Sensitivity and Model Calibration for Nitrate Transport Modeling in Eggleston Heights and Julington Creek Neighborhoods, Jacksonville

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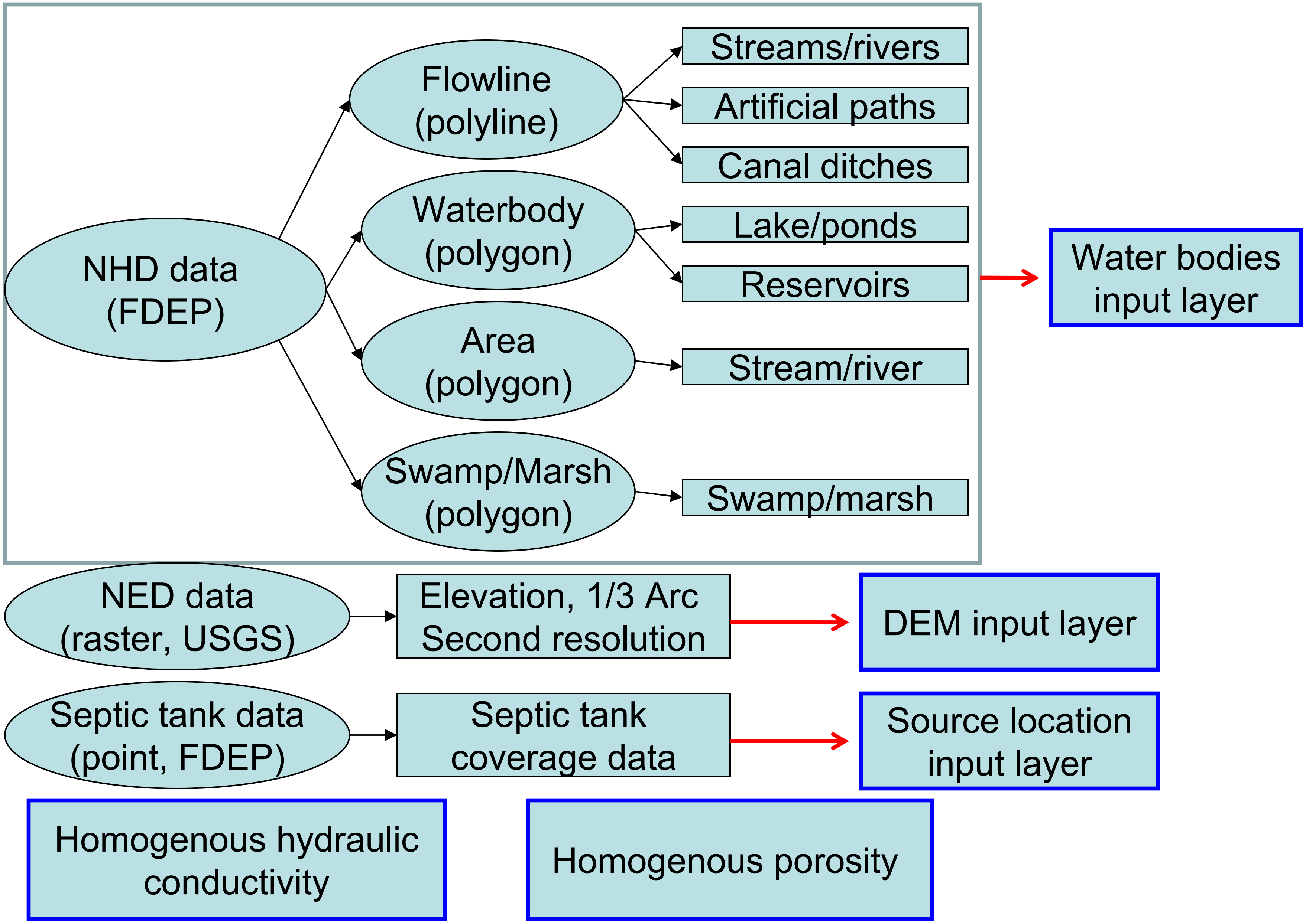
Outline

- Updating of Input Files (to incorporate more information or improve the quality)
- Sensitivity Analysis (to serve as guidelines for model calibration)
  - Local sensitivity
  - Global Sensitivity
  - Conclusions
- Calibration for the Eggleston Heights and Julington Creek Neighborhoods
  - Modeling domains
  - Field observations
  - Calibration procedure
  - Calibration results

Preparation of Input Files (User's Manual)



Updating of Input Files

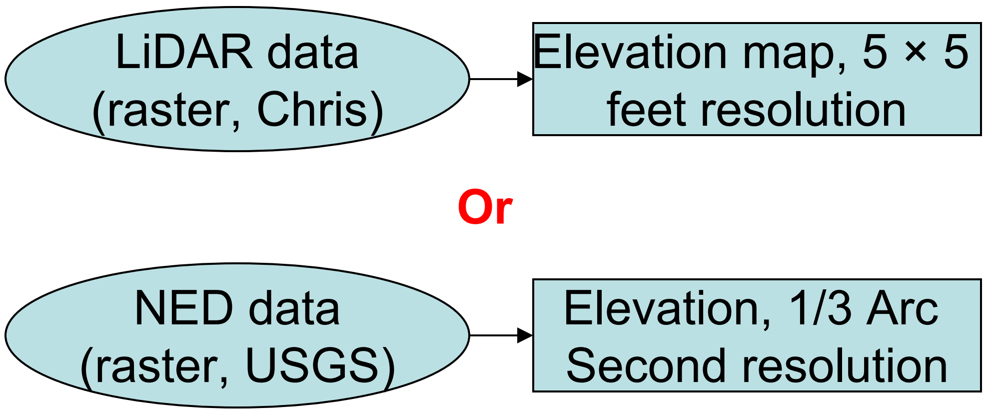
- Update DEM raster file by post-processing NED data or LiDAR data

- Update water body polygon file by combining the NHD data and ditches polygon file and update it based on LiDAR elevation map if necessary

- Generate heterogeneous hydraulic conductivity and soil porosity based on soil survey data

Only guidelines are shown here, more details please refer to the Application Manual

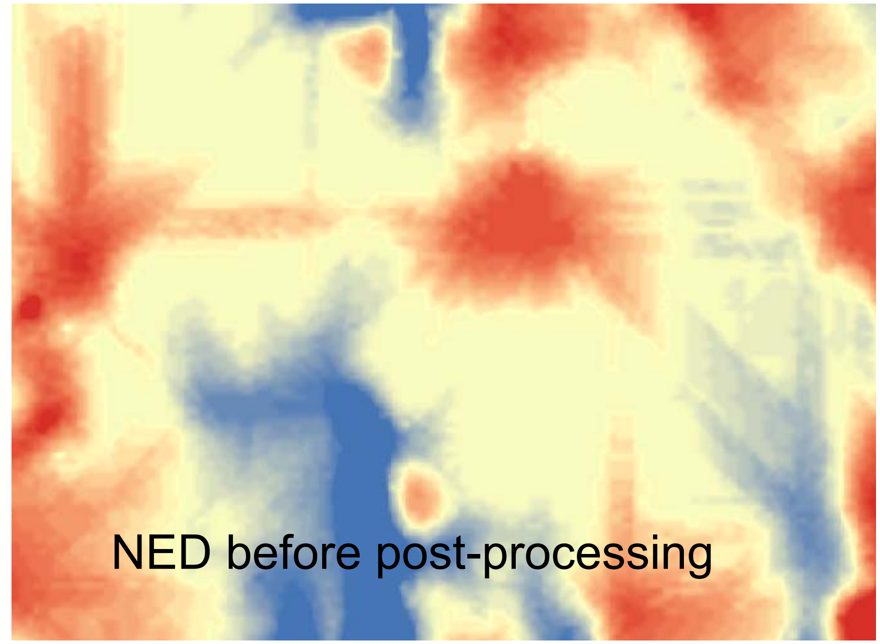
Updating of DEM File

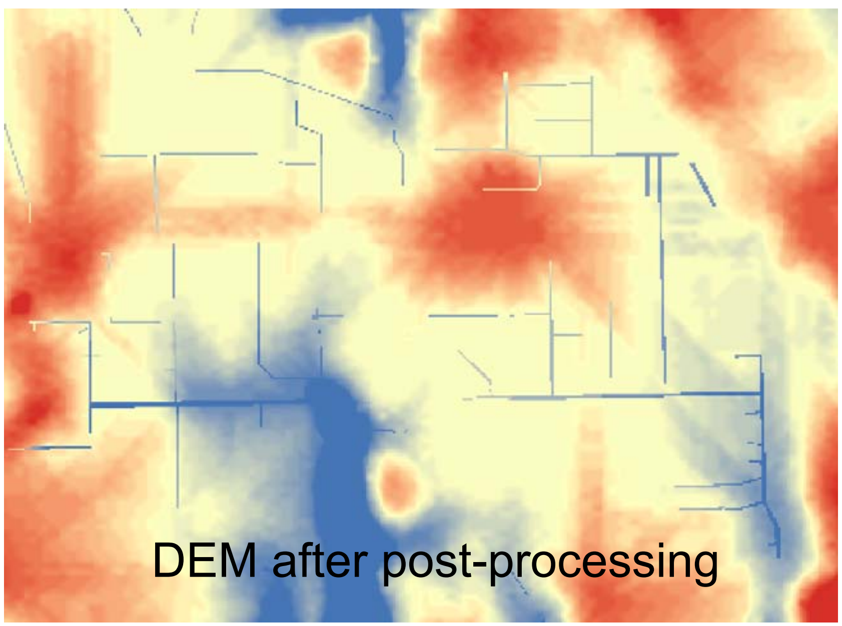


- NED data (USGS)
  - Must process the original NED data to incorporate the ditches information
- LiDAR Data (FDEP)
  - Must process the LiDAR data to reduce the resolution from 5 x 5 ft^2 to 10 x 10 m^2

Updating of DEM File
Post-process NED to Incorporate Ditches Information

Ditches polygon

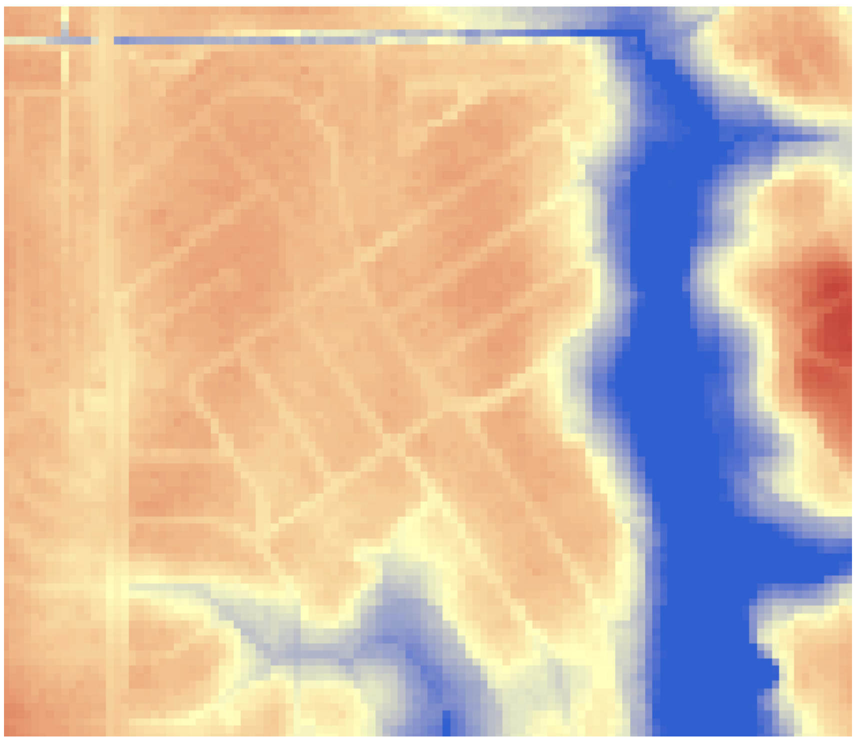

NED before post-processing


DEM after post-processing

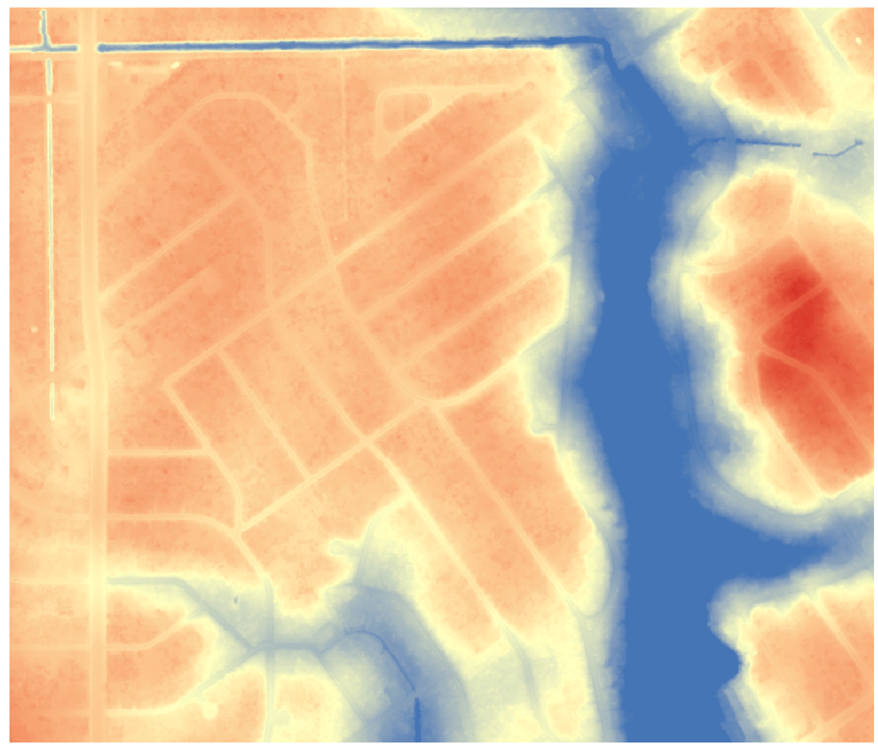
On the original NED, the elevation change around the ditches is not reflected. So we post-process the NED data using the survey ditch depth data associated in the attribute table of the ditch coverage polygon file and make the new elevation where the ditch located equal to the elevation of the original elevation value minus depth of that ditch.

Updating of DEM File
Post-process LiDAR Data

Method: nearest neighborhood re-sampling



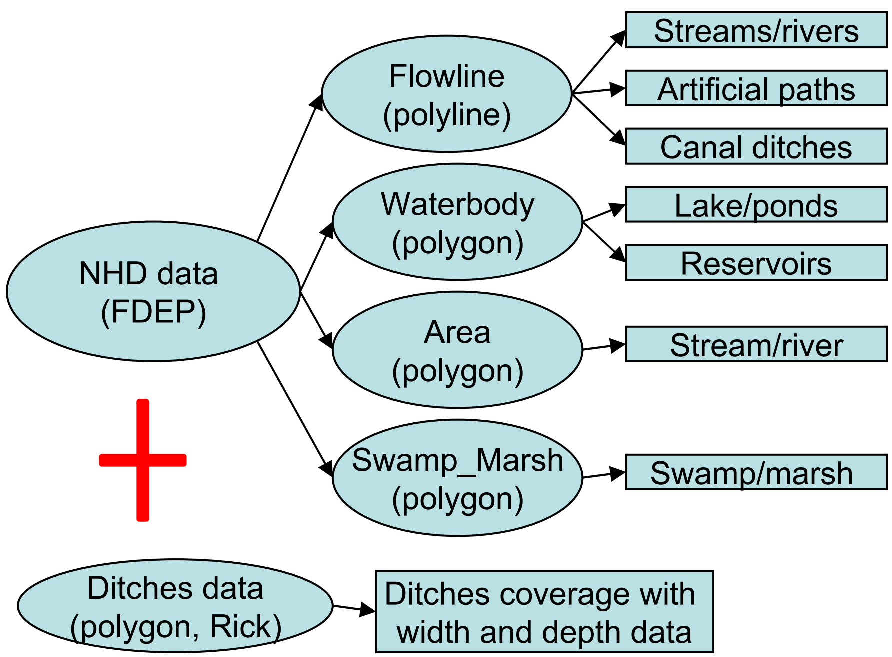
LiDAR after processing
(10×10m)

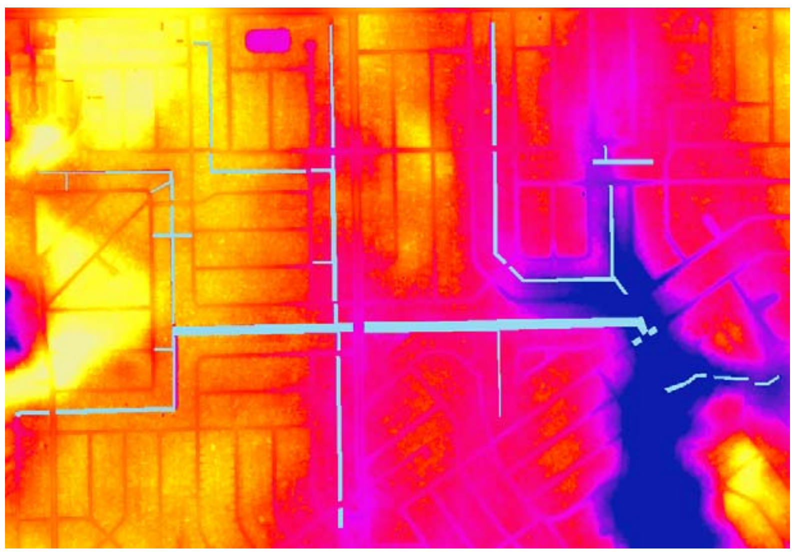


LiDAR before processing
(5×5 feet)

Updating of Water Bodies File

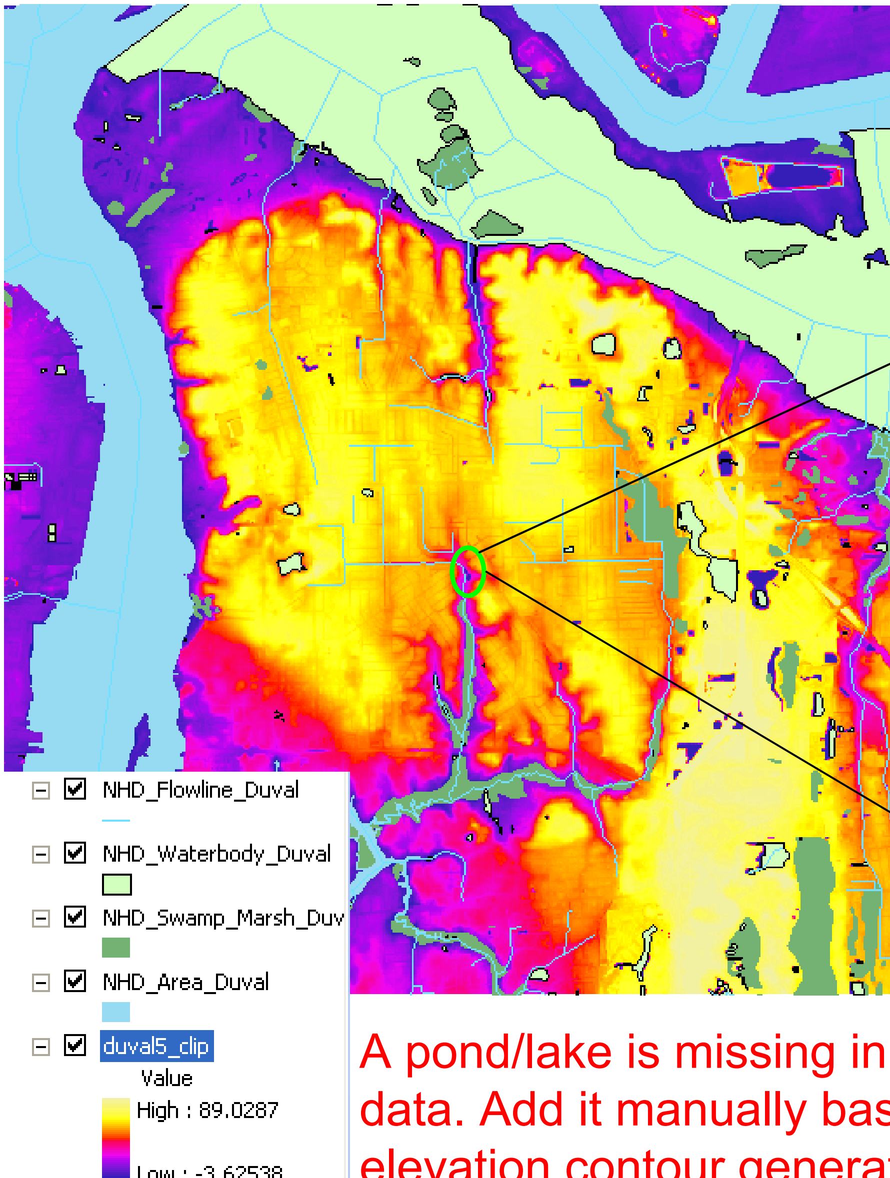
- Manually modify the ditch data to remove the gapes
- Replace the canal ditches component of the flowline file of NHD data with ditches data
- Buffer the flowline with a constant widths of 6m and turn the features into polygon
- Merge the five files together to generate water body polygon file
- Delete the overlap part
- Update base on LiDAR data if necessary

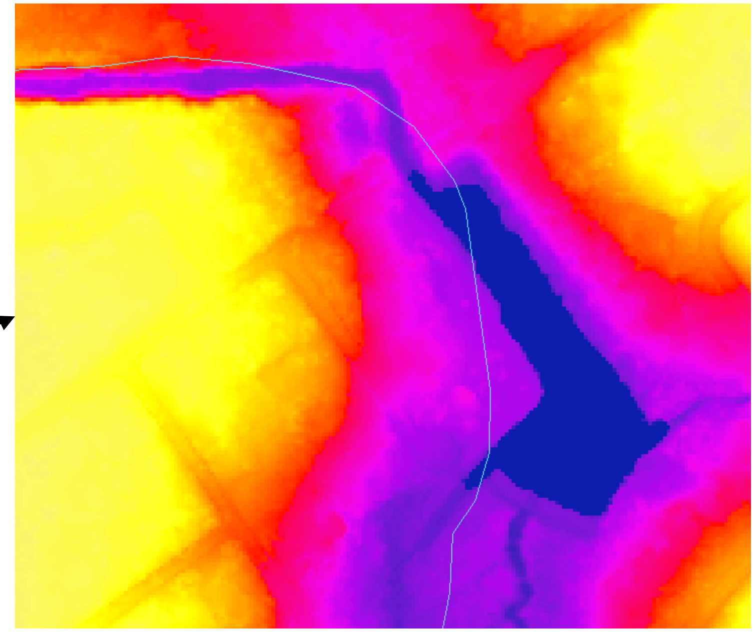




Discontinuity of ditches data

Update Water Bodies File Based on Elevation Contour



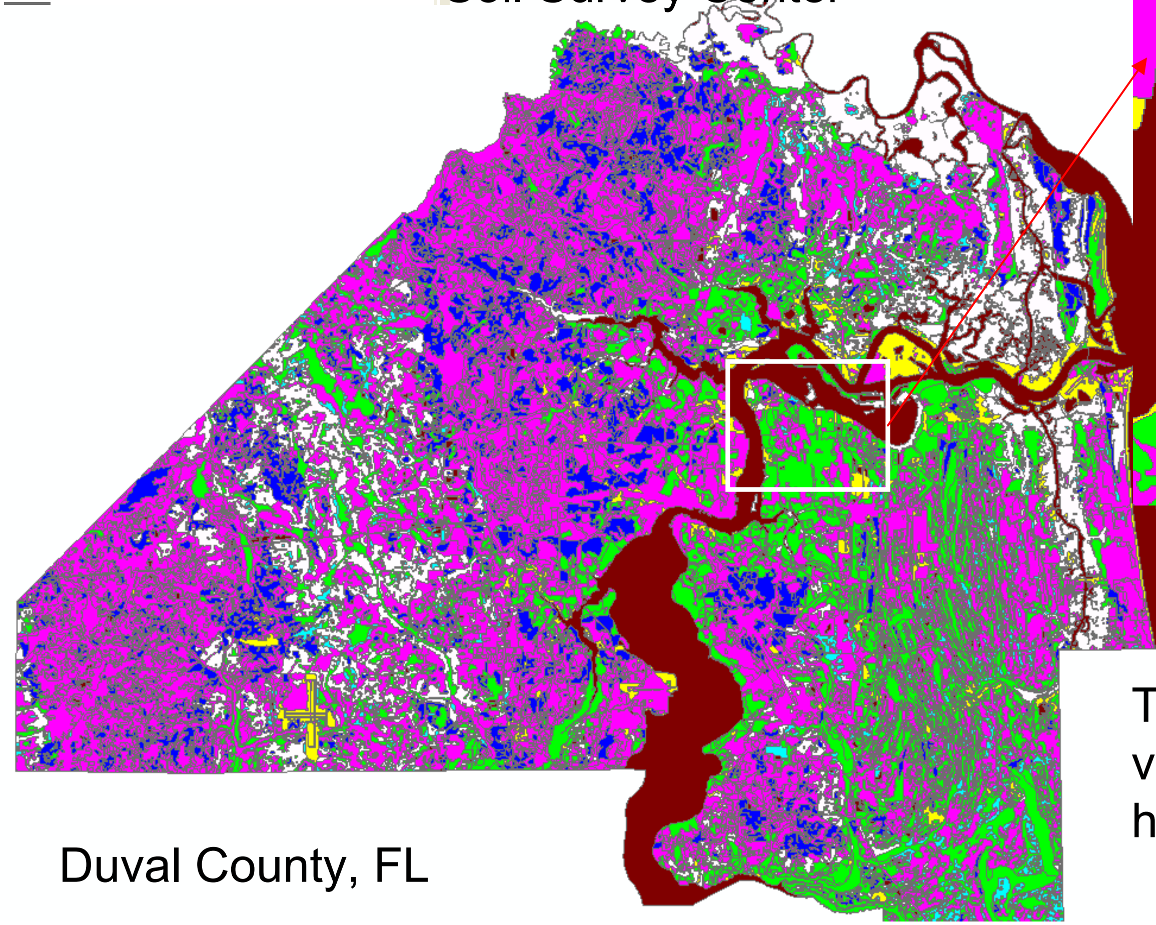


A pond/lake is missing in NHD data. Add it manually based on elevation contour generated from LiDAR DEM

Generate Heterogeneous Hydraulic Conductivity

- 0.017280 - 0.574425
- 0.574426 - 0.709984
- 0.709985 - 1.267129
- 1.267130 - 3.556981
- 3.556982 - 12.968218
- 12.968219 - 51.648178
- 51.648179 - 210.621884

The hydraulic conductivity data is derived from the vertical permeability data downloaded from Soil Data Mart, USDA NRCS National Soil Survey Center



Duval County, FL

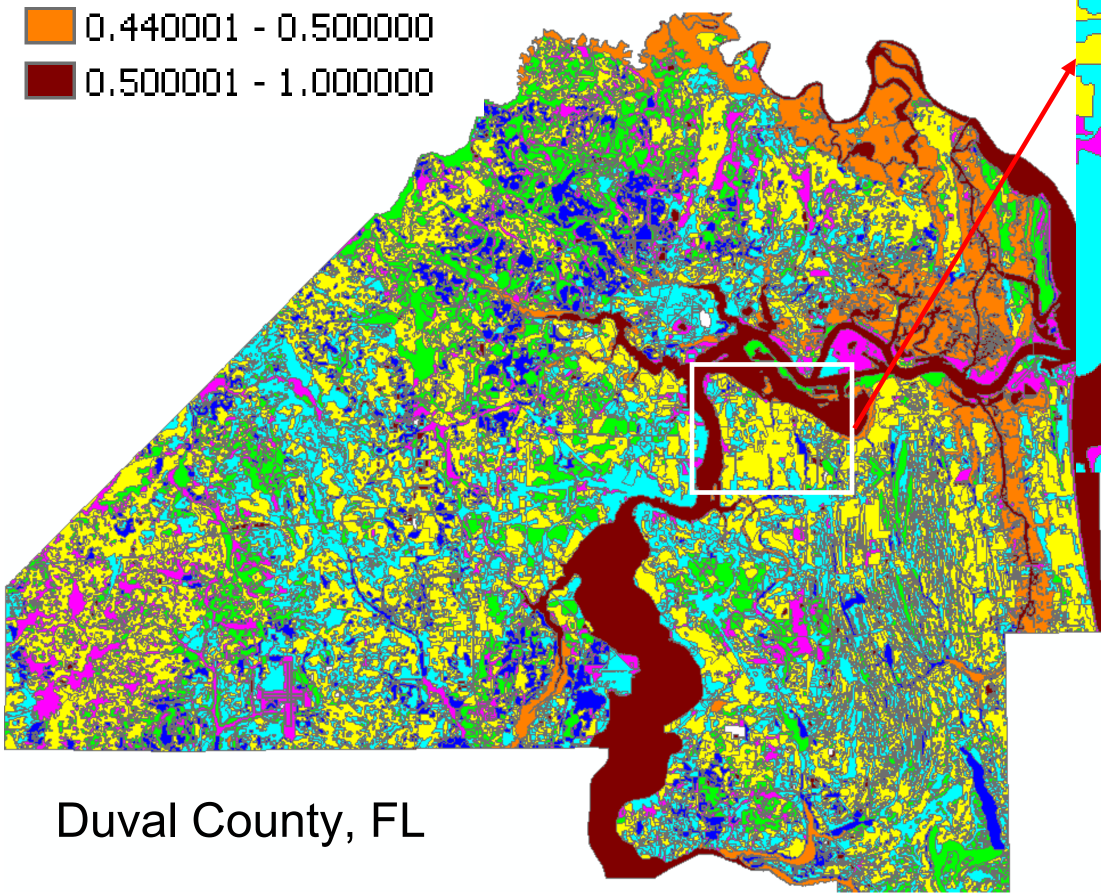
Eggleston Heights

There are three values for K : low value, representative value and high value

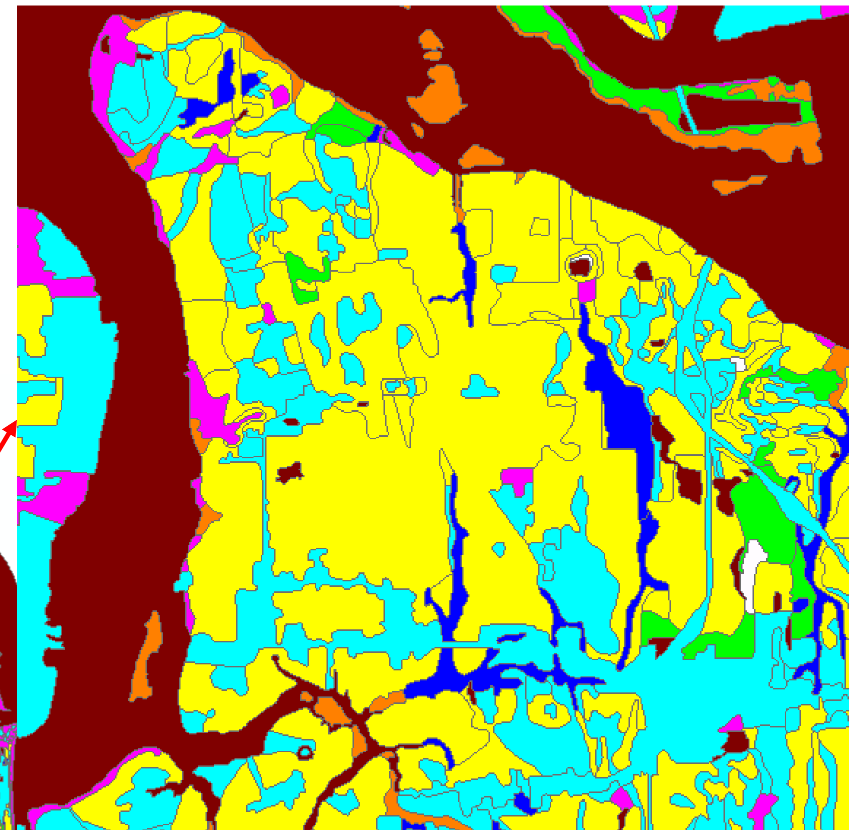
Generate Heterogeneous Soil Porosity

- 0.250000
- 0.250001 - 0.310000
- 0.310001 - 0.350000
- 0.350001 - 0.370000
- 0.370001 - 0.400000
- 0.400001 - 0.440000
- 0.440001 - 0.500000
- 0.500001 - 1.000000

The porosity data is derived from "the estimated volumetric soil water content at or near zero bar tension" data downloaded from Soil Data Mart, USDA NRCS National Soil Survey Center



Duval County, FL



Eggleston Heights

Calibrated Model Parameters

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

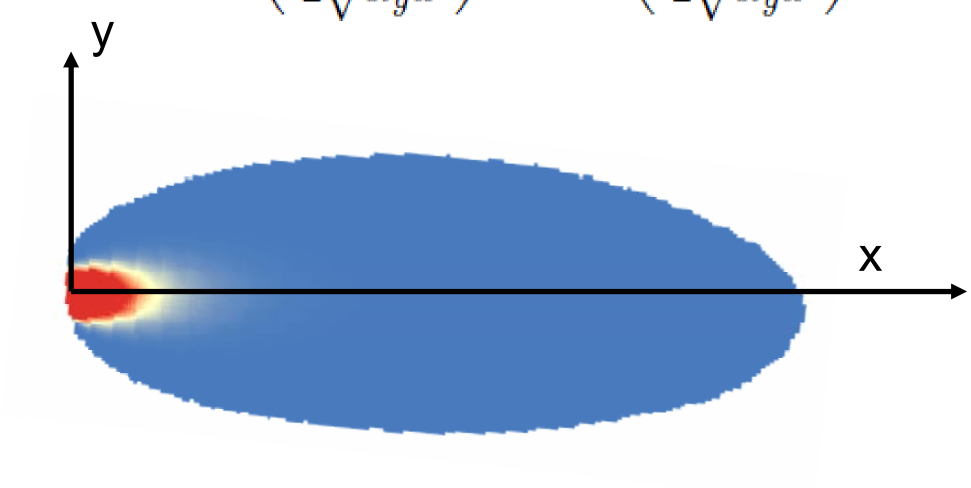
$$F_1 = exp\left[\frac{x}{2\alpha_x}\left(1 - \sqrt{1 + \frac{4k\alpha_x}{v}}\right)\right]$$

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

$$v = \sqrt{v_x^2 + v_y^2}$$

$$v_x = -\frac{K}{\phi}\frac{\partial h}{\partial x} = -\frac{K}{\phi} G_x$$

$$v_y = -\frac{K}{\phi}\frac{\partial h}{\partial y} = -\frac{K}{\phi} G_y$$



Example of a contaminate plume

Calibrated parameters include:

– Groundwater velocity: v
  - ✓Smoothing factor: s
  - ✓Porosity: Φ
  - ✓Hydraulic conductivity: K

– First-order decay coefficient: k

– Dispersivity: α_x and α_y

– Source concentration: C_0

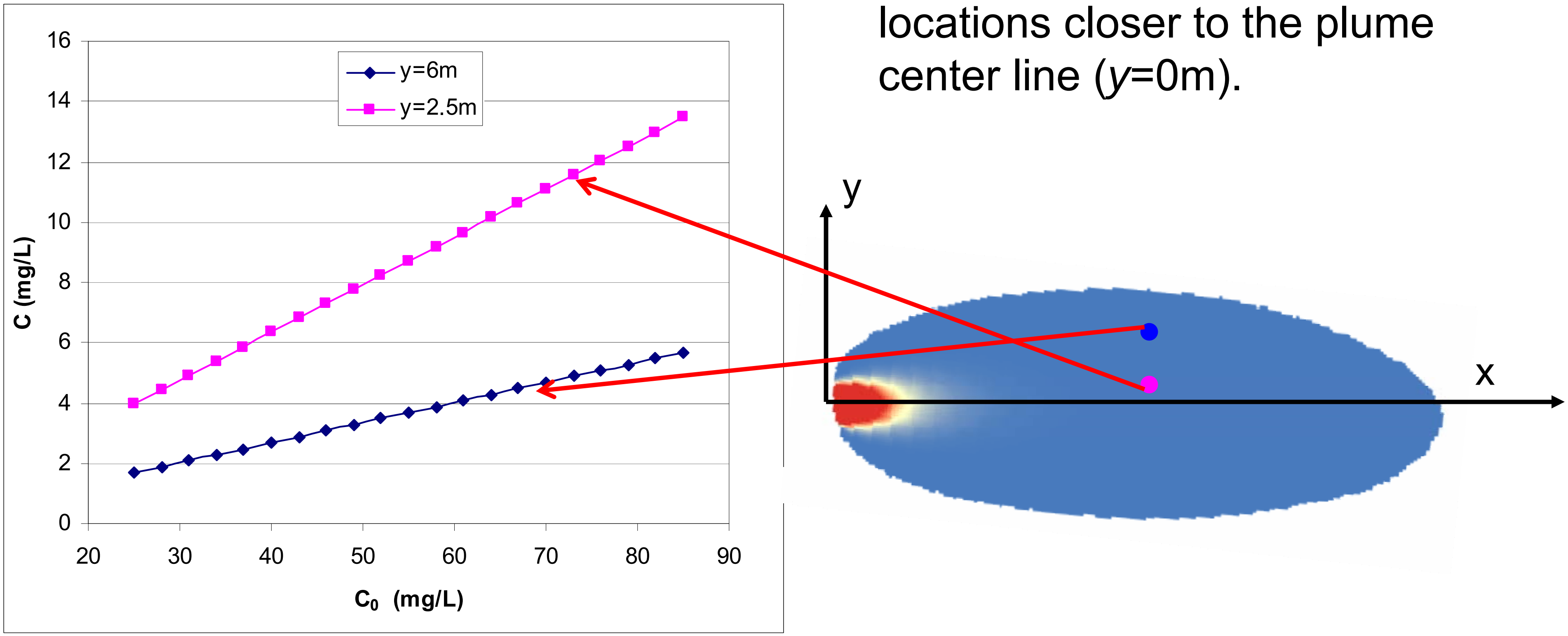
Nominal Parameter Values

- Seepage velocity: v = 0.2 m/d. This is the representative value of the domains of interest.
- Source plane concentration: C_0 = 40 mg/L. McCray et al. (2005).
- First-order decay coefficient: k = 0.008/d. McCray et al. (2005).
- Longitudinal dispersivity: α_x = 2.113 m. This value is similar to the work of Davis (2000) at a vicinity site in Jacksonville, FL.
- Horizontal transverse dispersivity: α_y = 0.234 m. This value is similar to the work of Davis (2000) at a vicinity site in Jacksonville, FL.
- Source plane length: Y = 6m. (Assuming the drainfield is 300 ft^2) .
- X coordinate: x = 30m. This is an arbitrary value selected for the demonstration

Local Sensitivity to Source Concentration

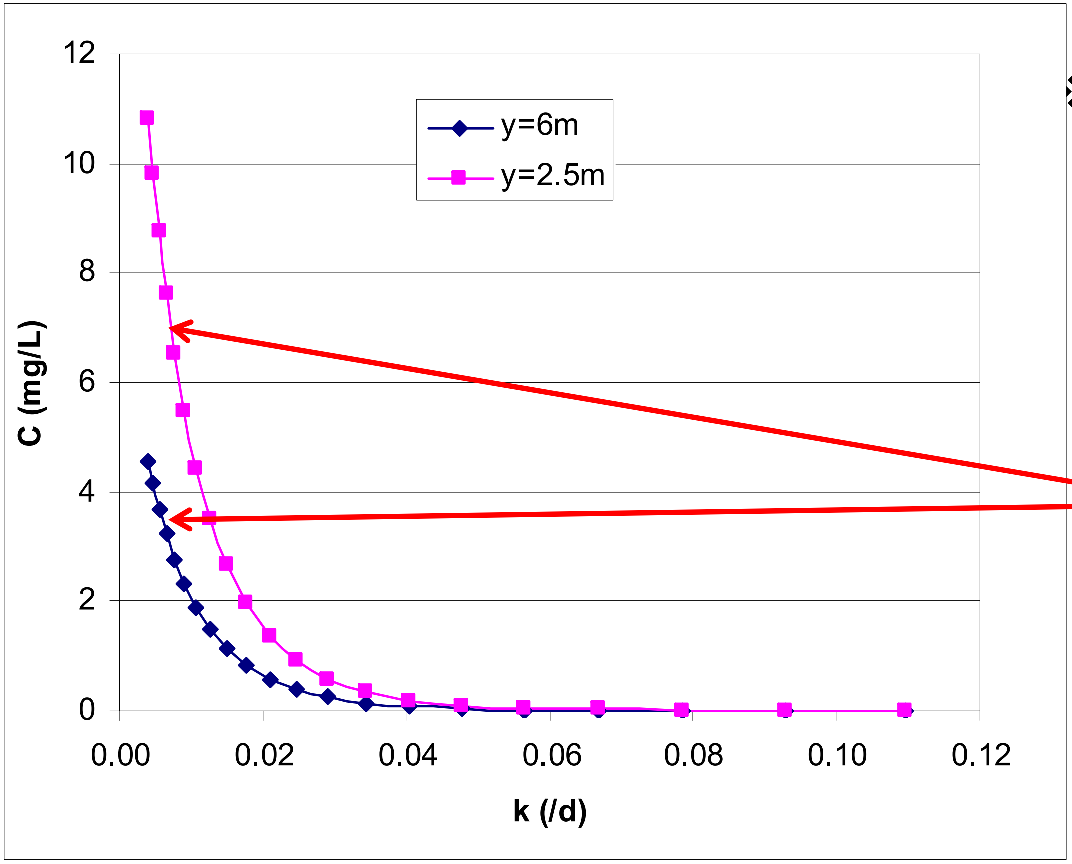
$$\frac{\partial C}{\partial C_0} = \frac{F_1 F_2}{2} > 0$$

- An increasing function of C_0.
- Increase of the source plane nitrate concentration will increase the simulated concentration within the plume.
- The increase is larger at locations closer to the plume center line (y=0m).

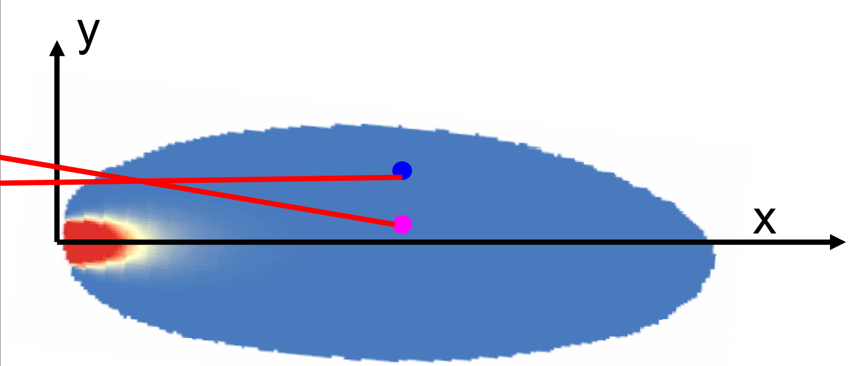


Local Sensitivity to First-order Decay Coefficient

$$\frac{\partial C}{\partial k} = \frac{C_0}{2} F_1 F_2 \frac{-x}{v\sqrt{1+\frac{4k\alpha_x}{v}}} < 0$$

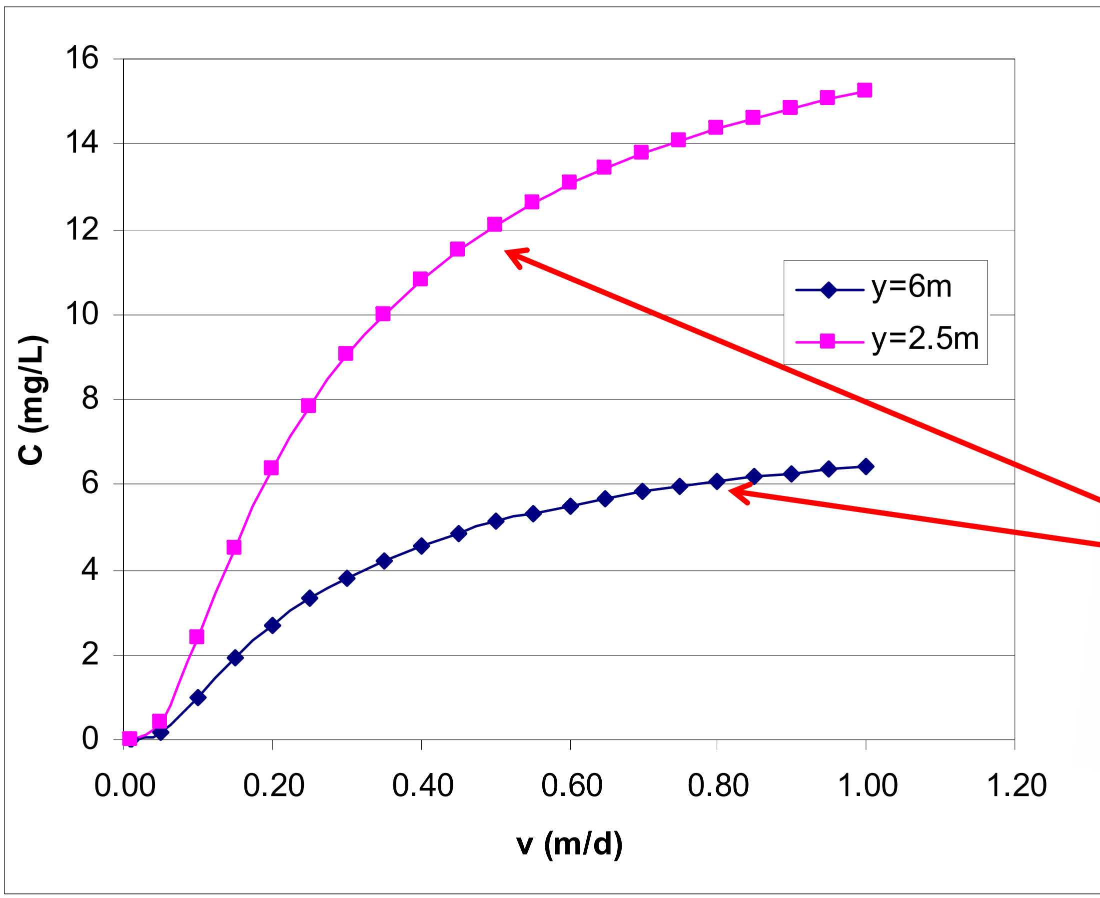


- A decreasing function of k.
- Increase of the first-order decay coefficient will result in decrease of the simulated concentration within the plume.
- The decrease is more rapid at locations closer to the plume center line (*y*=0m).

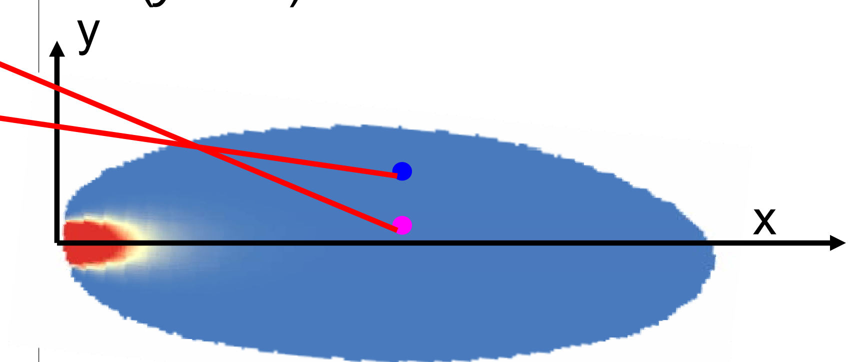


Local Sensitivity to Average Velocity

$$\frac{\partial C}{\partial v} = \frac{C_0}{2} F_1 F_2 \frac{kx}{v^2 \sqrt{1 + \frac{4k\alpha_x}{v}}} > 0$$

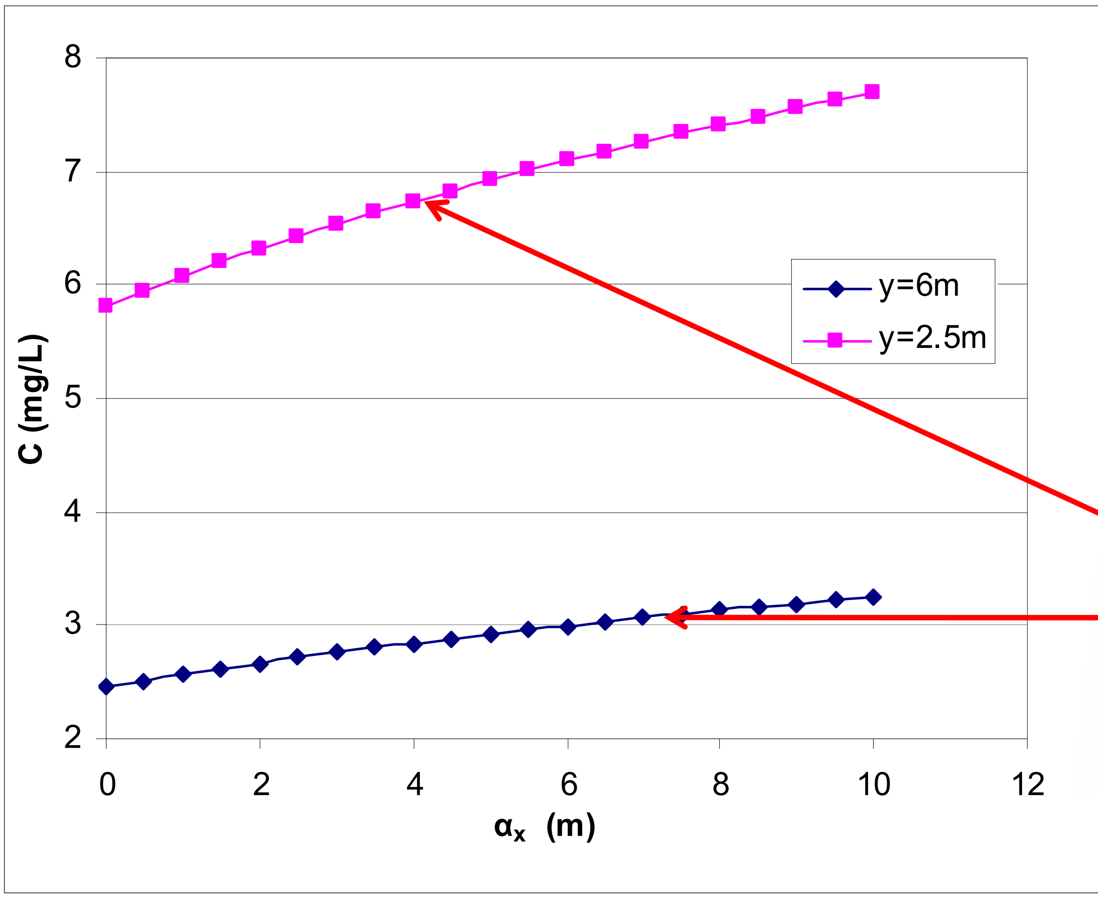


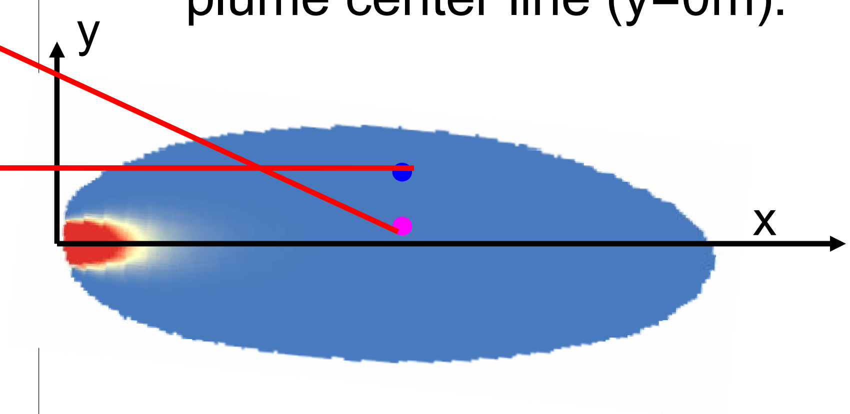
- An increasing function of v.
- Increase of the velocity is associated with increase the simulated concentration within the plume.
- The increase is more rapid at location closer to the plume center line (y=0m).



Local Sensitivity to Longitude Dispersivity

$$\frac{\partial C}{\partial \alpha_x} = \frac{C_0}{2} F_2 F_1 \frac{2xk^2}{v^2 \sqrt{1+\frac{4k\alpha_x}{v}} \left(\frac{2k\alpha_x}{v} + 1 + \sqrt{1+\frac{4k\alpha_x}{v}} \right)} > 0$$



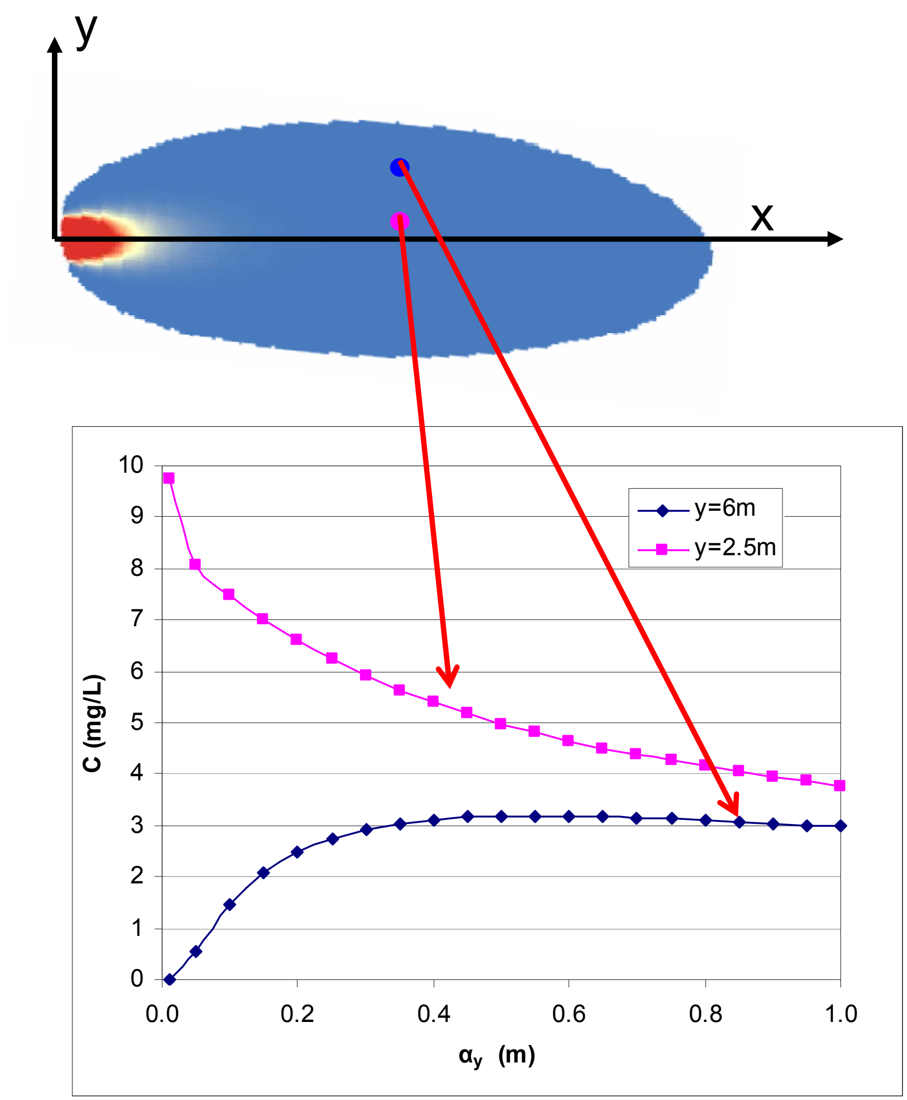


- An increasing function of α_x.
- Increasing α_x causes increase of the simulated concentration within the plume.
- The increase is more rapid at locations closer to the plume center line (y=0m).

Local Sensitivity to Transverse Dispersivity

$$\frac{\partial C}{\partial \alpha_y} = \frac{C_0}{2} F_1 \frac{1}{2\sqrt{\pi x}} \alpha_y^{-\frac{3}{2}} \exp\left(-\frac{y^2 + 0.25Y^2}{4\alpha_y x}\right)\left[(y-0.5Y)\exp\left(\frac{0.5yY}{2\alpha_y x}\right) - (y+0.5Y)\exp\left(-\frac{0.5yY}{2\alpha_y x}\right)\right]$$

$$= \begin{cases} \geq 0 & \alpha_y \leq \dfrac{0.5Yy}{x\ln\left(\dfrac{y+0.5Y}{y-0.5Y}\right)}, y > 0.5Y \\ \leq 0 & \alpha_y \geq \dfrac{0.5Yy}{x\ln\left(\dfrac{y+0.5Y}{y-0.5Y}\right)}, y > 0.5Y \\ < 0 & 0 \leq y \leq 0.5Y \end{cases}$$



- The relationship depends on the location.
- There is a threshold value.
- When α_y is smaller than the threshold value, the relationship is positive, but becomes negative if the threshold value is exceeded.

Recommended Parameter Range

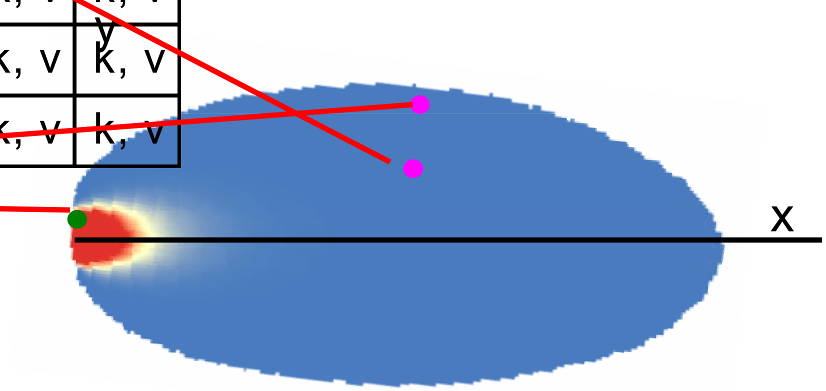
- using in global sensitivity study and model calibration

Dispersivity (m)		Hydraulic conductivity K (m/d) and soil porosity □	First-order decay coefficient (/d) k	Source concentration (mg/l) C_0
α_x	α_y			
0.21-21.34 Davis (2000), Gelhar et al.(1992)	0.021-2.134 Davis (2000), Gelhar et al.(1992)	Soil Survey Data (U.S. Department of Agriculture)	0.004-2.27 McCray et al. (2005)	25-80 McCray et al. (2005)

Global Sensitivity Analysis

Two parameters most critical to simulated nitrate concentration at selected locations of the plume

y(m) \ x(m)	0.0001	5	10	15	20	30	40	50
0	C_0, v	k, v	k ,v	k, v	k, v	k, v	k, v	k, v
1	C_0, v	k, v	k ,v	k, v	k, v	k, v	k, v	k, v
2	C_0, v	k, v	k ,v	k, v	k, v	k, v	k, v	k, v
3	C_0, v	k, v	k ,v	k, v	k, v	k, v	k, v	k, v
4	/	k, v	k ,v	k, v	k, v	k, v	k, v	k, v
6	/	α_y, k	k ,v	k, v	k, v	k, v	k, v	k, v
8	/	α_y, k	k , α_y	k, α_y	k, v	k, v	k, v	k, v
10	/	α_y, k	α_y, k	k, α_y	k, α_y	k, v	k, v	k, v
12	/	α_y, k	α_y, k	k, α_y	k, α_y	k, α_y	k, v	k, v



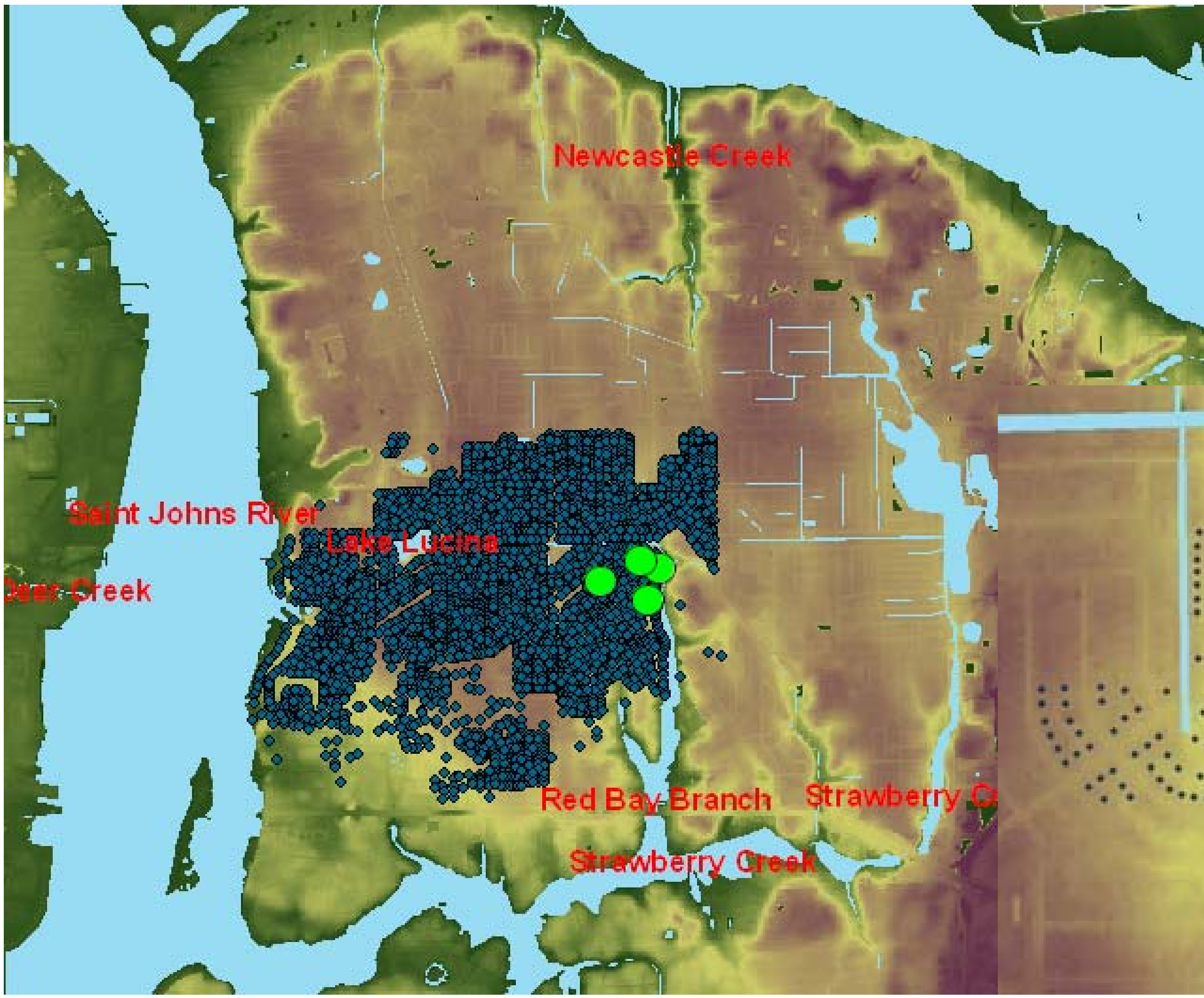
Conclusions of Sensitivity Analysis

- Increasing average velocity (i.e., increasing hydraulic conductivity and decrease soil porosity), longitude dispersivity, source concentration will cause increase of simulated concentrations at any locations. Increase of concentration is larger at locations near the source.
- Increasing the first-order decay coefficient will cause decrease of simulated concentrations at any locations.
- Increasing transverse dispersivity will cause
  - If $y<0.5Y$: decrease of simulated concentrations,
  - If $y>0.5Y$: increase of simulated concentrations at locations of $x>x_{critical}$ but decrease at $x<x_{critical}$.

$$x_{critical} = \frac{0.5Yy}{\alpha_y \ln\left(\frac{y+0.5Y}{y-0.5Y}\right)}$$

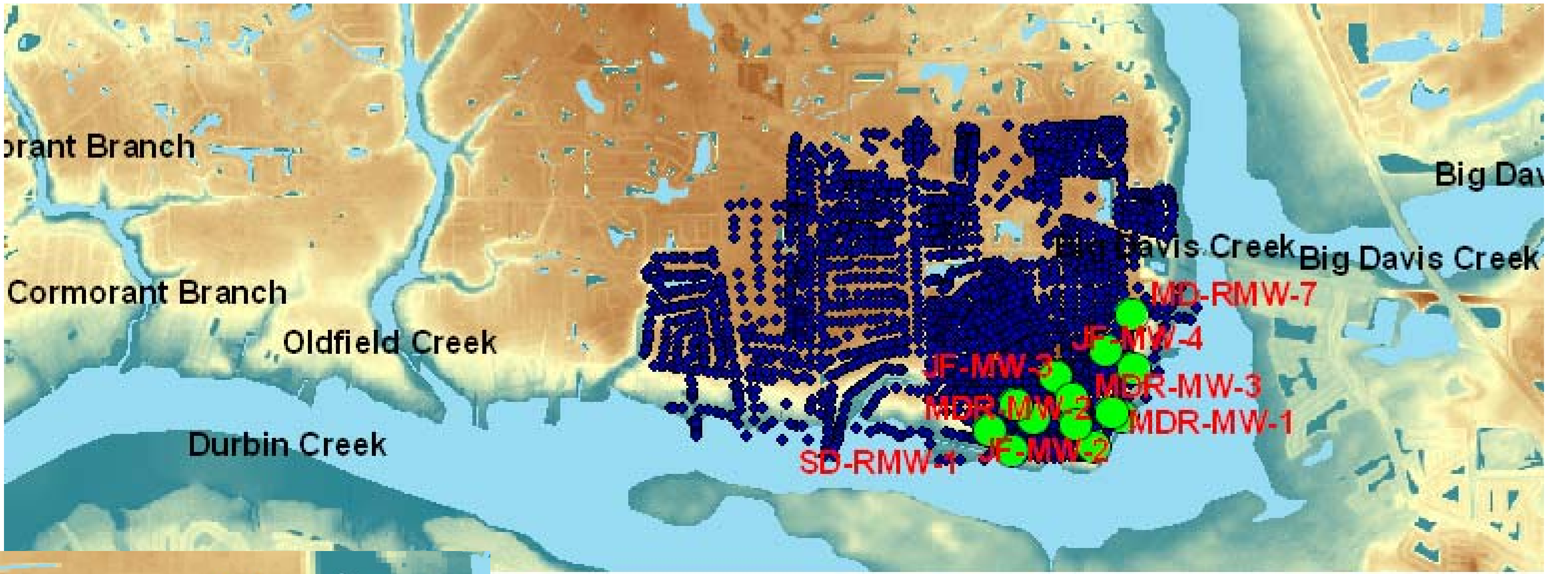
- When the locations are relatively close to the plume center line, the most critical parameter is first-order decay coefficient and flow velocity. Otherwise is first-order decay coefficient and transverse dispersivity

Study Domain: Eggleston Heights



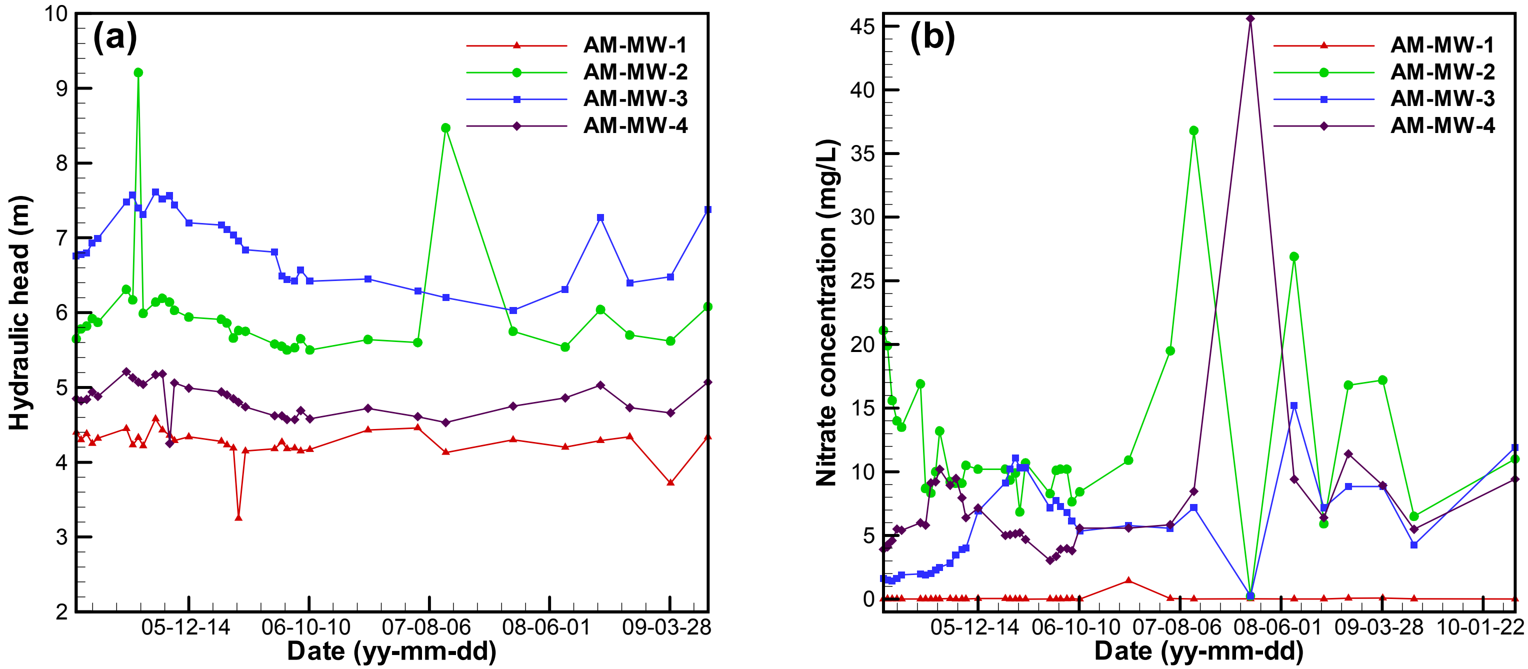
A total of 3517 septic tanks and 4 monitoring wells

Study Domain: Julington Creek



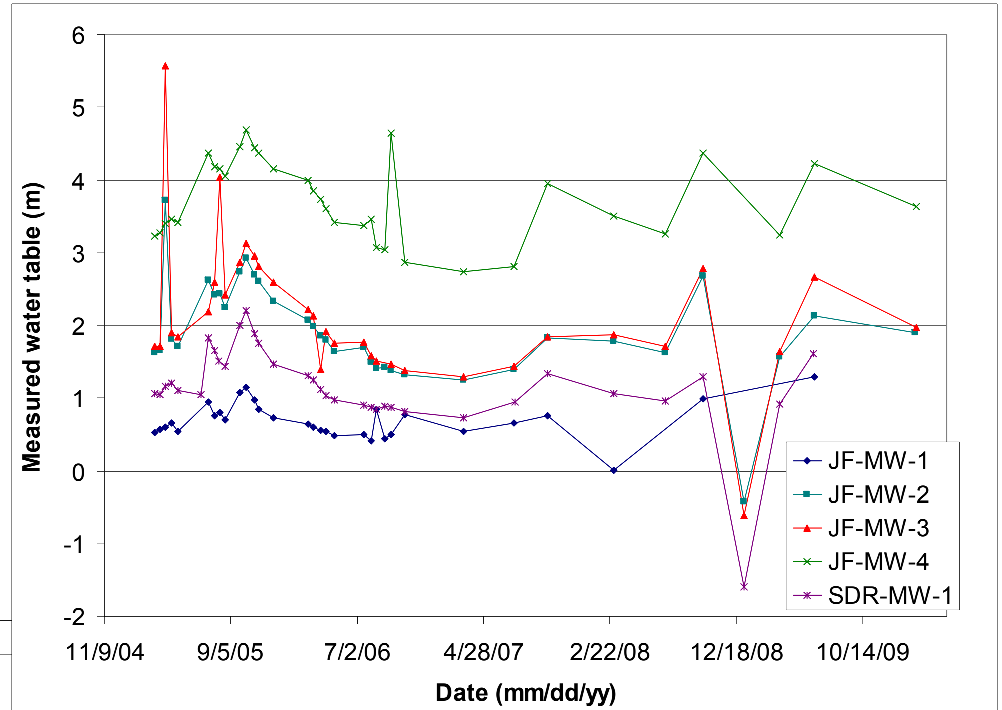
A total of 1978 septic tanks and 13 monitoring wells

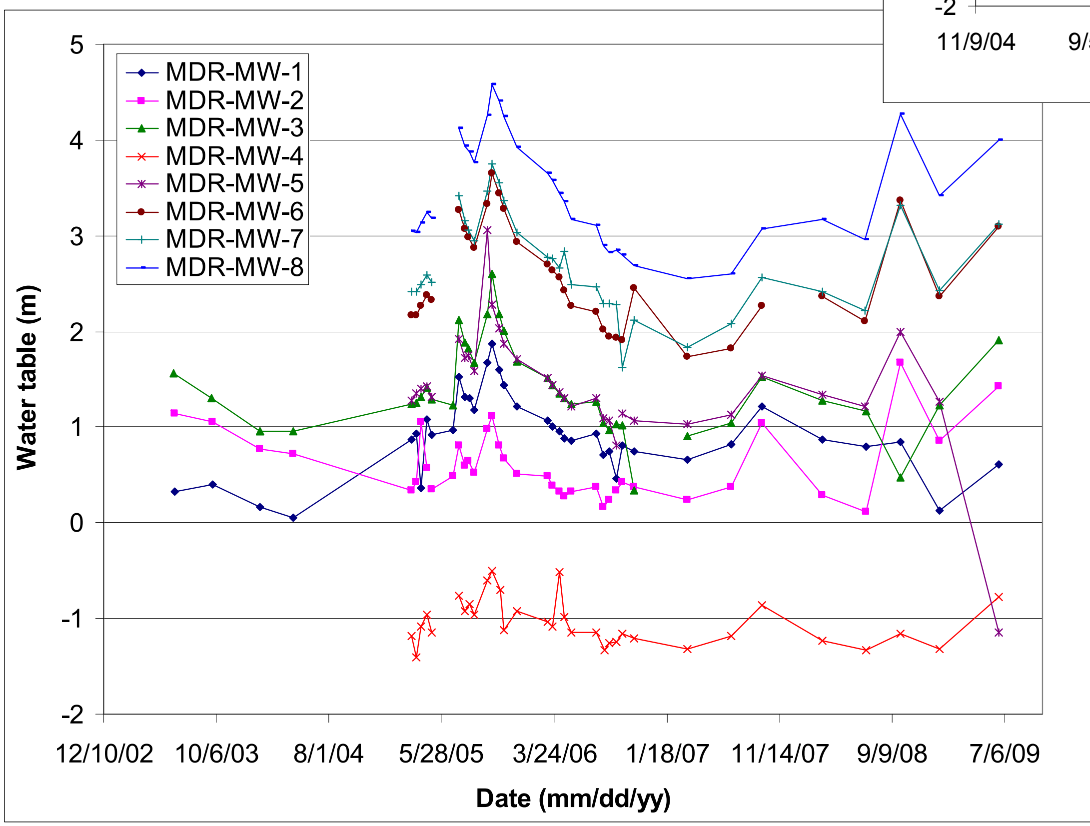
Field Observation Data (Eggleston Heights)



- A total of 136 observations of water level depth and 143 observations of nitrate concentration from the four monitoring wells were collected during the period from 03/08/2005 to 04/27/2010.
- The water table can be considered as steady, only the mean value is used in calibration
- The nitrate concentration measurement has big fluctuation, therefore the mean value, the upper and lower quartile as well as the maximum and minimum values are all considered in calibration

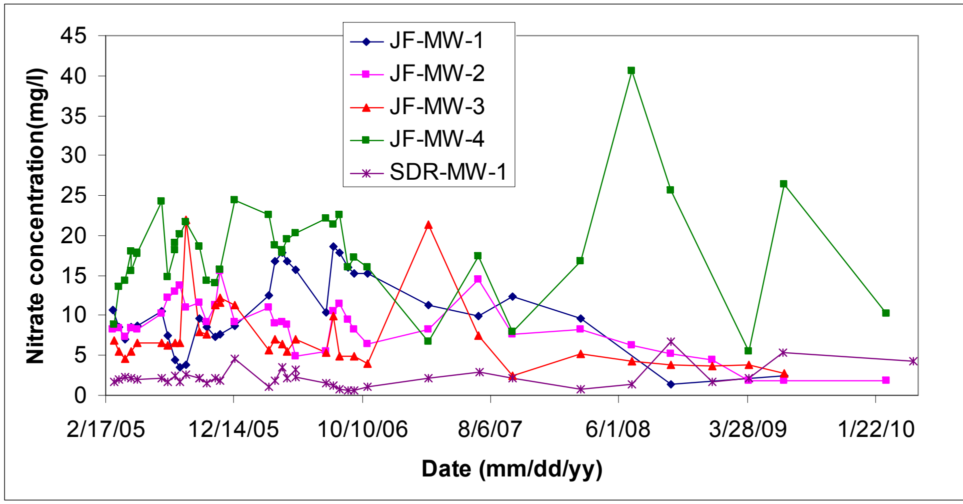
Field Observation Data (Julington Creek)

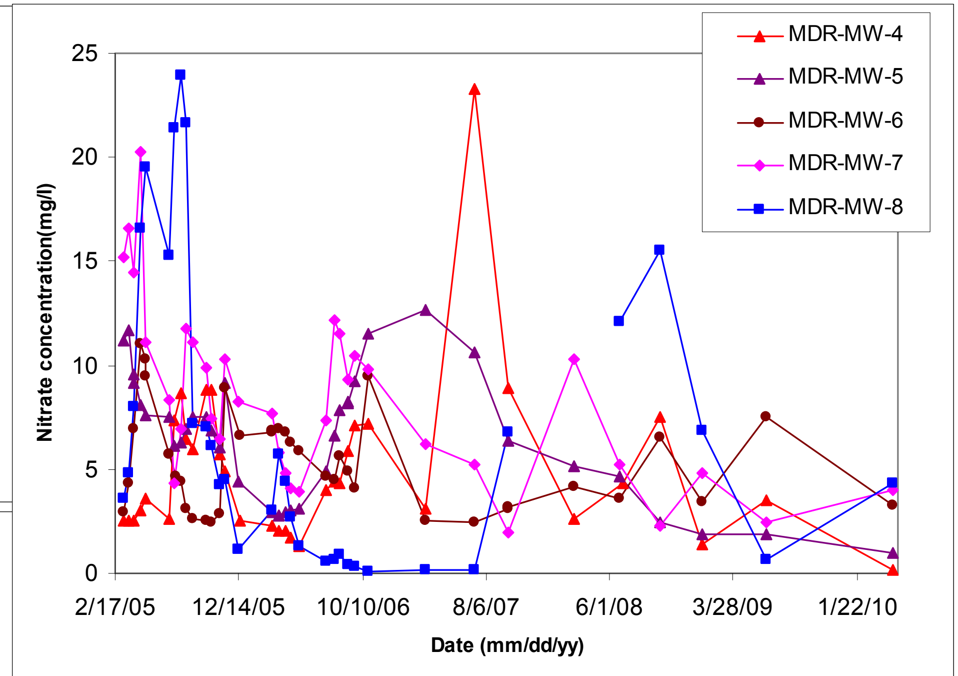


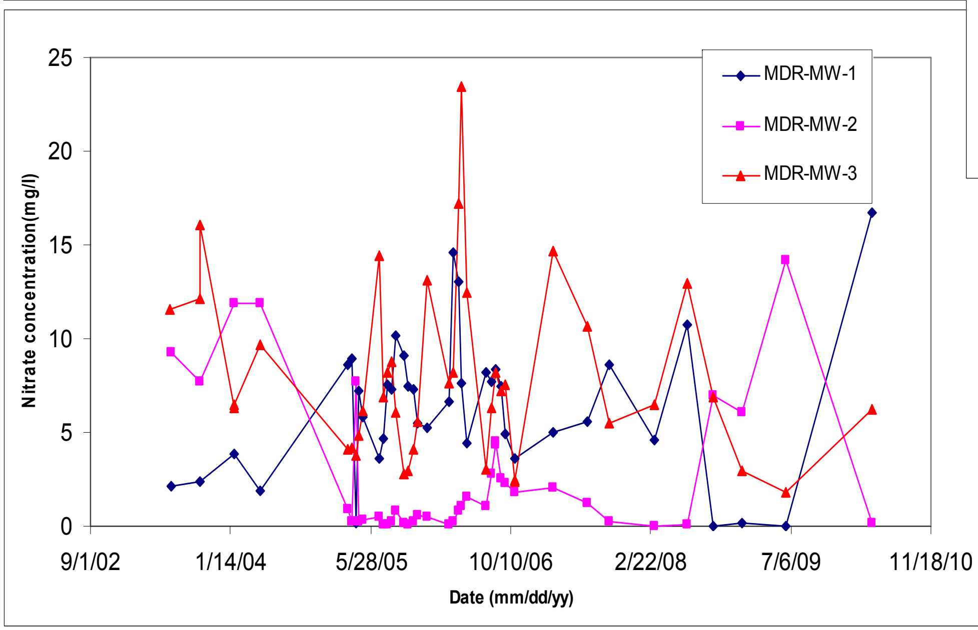


A total of 451 observations of water level depth from the 13 monitoring wells were collected during the period from 06/16/2003 to 02/17/2010.

Field Observations (Julington Creek)



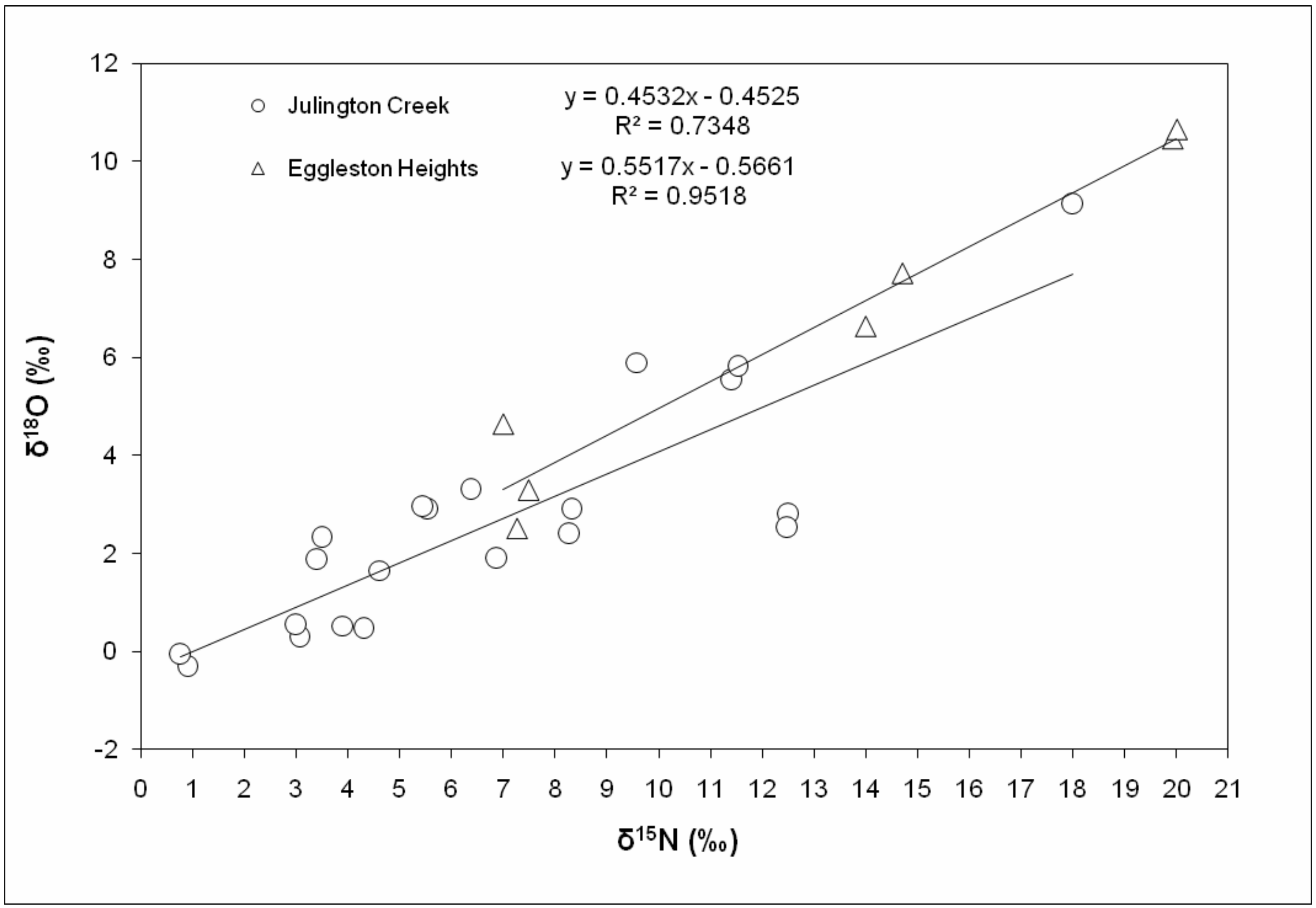




A total of 484 observations of nitrate concentration from the 13 monitoring wells were collected during the period from 06/16/2003 to 04/21/2010.

Isotopes Observations : $\delta^{15}N$ and $\delta^{18}O$

A linear relationship between $\delta^{18}O$ and $\delta^{15}N$ with a slope close to 0.51 (0.48 - 0.67) indicates that denitrification occurs. (Chen and Mcquarrie , 2005).



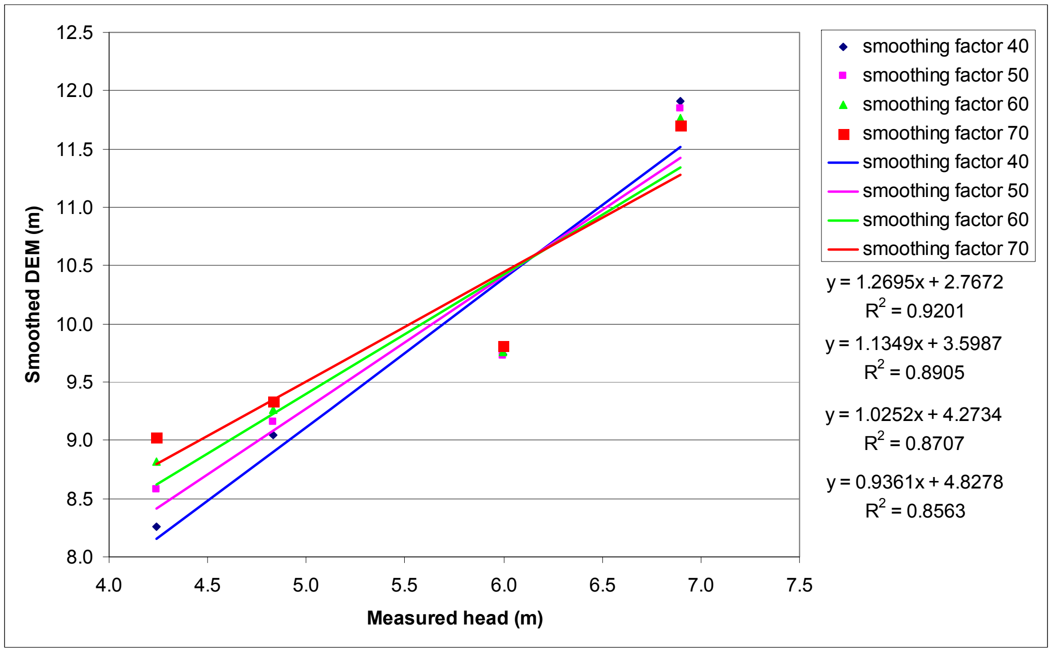
$\delta^{18}O$ vs. $\delta^{15}N$ Julington Creek and Eggleston Heights (Sep & Oct, 2010).

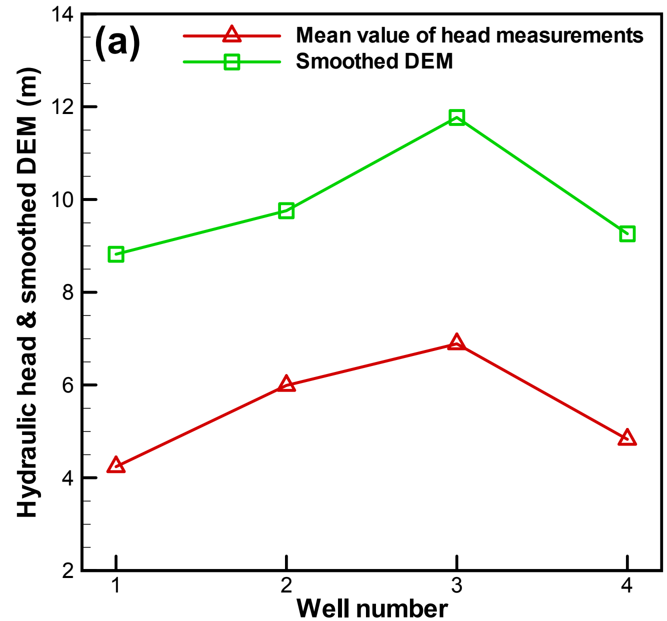
The linear relationship and the slope of a plot of $\delta^{18}O$ verses $\delta^{15}N$ data from Julington Creek and Eggleston Heights is an isotopic signature for denitrification

Calibrating Procedure

- Adjust smoothing factor to match head gradient measurements
- Adjust source concentration, hydraulic conductivity, dispersivity, first-order decay coefficient to match the concentration measurements.
- The model is capable of using different source concentration, dispersivity, first-order decay coefficient for every plume. But homogenous value of these parameters was recommended unless there is enough information

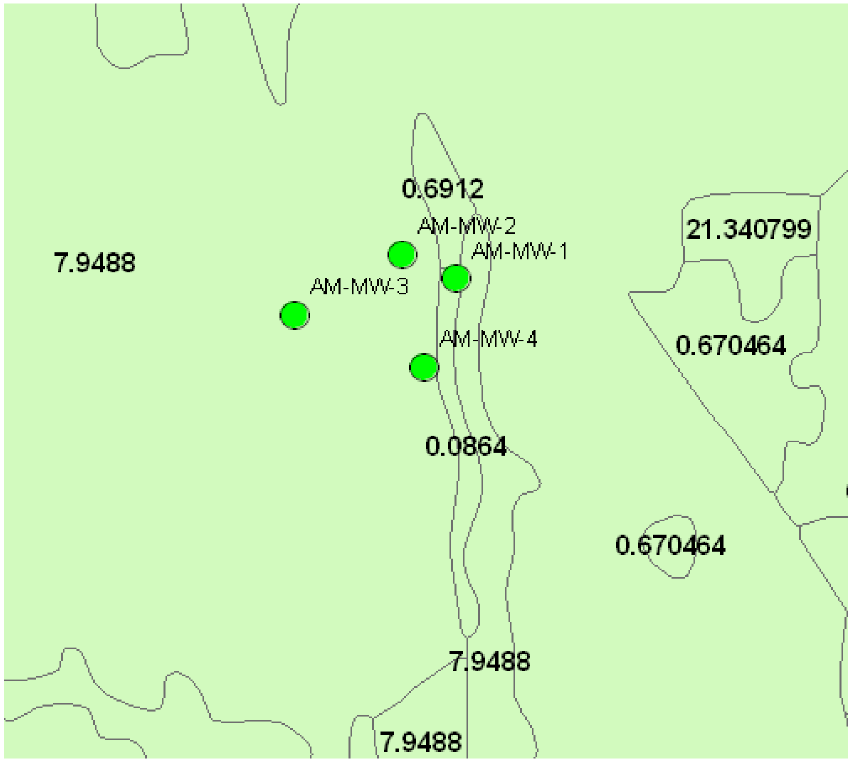
Calibrated Smoothing Factor (Eggleston Heights)

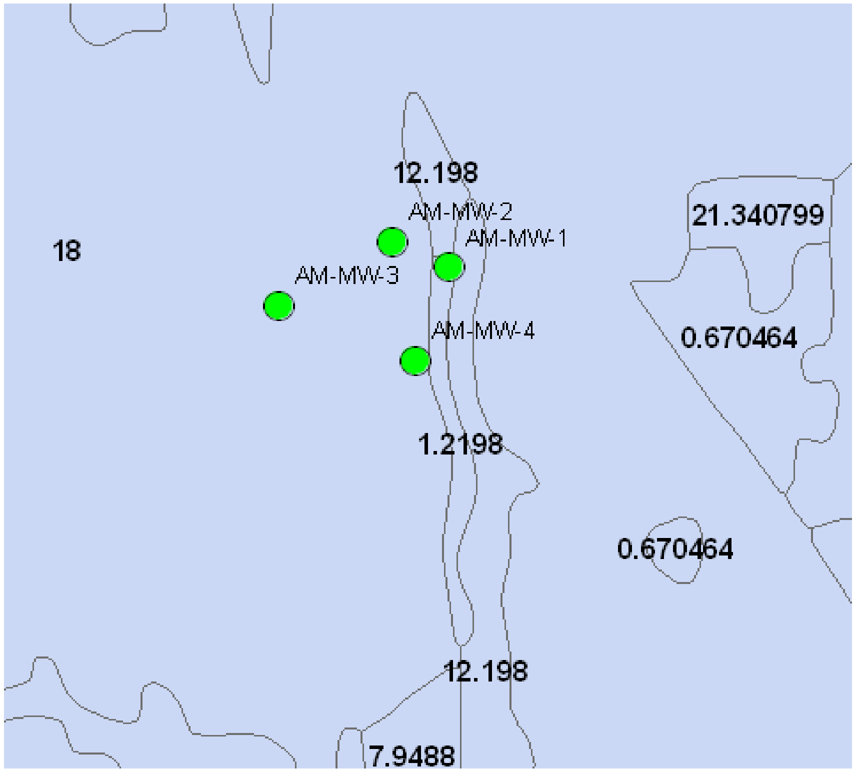




- Larger smoothing factors give smaller slopes of the regression lines and linear correlation coefficients.
- The best smoothing factor (i.e. 60 in this case) is selected for the slope close to unit with linear correlation coefficients larger than 0.9.

Calibrated Hydraulic Conductivity (Eggleston Heights)



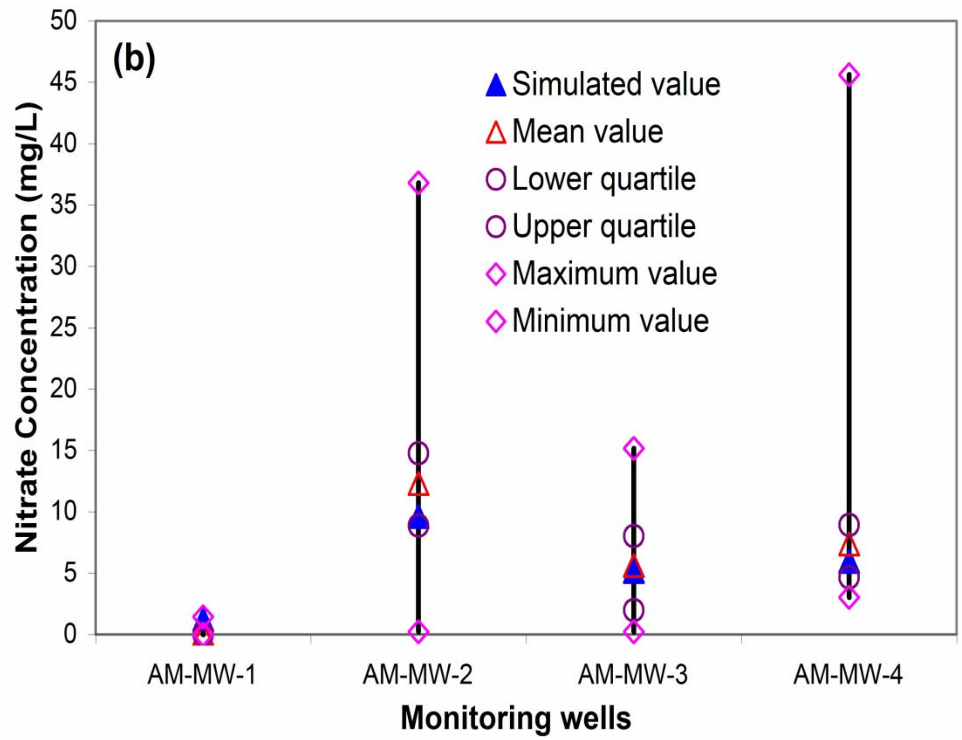


Zonal values of original (left) and calibrated (right) hydraulic conductivity

Calibration Results (Eggleston Heights)

Other parameters

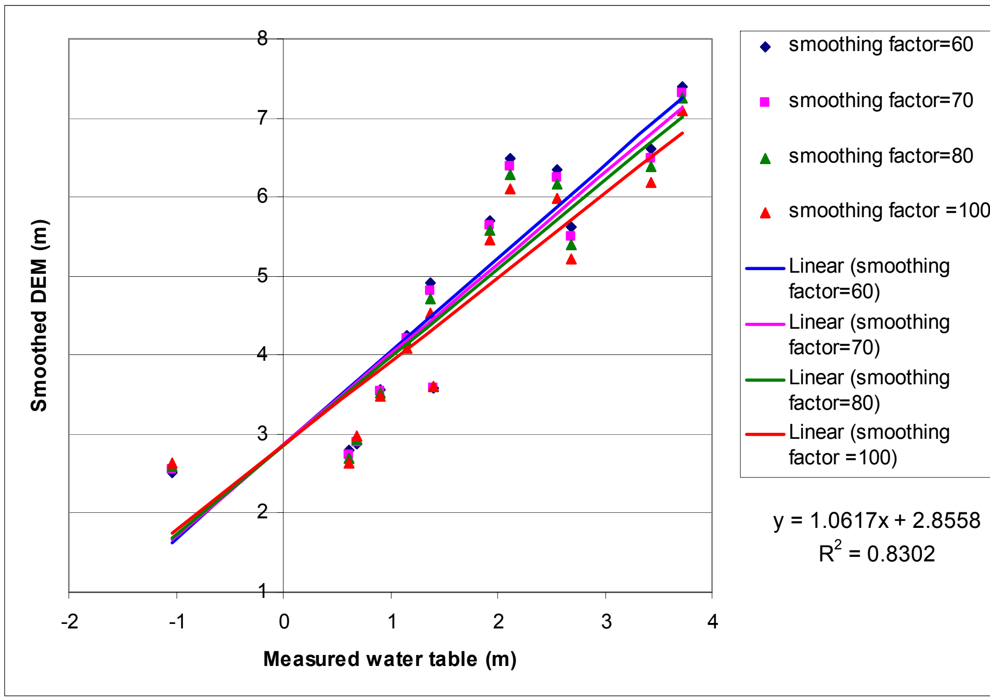
- –Width of the source plain Y=6m
- –Decay coefficient: k = 0.005 /d
- –Dispersivity: α_x = 10.0 m, α_y =1.0 m .
- –Porosity: Φ = the original values from the soil survey data

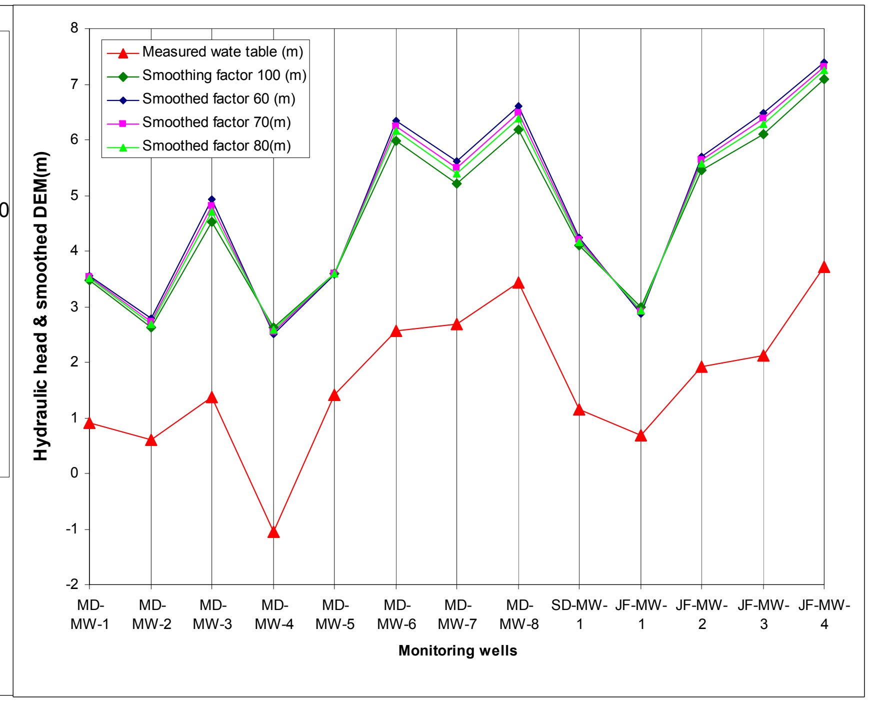


All of the simulated concentration are within the maximum and minimum range, 3 of them are within the lower and upper quartile and very close to mean values

Calibrated Smoothing Factor (Julington Creek)

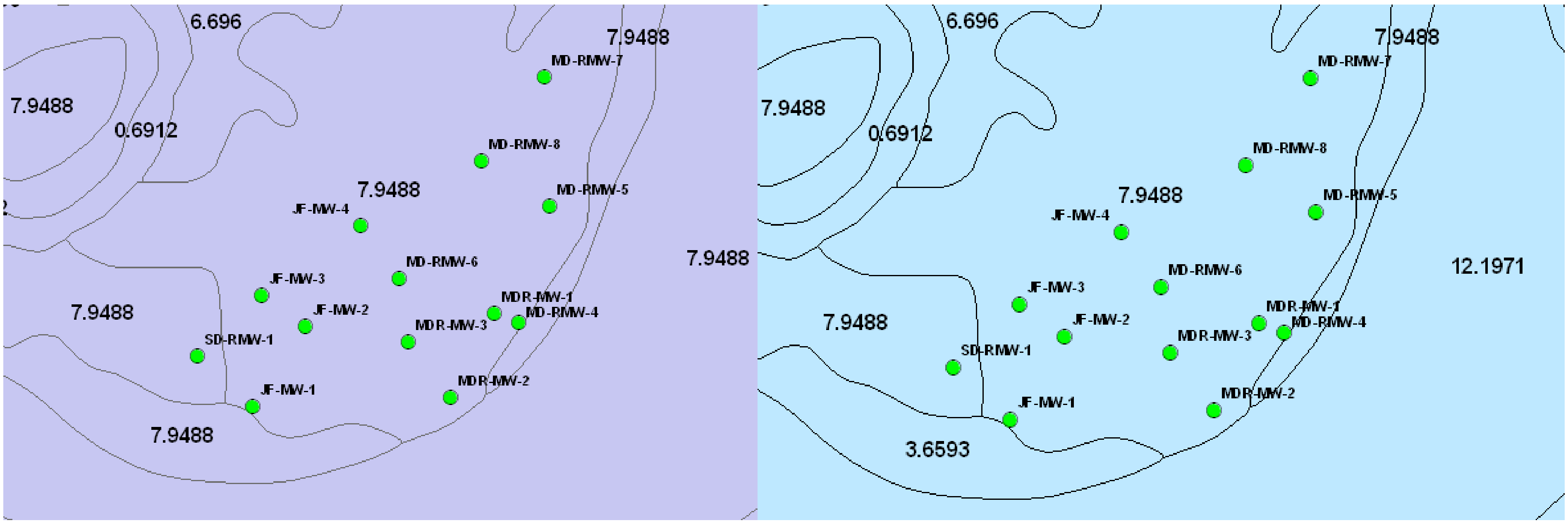
Smoothing factor of 100 is selected.





Larger smoothing factors give smaller slopes of the regression lines and linear correlation coefficients.

Calibrated Hydraulic Conductivity and Other Parameters (Julington Creek)

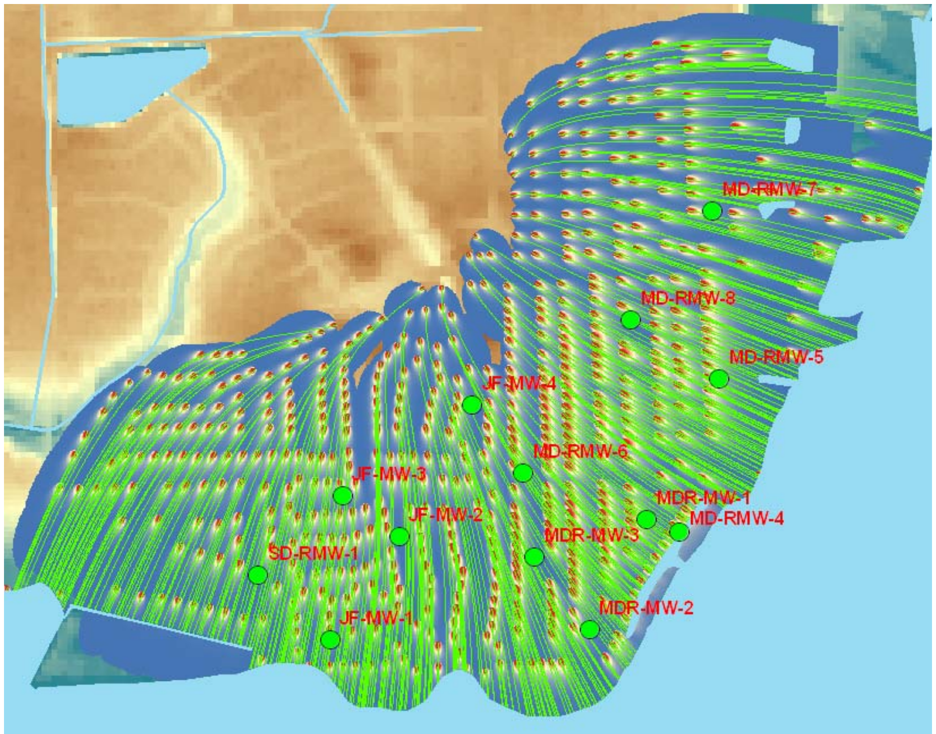


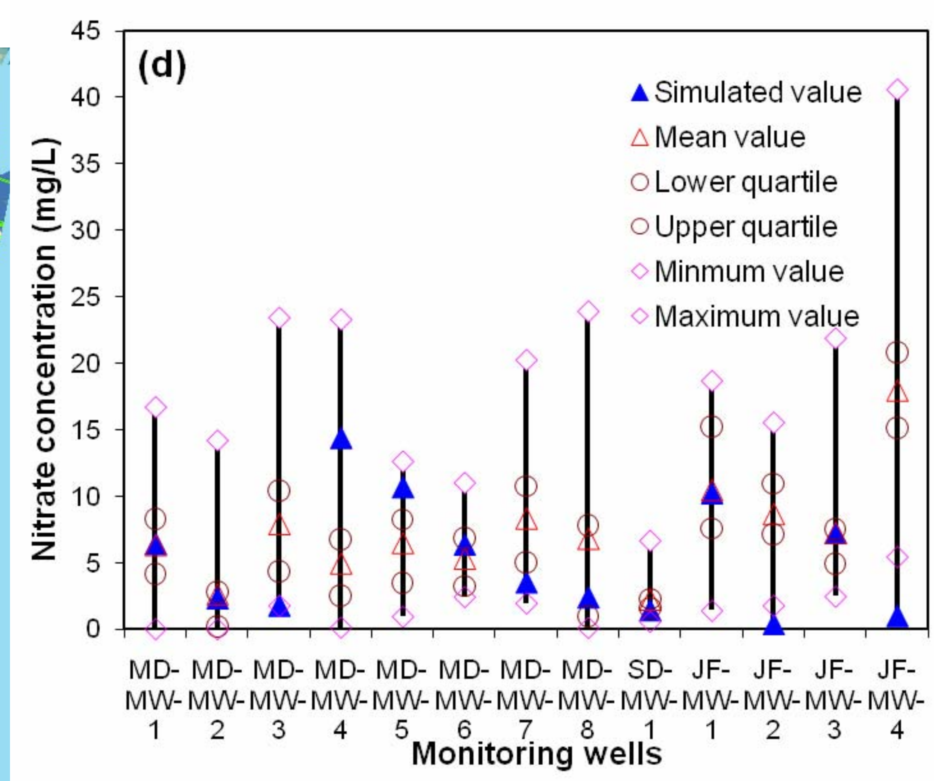
Zones of original hydraulic conductivity (left) and after calibration (right)

Other parameters

- Width of the source plain Y=6m
- Decay coefficient: k = 0.012 /d
- Dispersivity: α_x = 10.0 m, α_y =1.0 m.
- Soil porosity: Φ = the original values from the soil survey data
- Initial source concentration: C_0=100mg/L (fertilizer effect is considered)

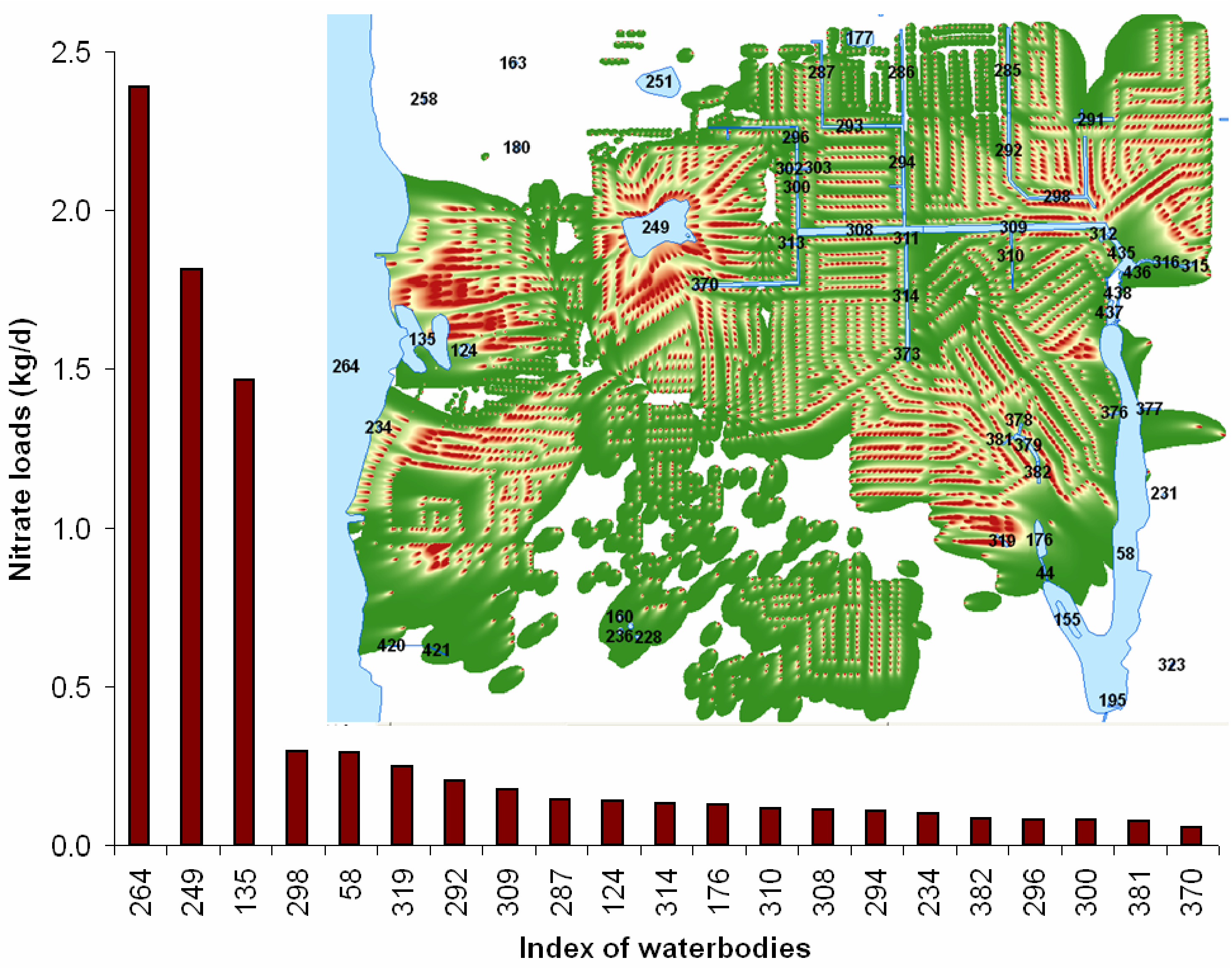
Calibration Results (Julington Creek)





- 11 of the simulated concentration are within the maximum and minimum range, 7 of them are within the lower and upper quartile and close to mean values
- 3 of the simulated concentration are underestimated, this can be improved by adjusting the source concentration individually

Nitrate Loads Estimation for Eggleston Heights Neighborhood



Estimated Source Input Mass Flux and Loads

- Based on the summary report of Anderson (2006) for Florida, average source nitrogen input mass flux is estimated as 20 g /sep/day.
- For Eggleston Heights, the estimated source input mass flux from 3495 septic systems is 115.4kg per day (33g/sep/day), about 92.5% of which is lost due to denitrification and 7.5% contributes to the loads to surface waterbodies.
- For Julington Creek, the estimated source input mass flux from 1924 septic systems is 59.4kg per day (31g/sep/day), about 97.6% of which is lost due to denitrification and 2.4% contributes to the loads to surface waterbodies.

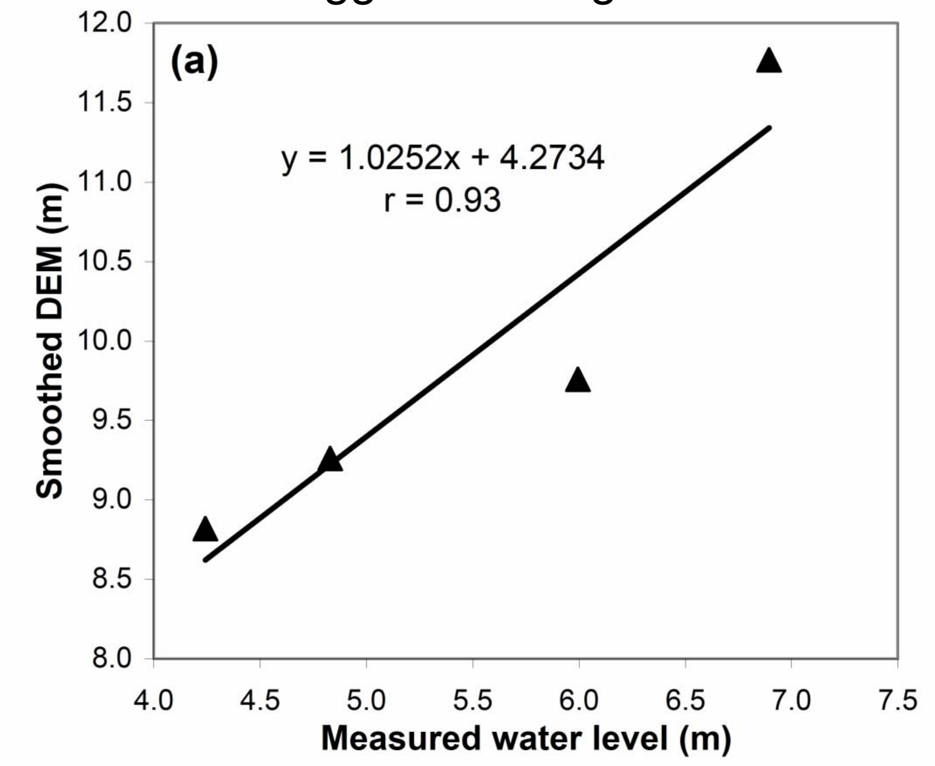
Conclusions

- Sensitivity analysis shows that the first-order decay coefficient, flow velocity and transverse dispersivity are critical parameters to the simulated concentration.
- Using LiDAR data, with an appropriate smoothing factor, the smoothed DEM simulates the hydraulic head gradient very well, the linear correlation coefficient is higher than 0.9.
- Using heterogeneous hydraulic conductivity, soil porosity and homogenous source concentration, dispersivity and first-order decay coefficient, most of the simulated concentration can meet the measurements range.
- The software gives reasonable estimation of source input mass flux, which is comparable with the estimate base on Anderson (2006).

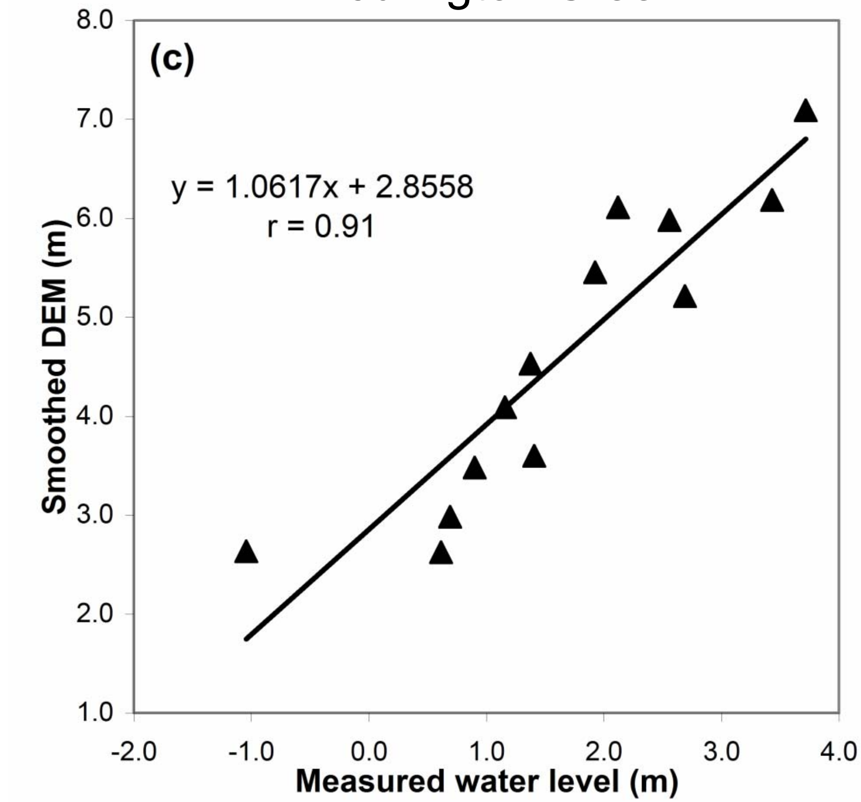
Thanks

Calibration Results of Hydraulic Gradient

Eggleston Heights



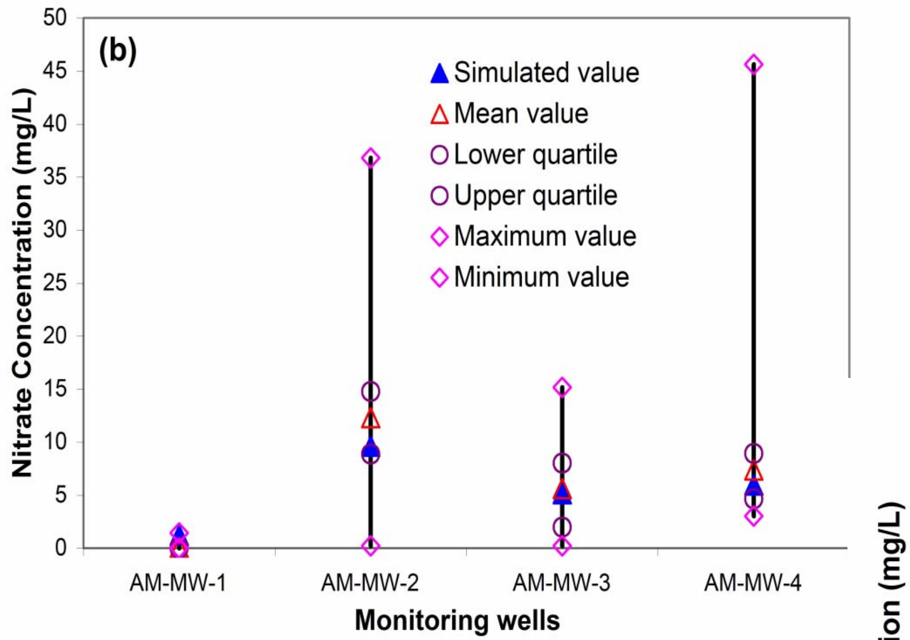
Julington Creek



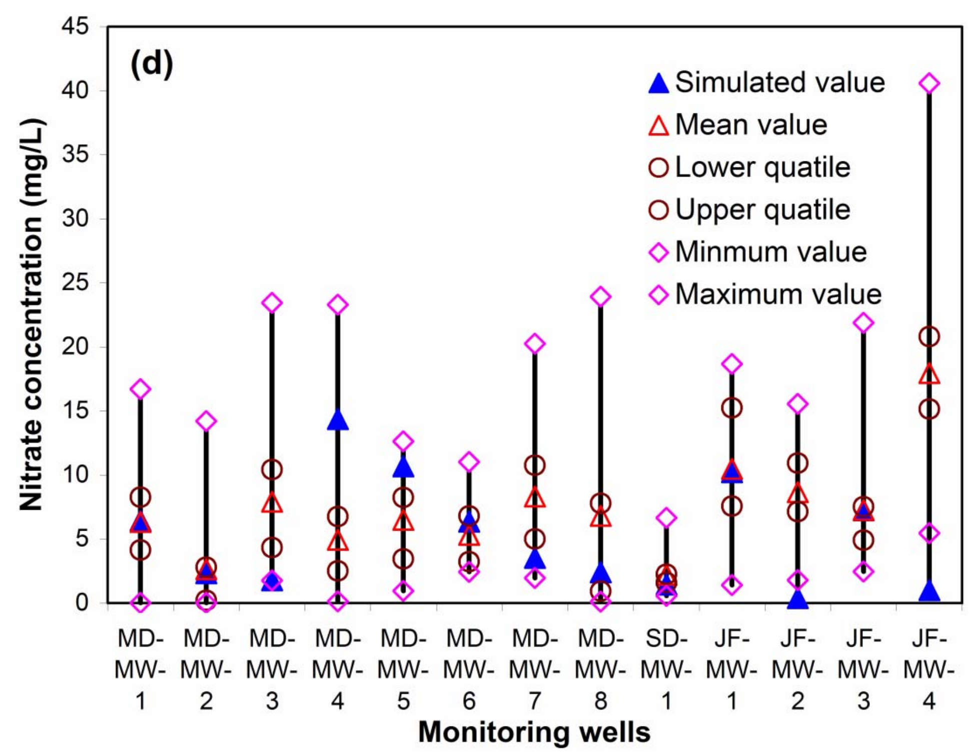
The smoothed DEM agree well with the observed water table shape with a linear correlation coefficient of more than 0.9 and slope of the linear regression close to 1.0

Calibration Results of Nitrate Concentration

Eggleston Heights



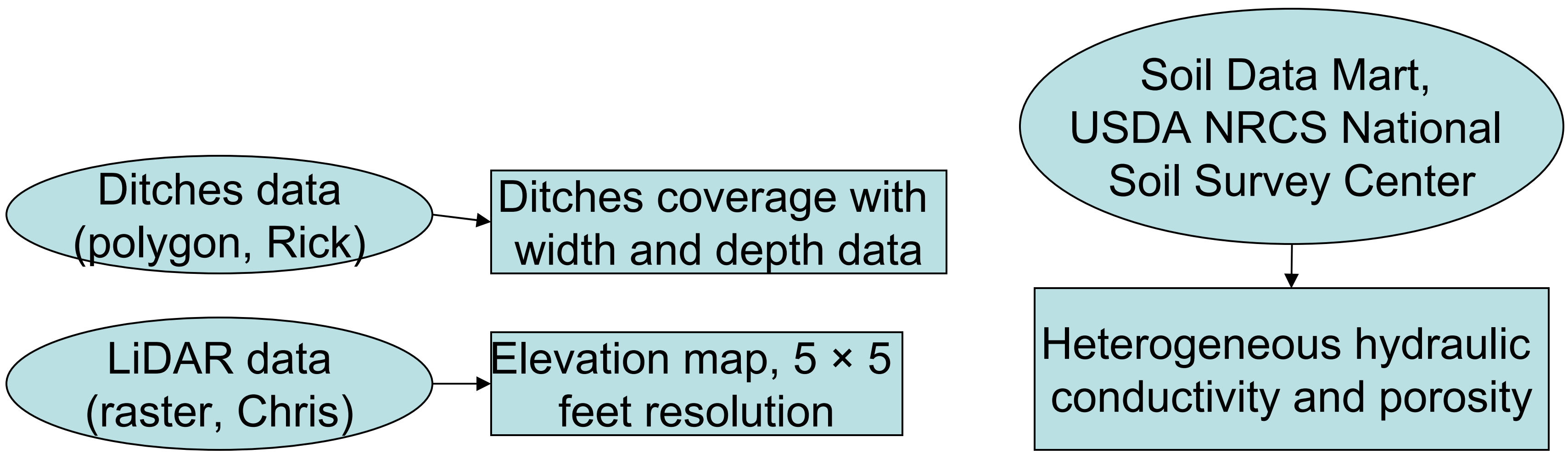
Julington Creek



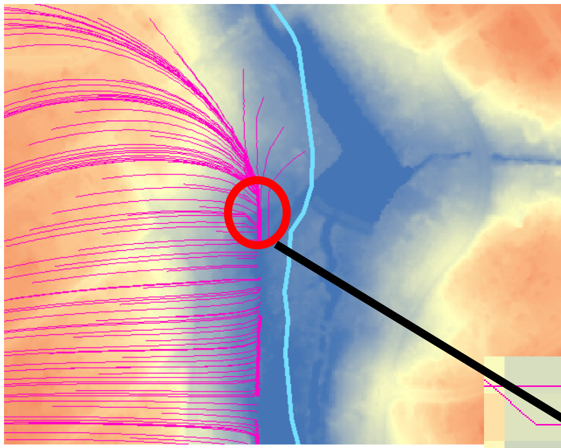
The simulated nitrate concentrations are close to the mean observations and within the inter-quartile of the observed concentrations in more than half of the monitoring wells.

Updating of Input Files

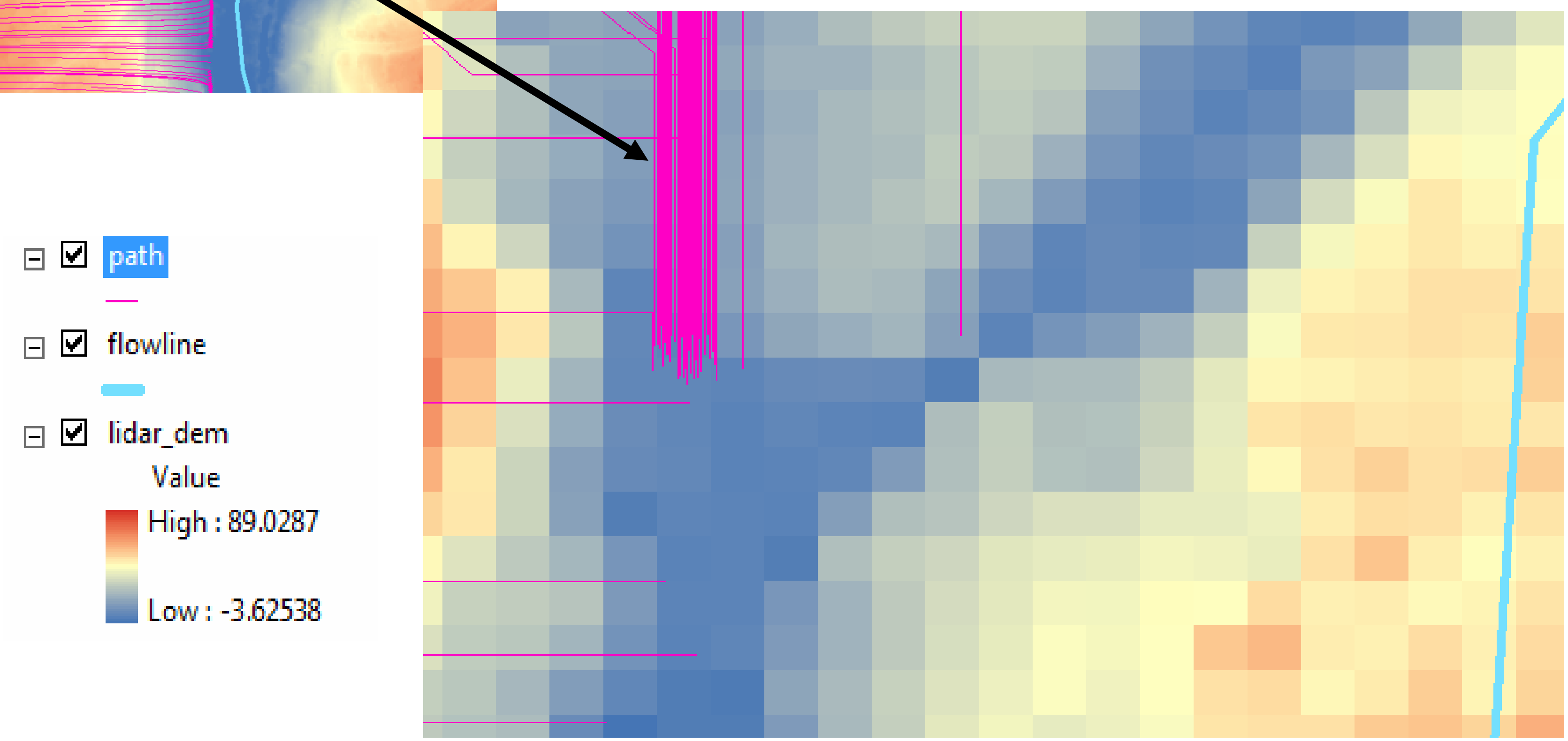
- Update DEM raster file by post-processing NED data or LiDAR data
- Prepare water body polygon file by combining the NHD data and ditches polygon file and update it based on LiDAR elevation map if necessary
- Generate heterogeneous hydraulic conductivity and soil porosity based on soil survey data



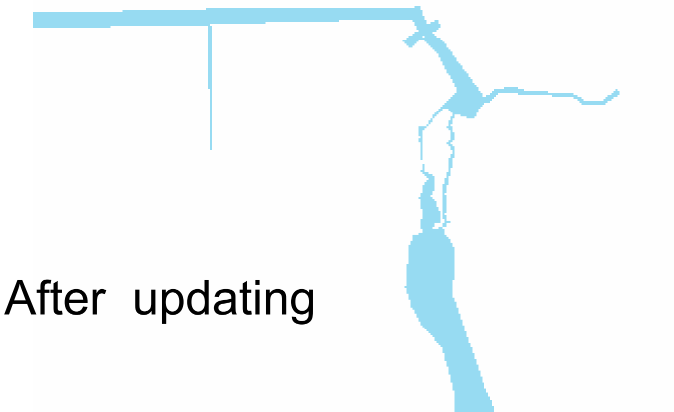
Problem Caused by Inconsistency of NHD data and DEM



When the water body is not located where the elevation value of DEM is lower, the calculated flow path may be "stopped" outside the water body.



Update Waterbody Based on Elevation Contour Generated from LiDAR DEM



After updating, the simulated flow paths of ArcNLET are more smooth and physically reasonable

Simulated flow paths after updating