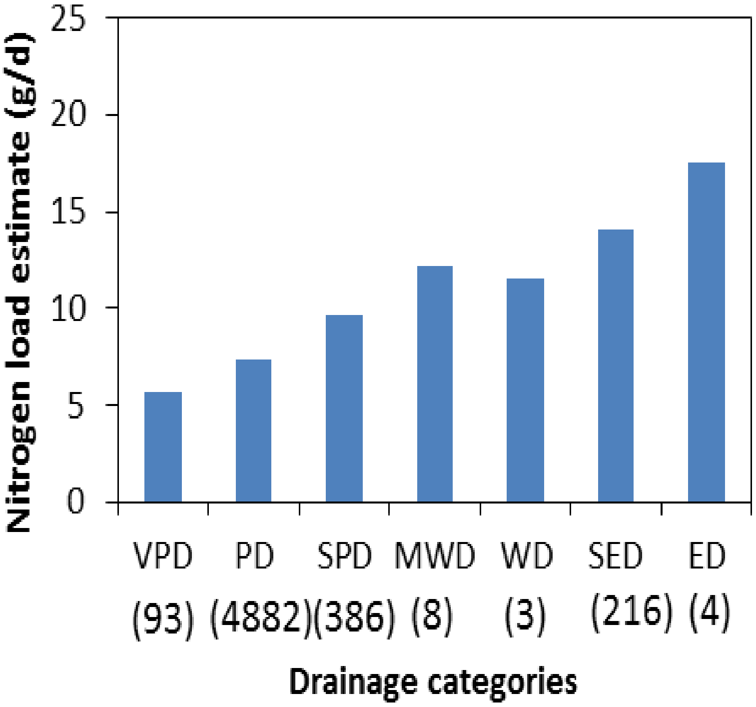
- Mean length of flow path (left): long mean length of flow path corresponds to more denitrification and thus less load estimate.
- Mean velocity (right): larger mean velocity results in shorter travel time, less denitrification, and thus more load estimate.





Factors Controlling Load Estimate

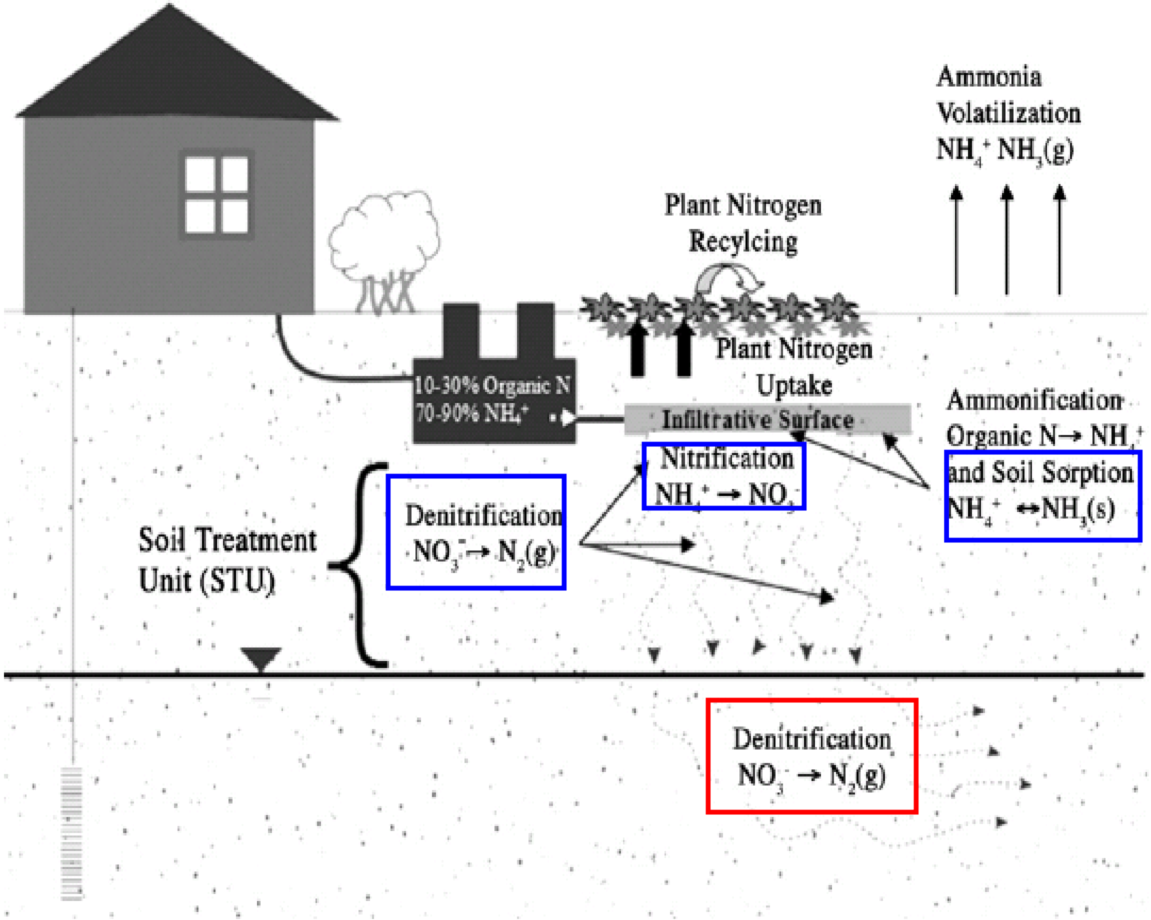
In the City of Port St. Lucie, the load estimate increases when the drainage condition changes from very poorly drained to excessively drained, because nitrogen transport is faster in well-drained soil is faster than in poorly drained soil.



VPD: very poorly drained
PD: poorly drained
SPD: somewhat poorly drained
MWD: moderately well drained
WD: well drained
SED: somewhat excessively drained
ED: excessively drained

The number of septic systems corresponding to each drainage condition is given in the parentheses

ArcNLET New Functions



From Heatwole and McCray (2007)

Vadose Zone Processes:

- Unsaturated flow (1-D)
- Ammonium and nitrate transport with sorption, nitrification, and denitrification

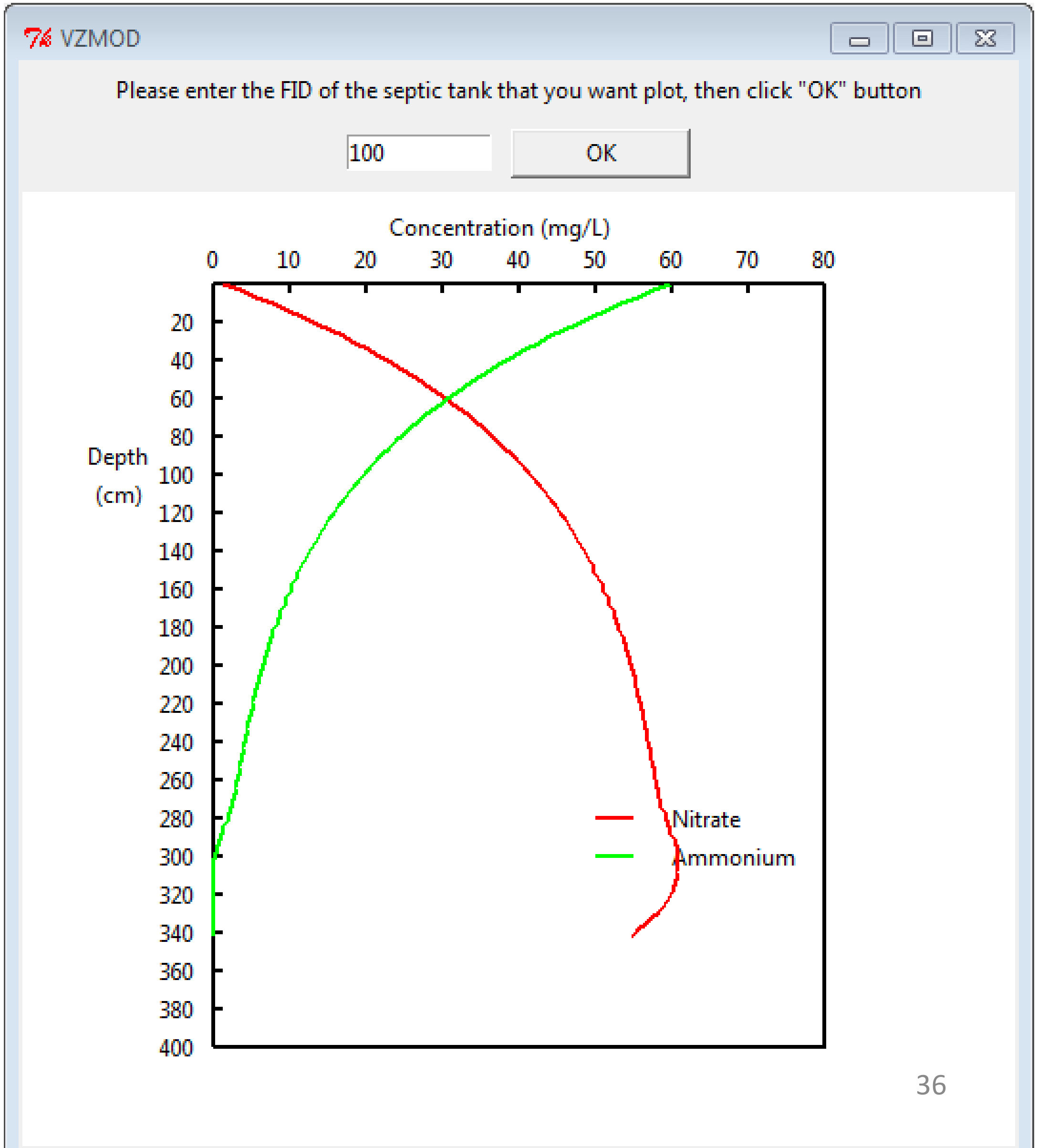
Groundwater Process:

- Groundwater flow (2-D)
- Ammonium and nitrate transport with sorption, nitrification, and denitrification

Surface processes for failed septic tanks have not been considered.

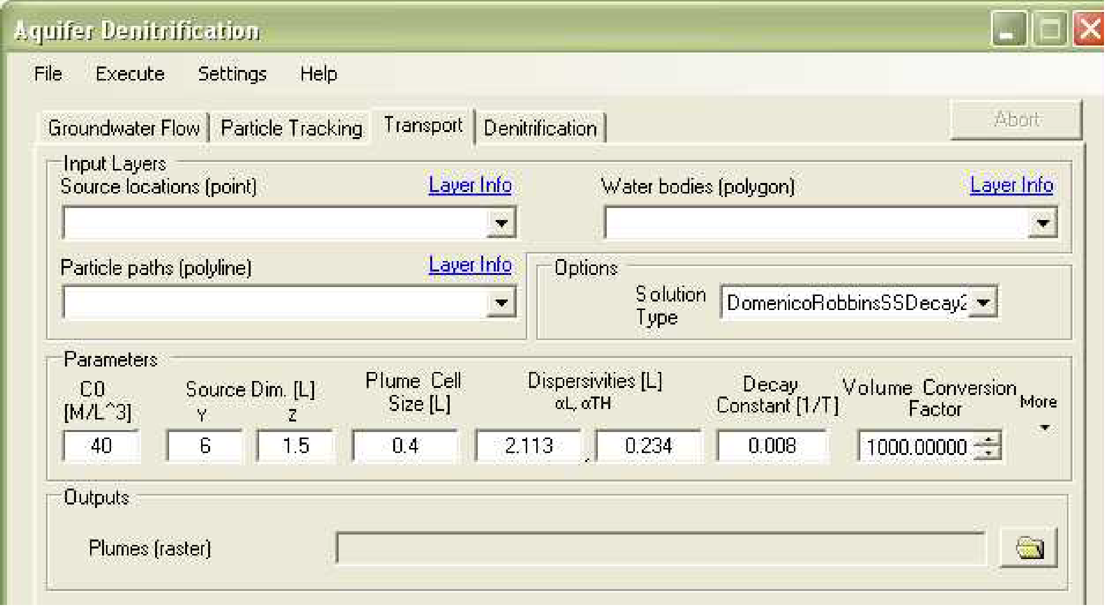
Importance of Ammonium Modeling

- Nitrification of ammonium may not be completed when water table is shallow.
- The analysis of the Jacksonville data by Ouyang and Zhang (2012) showed that the average concentrations in groundwater of organic nitrogen, ammonium, and NO_x (nitrate and nitrite) are 0.25 mg/L, 1.19 mg/L, and 5.67 mg/L, respectively.



Please enter the FID of the septic tank that you want plot, then click "OK" button

100



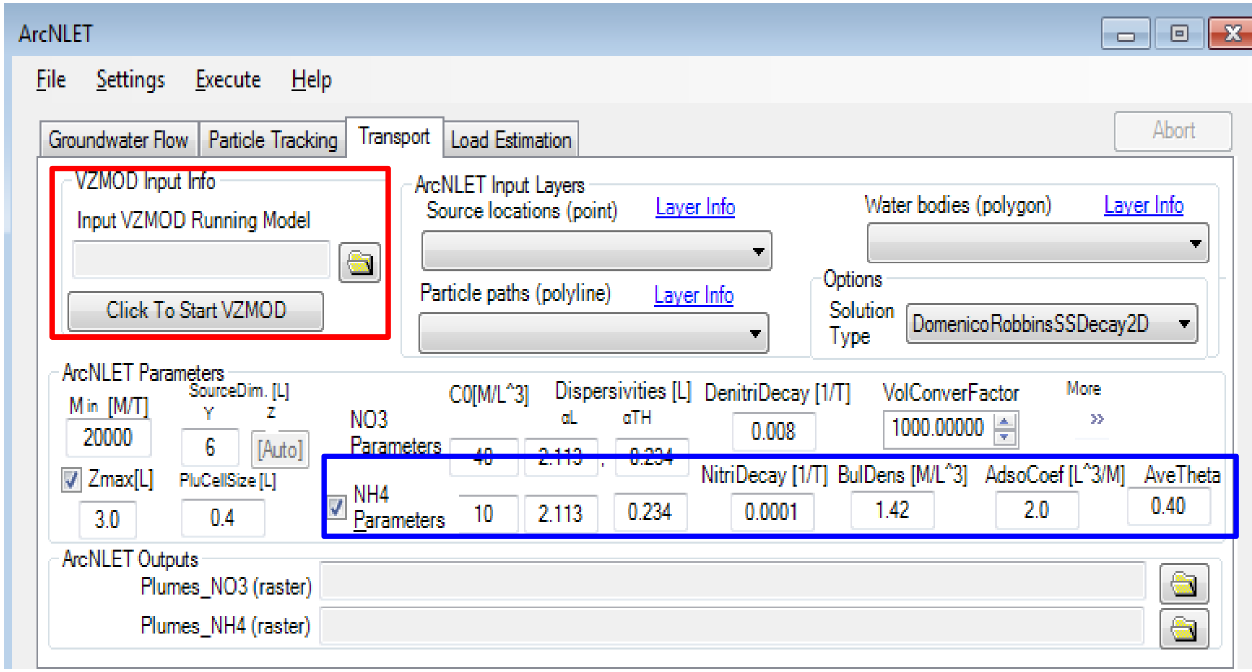
Solution Type: DomenicoRobbinsSSDecay2

C0 [M/L^3]	Source Dim. [L] Y	Source Dim. [L] Z	Plume Cell Size [L]	Dispersivities [L] αL	Dispersivities [L] αTH	Decay Constant [1/T]	Volume Conversion Factor
40	6	1.5	0.4	2.113	0.234	0.008	1000.00000

Original ArcNLET for nitrate transport in groundwater only

New ArcNLET for

- Ammonium and nitrate transport in vadose zone
- Ammonium transport in groundwater



Solution Type: DomenicoRobbinsSSDecay2D

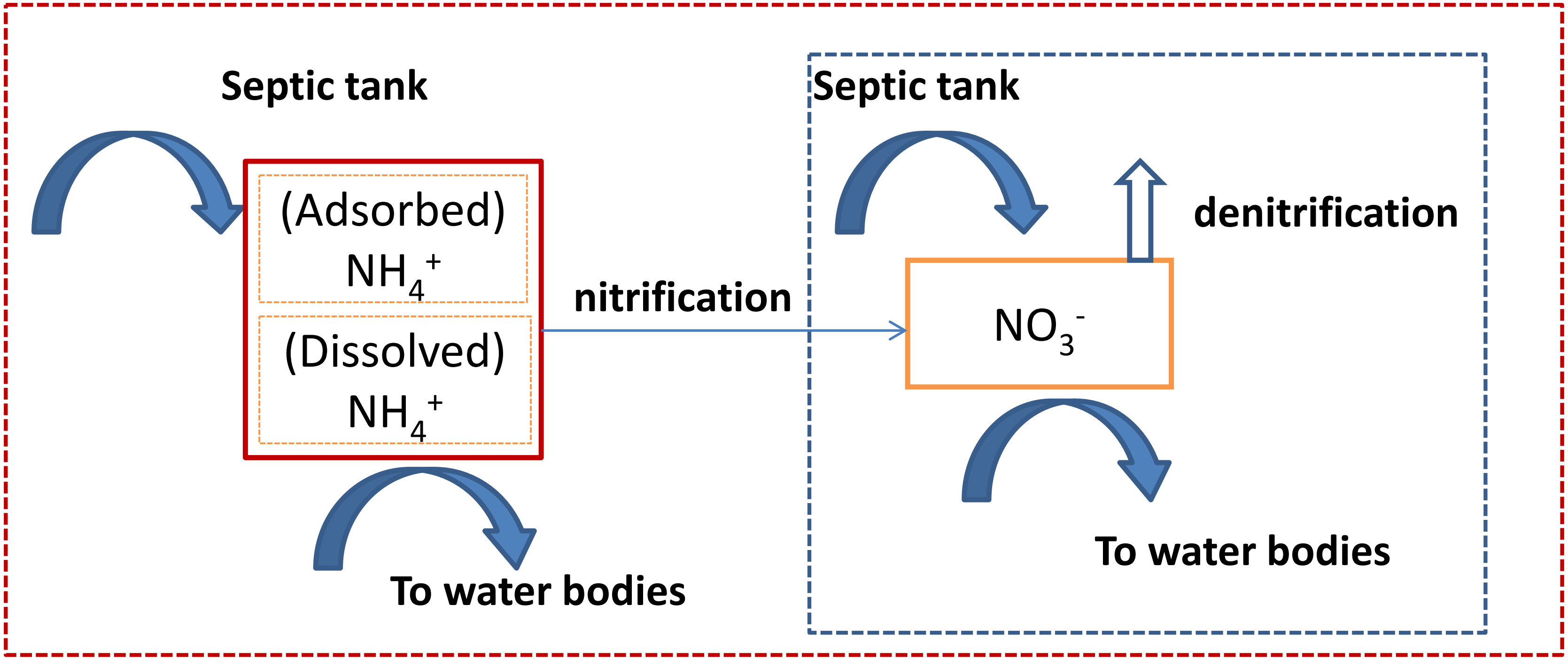
Min [M/T]	SourceDim. [L] Y	SourceDim. [L] Z	☑ Zmax[L]	PluCellSize [L]
20000	6	[Auto]	3.0	0.4

	C0[M/L^3]	Dispersivities [L] αL	Dispersivities [L] αTH	DenitriDecay [1/T]	VolConverFactor
NO3 Parameters	40	2.113	0.234	0.008	1000.00000

	C0[M/L^3]	Dispersivities [L] αL	Dispersivities [L] αTH	NitriDecay [1/T]	BulDens [M/L^3]	AdsoCoef [L^3/M]	AveTheta
☑ NH4 Parameters	10	2.113	0.234	0.0001	1.42	2.0	0.40

Conceptual Model

Ammonium and nitrate transformation and transport in the groundwater system.



Septic tank

(Adsorbed)
NH_4^+

(Dissolved)
NH_4^+

To water bodies

nitrification

Septic tank

denitrification

NO_3^-

To water bodies

Mathematical models

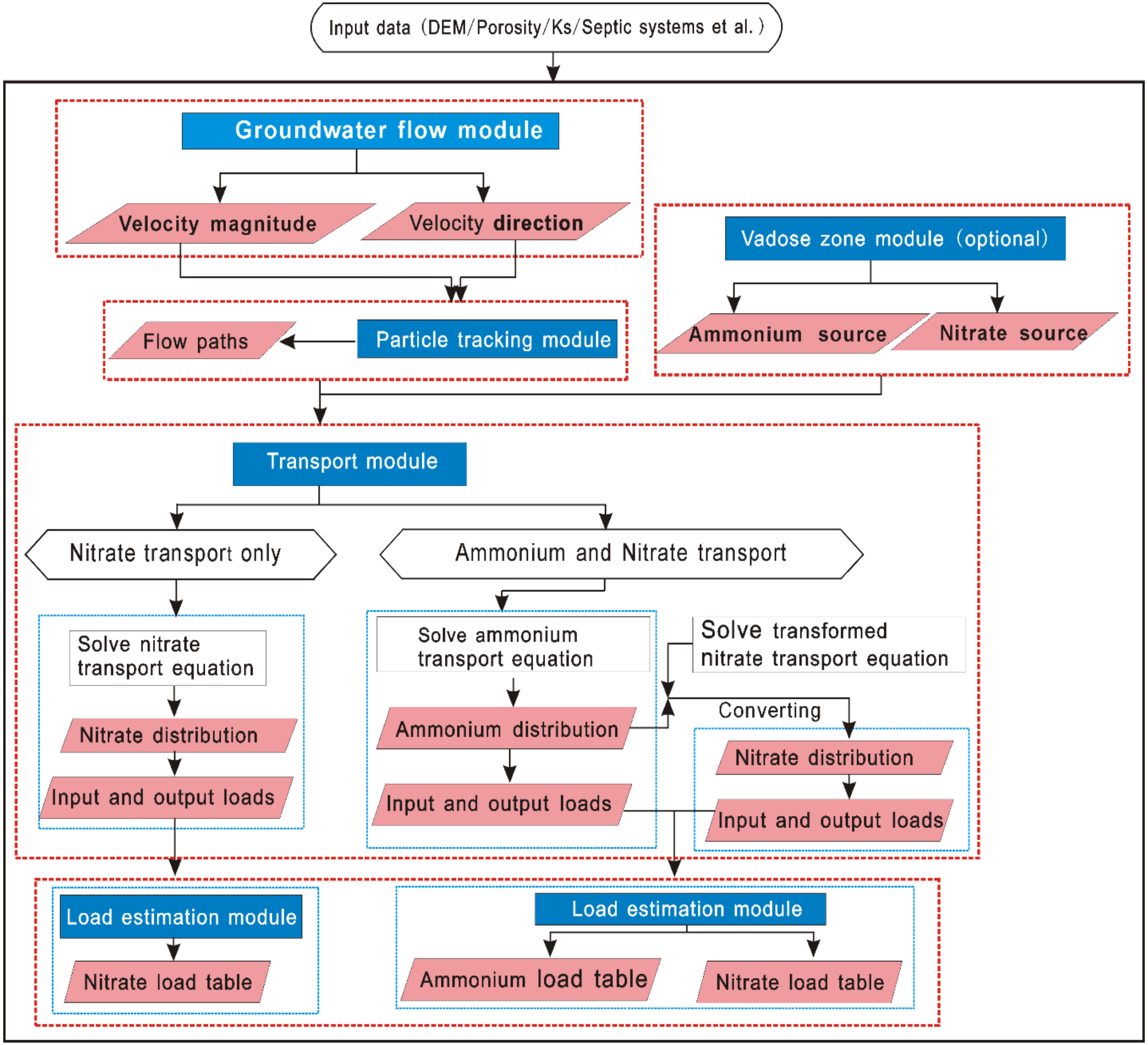
Ammonium transport equation

$$\underbrace{0}_{\text{Total mass change}} = \underbrace{D_x \frac{\partial^2 c_{NH_4^+}}{\partial x^2} + D_y \frac{\partial^2 c_{NH_4^+}}{\partial y^2}}_{\text{dispersion}} \underbrace{- v \frac{\partial c_{NH_4^+}}{\partial x}}_{\text{advection}} \underbrace{- k_{nit} \left(1 + \frac{\rho k_{adsop}}{\theta}\right) c_{NH_4^+}}_{\text{nitrification}} \qquad (1)$$

Nitrate transport equation

$$\underbrace{0}_{\text{Total mass change}} = \underbrace{D_x \frac{\partial^2 c_{NO_3^-}}{\partial x^2} + D_y \frac{\partial^2 c_{NO_3^-}}{\partial y^2}}_{\text{dispersion}} \underbrace{- v \frac{\partial c_{NO_3^-}}{\partial x}}_{\text{advection}} \underbrace{+ k_{nit} \left(1 + \frac{\rho k_{adsop}}{\theta}\right) c_{NH_4^+}}_{\text{nitrification}} \underbrace{- k_{denit} c_{NO_3^-}}_{\text{denitrification}} \qquad (2)$$

Flowchart



Input data（DEM/Porosity/Ks/Septic systems et al.）

Groundwater flow module

Velocity magnitude

Velocity direction

Vadose zone module（optional）

Ammonium source

Nitrate source

Flow paths

Particle tracking module

Transport module

Nitrate transport only

Ammonium and Nitrate transport

Solve nitrate transport equation

Nitrate distribution

Input and output loads

Solve ammonium transport equation

Ammonium distribution

Input and output loads

Solve transformed nitrate transport equation

Converting

Nitrate distribution

Input and output loads

Load estimation module

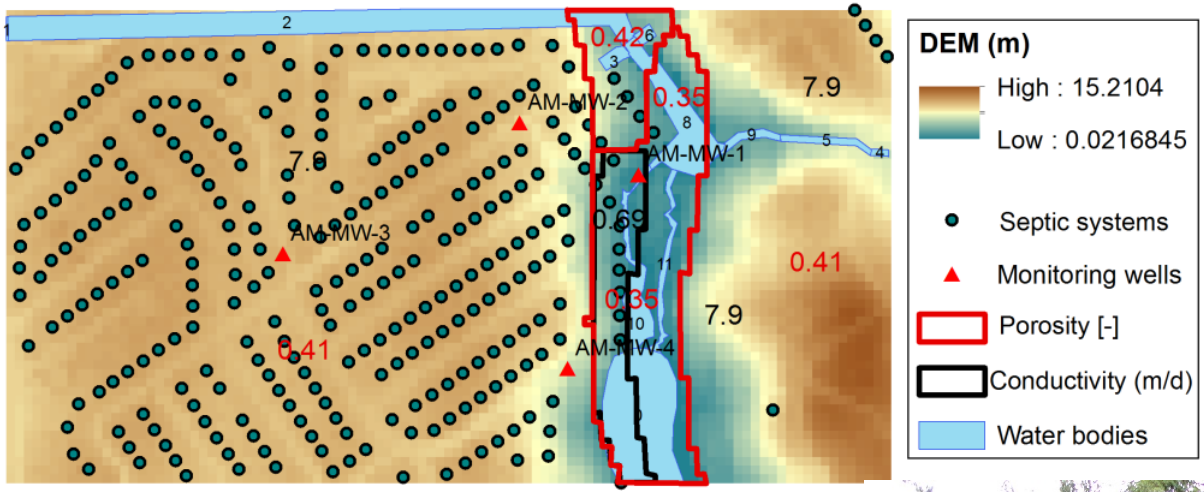
Nitrate load table

Load estimation module

Ammonium load table

Nitrate load table

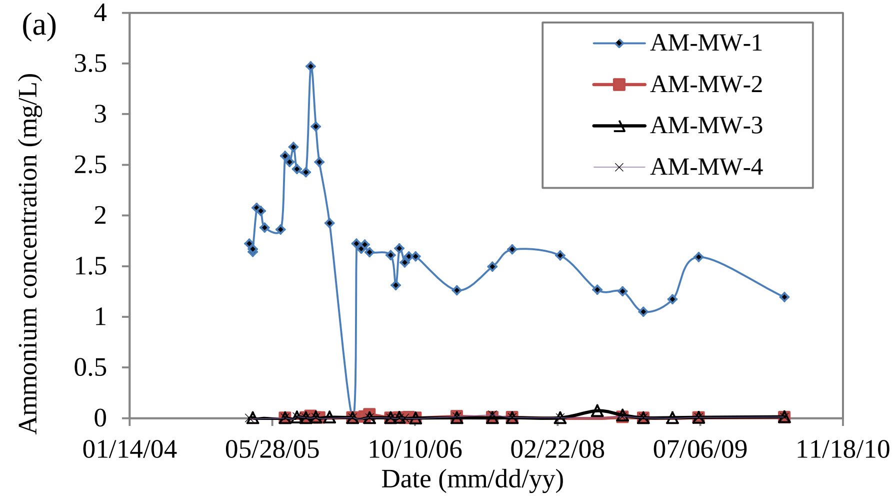
Application of New ArcNLET

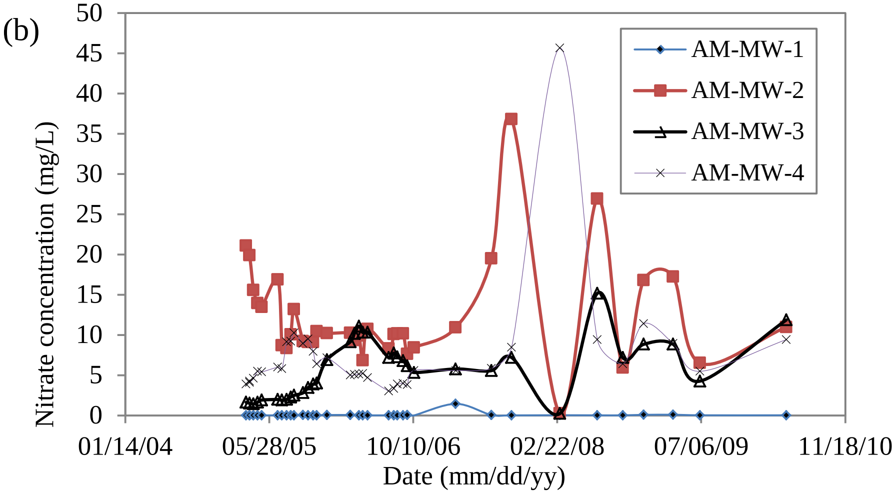


Modeling domain

Monitoring well AM-MW-1 is very close to Red Bay Branch.

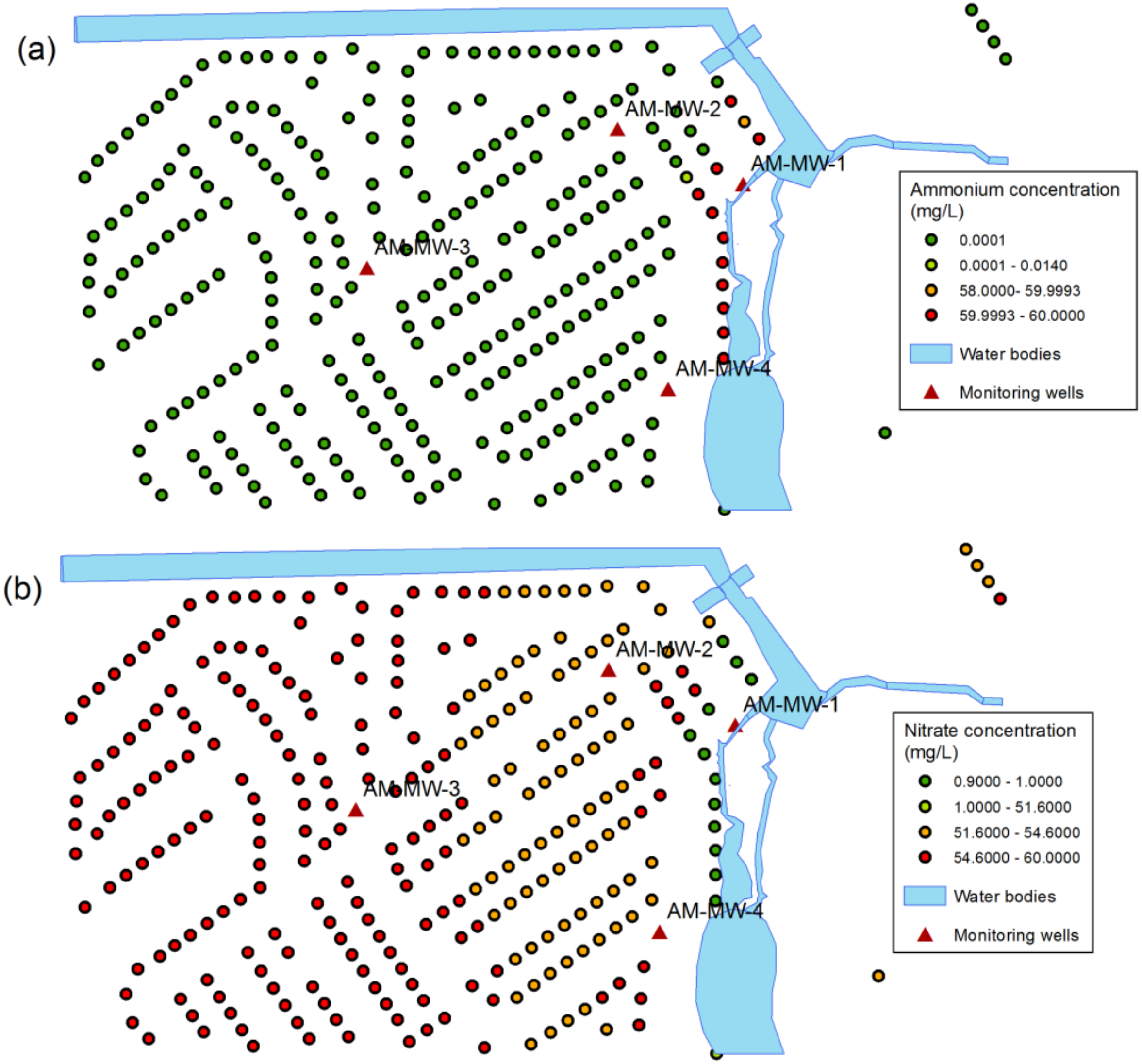
Ammonium and Nitrate Concentrations in Groundwater





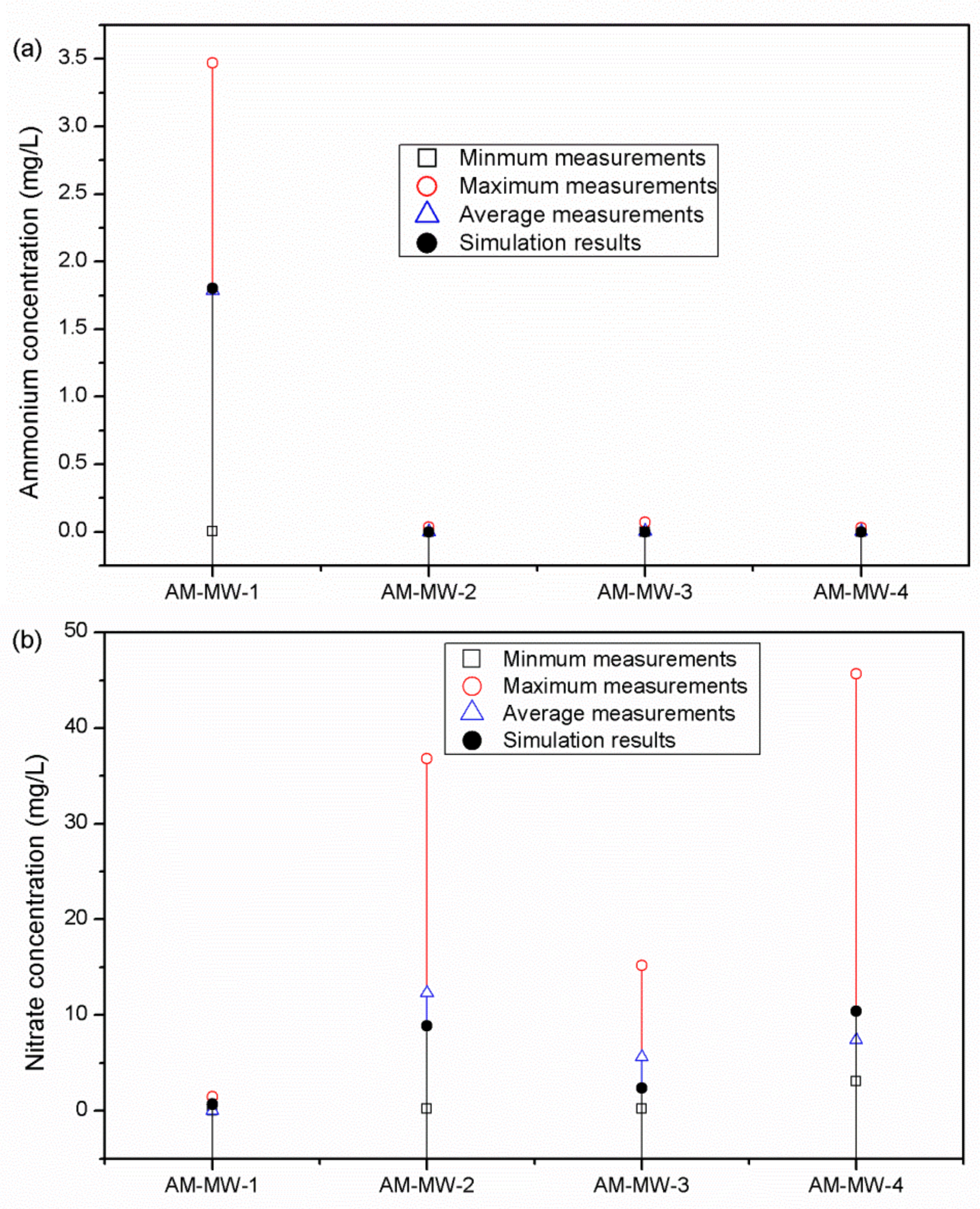
- High ammonium concentration
- Low nitrate concentration

Vadose Zone Modeling Results



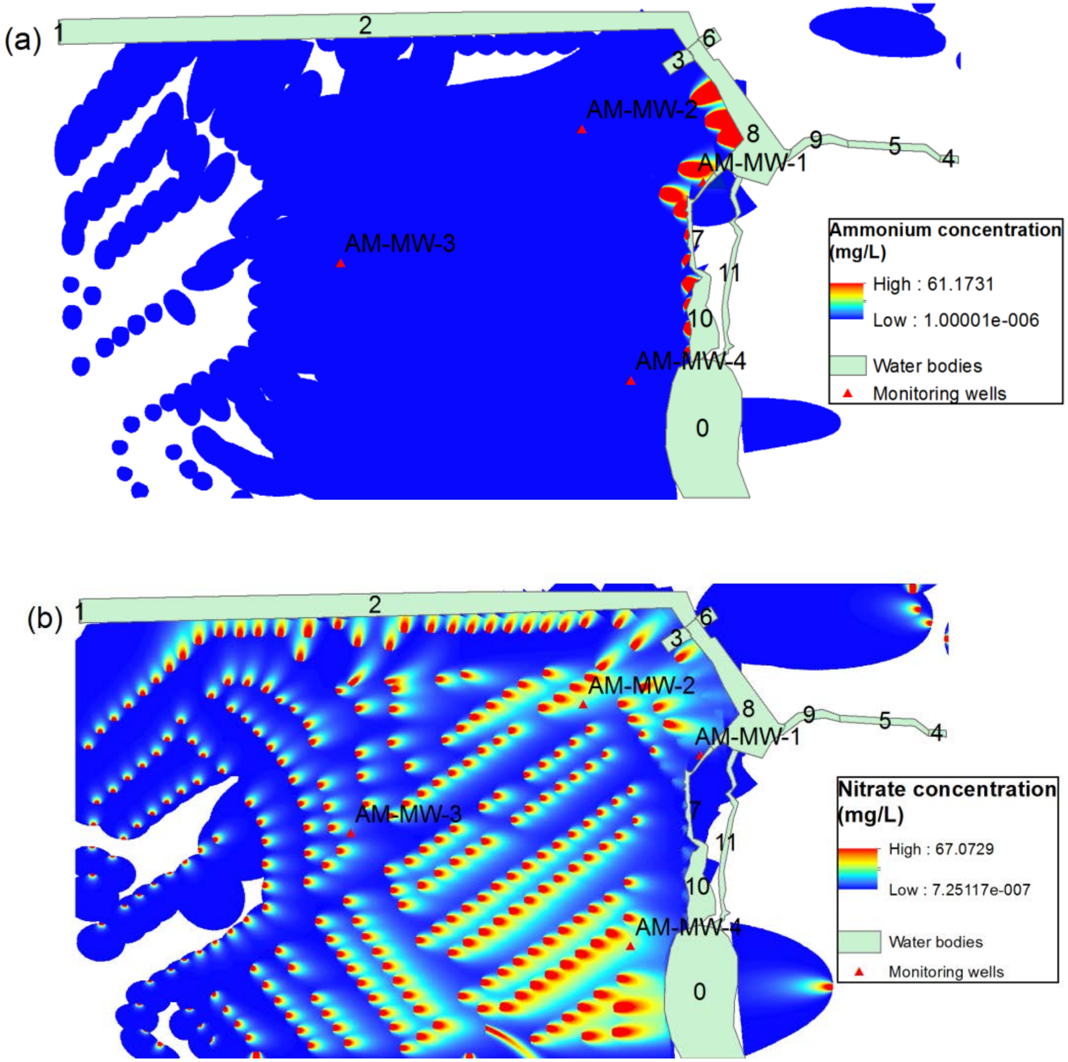
Simulated concentrations of ammonium and nitrate at water table

Groundwater Modeling Results



Simulated concentrations of ammonium and nitrate at monitoring wells.

Groundwater Modeling Results



Simulated plumes of ammonium and nitrate in groundwater.

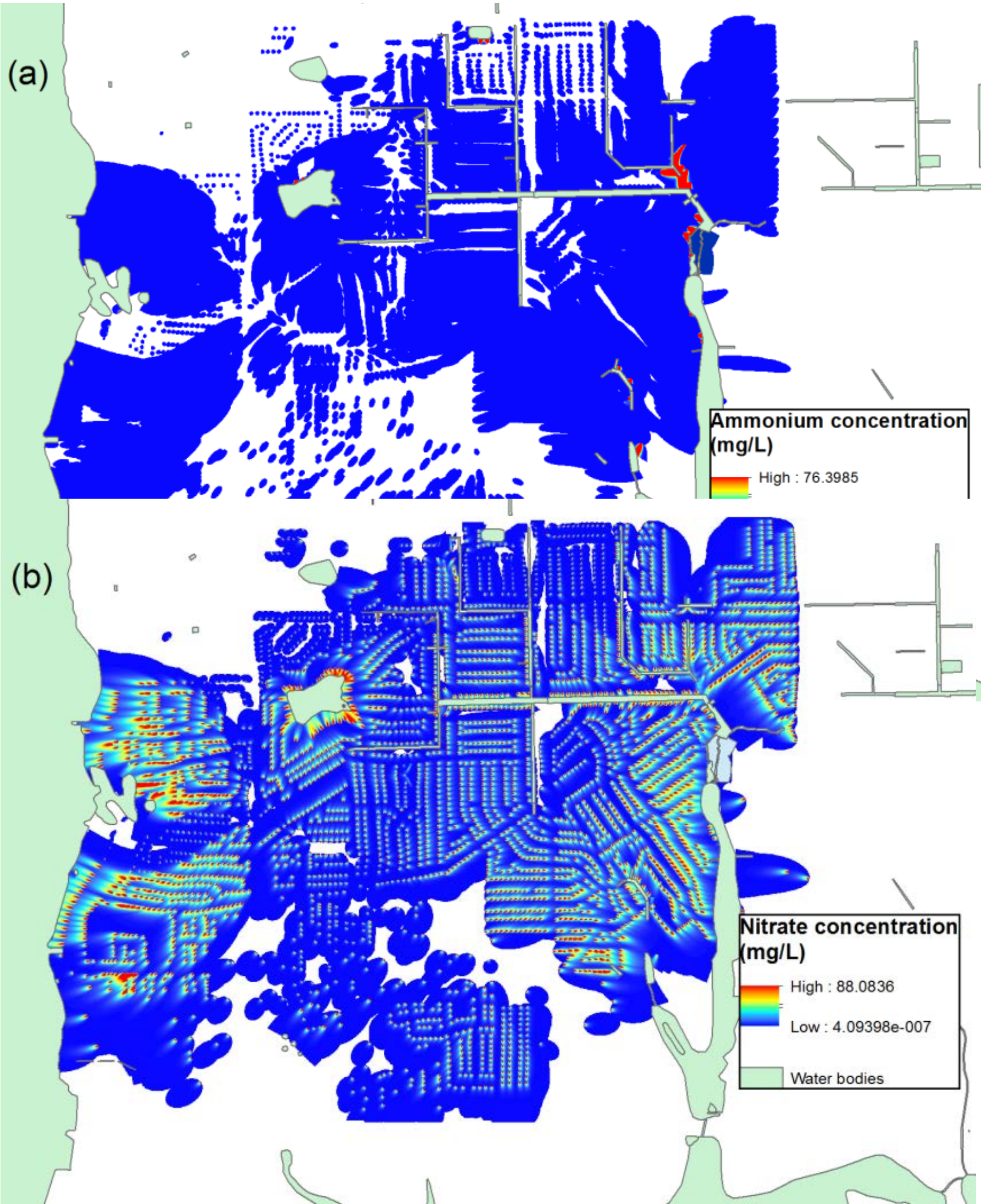
For a portion of the entire Eggleston Heights neighborhood

	Ammonium	Nitrate	Total
Loading to groundwater (kg d^{-1})	0.30	6.69	6.99
Loading to surface water bodies (kg d^{-1})	0.25	1.10	1.35
Percentage of removal (%)	15.88	83.54	80.67
Percentage of loading to water bodies (%)	18.46	81.54	100.00

For the entire Eggleston Heights neighborhood

	Ammonium	Nitrate	Total
Loading to groundwater (kg d^{-1})	1.54	82.34	83.87
Loading to surface water bodies (kg d^{-1})	1.30	11.13	12.43
Percentage of removal (%)	15.52	86.48	85.18
Percentage of loading to water bodies (%)	10.45	89.55	100.00

Groundwater Modeling Results



Simulated plumes of ammonium and nitrate in groundwater.

Conclusions

- Data and information needed to establish ArcNLET models for nitrogen load estimation are readily available in the modeling areas.
- After calibrating the ArcNLET flow and transport models, model simulations can reasonably match corresponding field observations.
- ArcNLET estimated nitrogen loads in the modeling sites vary substantially in space, and the spatial variability is useful to management of nitrogen pollution.
- The load estimates can be used directly to facilitate TMDL and BMAP planning.

Questions, Suggestions, and Comments?