

Picture from USGS Scientific Investigations Report 2008–5220

## A Brief Summary of ArcNLET and Associated Tools for Estimation of Nitrate Load from Septic Systems to Surface Water Bodies Ming Ye (<u>mye@fsu.edu</u>), Department of Scientific Computing, Florida State University January 26<sup>th</sup>, 2012

## Presentation at the City of Jacksonville

Last presentation to the City was December 9th, 2010

# Outlines

- Development of ArcNLET and its applications at Julington Creek and Eggleston Height neighborhoods
- New understanding gained last year
- New tools (developed and under development) associated with ArcNLET to facilitate nitrate load estimation
- Suggestion and comments

# What is ArcNLET?

## ArcGIS-based Nitrate Load Estimation Toolkit

- A simplified conceptual model of groundwater flow and solute transport
- Implementation as an ArcGIS extension
- Calculation of nitrate plume and nitrate load



Compatible with ArcGIS 9.3 and 10

# ArcNLET Development History

- It was developed during January 2009 July 2011.
- The first workshop was offered in July 2011.
- Software is available for free download at FSU website http://people.sc.fsu.edu/~mye/ArcNLET/.
- The project was reported on Florida State News as a FSU front page story, and listed as one of the twelve FSU 2011 research highlights.
- We were invited to contribute an article to ESRI Hydro Blog.
- Education and scholarly activities: The project supported two master students and produced two journal articles, one conference proceeding, and a number of conference presentations.

# Why Do We Develop ArcNLET?

- There is no suitable tool for estimation of nitrate load to meet TMDL requirements and perform LSJR Nitrogen BMAP. Existing tools are either too simple or too complex.
- Develop a simplified model that consider key hydrogeologic processes of groundwater flow and nitrate fate and transport.
- Implement the model by developing a user-friendly ArcGIS extension to
  - Simulate nitrate fate and transport including the denitrification process
  - Consider either individual or clustered septic tanks
  - Provide a management and planning tool for environmental management and regulation
- Use the software to facilitate DEP environmental management and regulation.
- Disseminate the software and conduct technical transfer to DEP staff and other interested parties.

## Simplified Conceptual Model to consider key hydrogeologic processes involved in nitrate transport:





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

#### Example Graphic User Interface

ifer Denitrification				
le Execute Settings Help				
Groundwater Flow Particle Tracking Transport Denitrification	n	Abort		
Input Layers DEM surface elevation map (L1 (raster) Layer Info	Hydraulic conductivity [L/T] (raster)	Laver Info		
<b>•</b>				
Water bodies (polygon)	Soil porosity (raster)	Laver Info		
·		<b>_</b>		
Options & Parameters			Example simulated nitrate nlu	imas
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# **Requirements on Potential Users**

• The GUI make it easier for some with little experience in analyzing groundwater transport problems to apply a solute-transport model to a field problem.

#### Use of ArcNLET requires

- 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 by which 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
- It may be useful to test and tune the model for several representative sites before using the model for general purposes.

# What Challenges Do We Face?

#### • Keith Beven (2001): The Dalton Lecture

How far can we go in distributed hydrological modeling?

"The principles are general and we have at least a qualitative understanding of their implications, but the difficulty comes in the fact that we are required to apply hydrological models in particular catchments, all with their own unique characteristics."

 Warren Wood (2000), Editorial of Ground Water (one of the most widely read groundwater journal) It's the heterogeneity!

"If all aquifer systems were homogeneous, then hydrogeologic problems would be reduced to handbook applications, and there would be no ground water hydrologists as we know them."

"It is my guess that ... it will be many years before we can effectively deal with heterogeneity on societally important scales."

**Leonard Konikow** (2011, Ground Water): "the secret to successful solute-transport modeling may simply be to lower your expectations." <sup>9</sup>

# What Do We Find?

- Default parameters obtained from literature
- Site-specific observations and <u>manual</u> model calibration for Julington Creek neighborhood, Jacksonville



# Manual Model Calibration: Trial and Error



# What Do We Find?





**Default** parameter values (91g/d): ➢hy con: 2.113m/d ← Too small Porosity: 0.25  $\geq \alpha_{1}: 2.113 \text{m}$  $\succ$  C<sub>0</sub>: 40mg/L ≻ k<sub>den</sub>: 0.008/d  $\succ$  smthF: 50 Too small number of plumes reaching river: 228 Calibrated parameter values (1023g/d): ➢hy\_con: see the map

- Porosity: soil data
- $\succ \alpha_1$ : 10m
- > α<sub>τ</sub>: 1.0m
- $\succ$  C<sub>0</sub>: 100mg/L
- ≻ k<sub>den</sub>: 0.012/d
- ➢ smthF: 100
- Adjusted to match observed plumes
- number of plumes reaching river: 354

# **Does God Play Dice?**

- Different sets of model parameters give similar results of model calibration. Computer can do a better job of calibration.
- The calibrated parameter set is one of the realizations (*E pluribus unum*).
- Parametric Uncertainty:

"However, we should accept that there may be many different model structures and parameter sets that will be acceptable in simulating the available data." (Keith Beven, 2001, Dalton Lecture)



# Why Are Model Parameters Uncertain?

Poetry of Donald H. Rumsfeld:

Feb. 12, 2002

Department of Defense news briefing

#### The Unknown

As we know, There are *known knowns*.

There are things we know we know.

We also know

There are known unknowns.

That is to say

We know there are some things We do not know.

But there are also *unknown unknowns*,

The ones we don't know We don't know.



"All inputs used in estimation of inputs and loadings are uncertain to some extent."

"Significant uncertainties have been identified throughout this report."



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How to Address and Reduce Parametric Uncertainty?

- Select random parameters whose values are largely unknown.
- Determine the ranges and probability distributions of the parameters.
- Conduct sensitivity analysis to identify the parameters that are most influential to the load estimate.
- Calibrate the model against field observations to reduce parametric uncertainty.
- Conduct Monte Carlo simulation to quantify uncertainty in nitrate load estimation.
- An example for the Lakeshore neighborhood, where observations are not available.

## **Random Parameter and Their Distributions**



# Maximum, minimum and representative values of hydraulic conductivity is derived from soil data

Parameter	Distribution	Max	Representative	Min
hy_con23	TRIANGULAR	3.6593	7.9488	12.1976
hy_con65	TRIANGULAR	3.6593	7.9488	12.1976
hy_con71	TRIANGULAR	0.122	0.6705	1.2198
hy_con73	TRIANGULAR	0.122	0.6705	1.2198
hy_con116	TRIANGULAR	3.6593	7.9488	12.1976
hy_con117	TRIANGULAR	0.122	0.6705	1.2198
hy_con120	TRIANGULAR	1.2198	6.696	12.1976
hy_con164	TRIANGULAR	0.122	0.6912	1.2198
hy_con165	TRIANGULAR	12.1824	21.3408	30.4992
C	NORMAL	25		80
α	NORMAL	0.21		21.34
k	IOGNORMAL	0.004		1.08
smthF	UNIFORM	20		80

#### **Distributions of LHS Samples**

## Identify Influential Model Parameters





# **Uncertainty Analysis**





The load estimation has large uncertainty, and the uncertainty may be even larger if there are ditches within the neighborhood.



# Similarity With CDM Method Green zone at right is the 300-meter buffer zone based on

- the NHD.
- The number of failed septic tanks in the buffer zone and used for the load calculation is 223.
- The total amount of nitrate load is 223 x [11.2 g/d x 2.51 x 0.8] = 5015 g/d. Denitrification is not considered.



### Parameter values of the largest load estimate:

- $\succ$  hy con: see the map (hy con169: 23.9 m/d)
- Porosity: soil data
- > α<sub>x</sub>: 9.351m
- > α<sub>v</sub>: 0.935m
- ≻ C<sub>0</sub>: 54.76mg/L
- ≻ k<sub>den</sub>: 0.004/d
- $\succ$  smthF: 24

Smallest value from literature

### **Estimated load:**

4654 g/d from <u>205</u> out of 265 plumes that reach the river

# Isotope Signature of Denitrification

Indication of denitrification occurrence (Chen and Mcquarrie, 2005):

- Linear relationship
- Slope close to 0.51



 $\delta^{18}$ O vs.  $\delta^{15}$ N at Julington Creek and Eggleston Heights (Sep & Oct, 2010).

## How Much Parametric Uncertainty Can Be Reduced by Field Observations?

- The parametric uncertainty can be reduced dramatically by incorporating the field observations into model calibration.
- Take the first-order decay coefficient as an example.



## **Reduction of Load Estimation Uncertainty**

Load estimates before incorporating field observations.





CDM estimate is 7624/8292 g/d

Mean	1334.48
Median	1225.43
Standard	
Deviation	652.61
Minimum	177.62
Maximum	5655.87
Realizations	2000
95 <sup>th</sup> percentile	2581.89
5 <sup>th</sup> percentile	513.28

Mean	1504.24
Median	1466.39
Standard Deviation	257.08
Minimum	1048.57
Maximum	2078.18
Realizations	19
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# What Have Been Developed After ArcNLET?

- Python codes of sensitivity analysis to identify the most influential model parameters to load estimation.
- Python code of uncertainty analysis and automated model calibration.
- GUIs are not available, but can be developed in several weeks.
- Python code of simulating nitrate fate and transport modeling in unsaturated soil. We are at the last stage of verification and validating. GUI is available.

Illustration for loamy soil

- Share data files of ArcNLET such as raster files of DEM, hydraulic conductivity and porosity.
- Model parameters for various soil types.
- Estimate nitrate load to groundwater for multiple septic tanks.

74 Nitrate Fate And Trans	oort In Soil						
Select Soil Types	Hydraul	ic Parameters	Nitrificat	ion Parameters	Denitrifica	tion Parameters	29.4534195829 mg/l
C Clay	HLR	2.0	Kr-max	56.0	Vmax	2.56	Nitrate concentration of Septictank 579 is 28.0753677696 mg/l
C Clay Loam	αG	0.021	Km-nit	5.0	Kan dat	50	Nitrate concentration of Septictank 580 is 26.0708917094 mg/l
Loam	αVG	0.011	e2	2.267	KIII-GIIL		Nitrate concentration of Septictank 581 is
C. Learne Sand	Ks	12.04	e	1.104	e-dnt	3.//4	Nitrate concentration of Septictank 582 is
Coarriy Sand	θr	0.061	βnit	0.347	βdnt	0.347	Nitrate concentration of Septictank 583 is
C Sand	θs	0.399	fs	0.0	sdn	0.0	26.2275453238 mg/l Nitrate concentration of Septictank 584 is
C Sandy Clay	n	1.474	fwp	0.0			26.144834313 mg/l Nitrate concentration of Sentictank 585 is
C Sandy Clay Loam	m	0.321	swp	0.154	Water Tab	le Depth	27.6454796131 mg/l
C Sandy Loam	I	0.5	sl	0.665	Distance	288	30.7648848965 mg/l
⊂ Silt	 	atura Daramatan	sh	0.809	Output Co	oncentrations	Copying the source point file to the workspace and adding the calculation results to it
C Silby Clay	T	18.5	C C C C C C C C C C C C C C C C C C C		C-NH4	1e-05	A new shape file has been created with calculated nitrate concentrations added to the
	Tont nit	25.0		60.0	C NO2	30 764884806	field "N0_Conc" Calculation is done, you can check the
Silty Clay Loam	Tant de	. 25.0	C0 NO2	1.0	10-1105	30.704004030	concentration profile of individual septic tank by
C Silty Loam	Topt-ar	10 20.0	100-1405	1.0			
Multiple source		Heterogeneous I	vdraulic cond	uctivity and soil p	orosity 🔽 Us	ing smoothed DE	M to calculate WTD
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Hydraulic conductivity fil	e(raster)	E:/julingtonUA/hyd	_cond_t.img				Browse
Soil porosity file(raster)					Rrowse Run		
					Check results		
Smoothed Delvi file (raste	a) [	e a la serie si su ana	, .				Quit
DEM file (raster)		E:/julingtonUA/lidar	dem.img				Browse



#### Illustration for sandy soil

elect Soil Types	Hudraul	ic Parameters	Nitrificati	on Parameters		1. 4	53 201893354 mg/l	
	Hydraul	ic Parameters	Nitrification Parameters		Denitrification Parameters		Nitrate concentration of Septictank 579 is	
Clay	HLR	2.0	Kr-max	56.0	Vmax	2.58	53.0670471461 mg/l	
Clay Loam	αG	0.09	Km-nit	5.0	Km-dnt	5.0	S2.850533884 mg/l	
Loam	aVG	0.035	e2	2.267			Nitrate concentration of Septictank 581 is	
·	Ks	642.98	6	1.104	e-dnt	2.865	Nitrate concentration of Septictank 582 is	
Loamy Sand	θr	0.053	βnit	0.347	βdnt	0.347	53.138154856 mg/l Nitrate concentration of Septictank 583 is	
Sand	θs	0.375	fs	0.0	sdn	0.0	52.8681605868 mg/l Nitrate concentration of Septictank 584 is	
Sandy Clay	n	3.18	fwp	0.0			51.8469302575 mg/l	
Sandy Clay Loam		0.686	swp	0.154	Water Tab	le Depth	53.0224333877 mg/l	
Sandy Loam	1	0.5	Swp	0.665	Distance	288	Nitrate concentration of Septictank 586 is 53.3170989658 mg/l	
Sundy Louin	1	0.0	SI	0.000			Copying the source point file to the workspace	
Silt	Temper	rature Parameters sh 0.809		Output Concentrations		A new shape file has been created with		
Silty Clay	Т	18.5	Effluent Concentrations		C-NH4	1e-05	calculated nitrate concentrations added to the	
Silty Clay Loam	Topt-nit	t 25.0	C0-NH4	60.0	C-NO3	53.317098965	Calculation is done, you can check the	
Silty Loam	Topt-dr	nt 26.0	C0-NO3	1.0	1		concentration profile of individual septic tank by the FID	
] Multiple source		Heterogeneous	hydraulic cond	uctivity and soil po	orosity 🔽 Usi	ng smoothed DEI	M to calculate WTD	
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Soil porosity file(raster) E:/julingtonUA/porosity_heter.img			6			Browse		
moothed DEM file (raster) E:/temp/smoothedDEM.img					Browse			
					Ouit			



Nitrate

Ammonium

# What are Being Developed?

 Python code of data-worth analysis for design of monitoring network and field investigation. It is based on the OPR-PPR method of U.S. Geological Survey.



Potential locations of new monitoring wells

# General Ideas for Moving Forward

- Select several representative sites measured by, for example, values of organic carbon (OC) and groundwater velocity
- Conduct field investigation to measure, for example, OC, pH, water content, nitrate concentration, and seepage velocity.
- Calibrate the model against field observations and conduct sensitivity and uncertainty analysis to obtain
  - Representative parameter values and distributions: use them for similar sites to simulate nitrate load, if resources are available
  - Representative load values and distributions: use them for similar sites directly, if resources are unavailable

## Questions, Suggestions, and Comments?

