



Practical Application of ArcNLET-Py: A Case Study of the Turkey Creek Sub-Basin

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CONTENTS

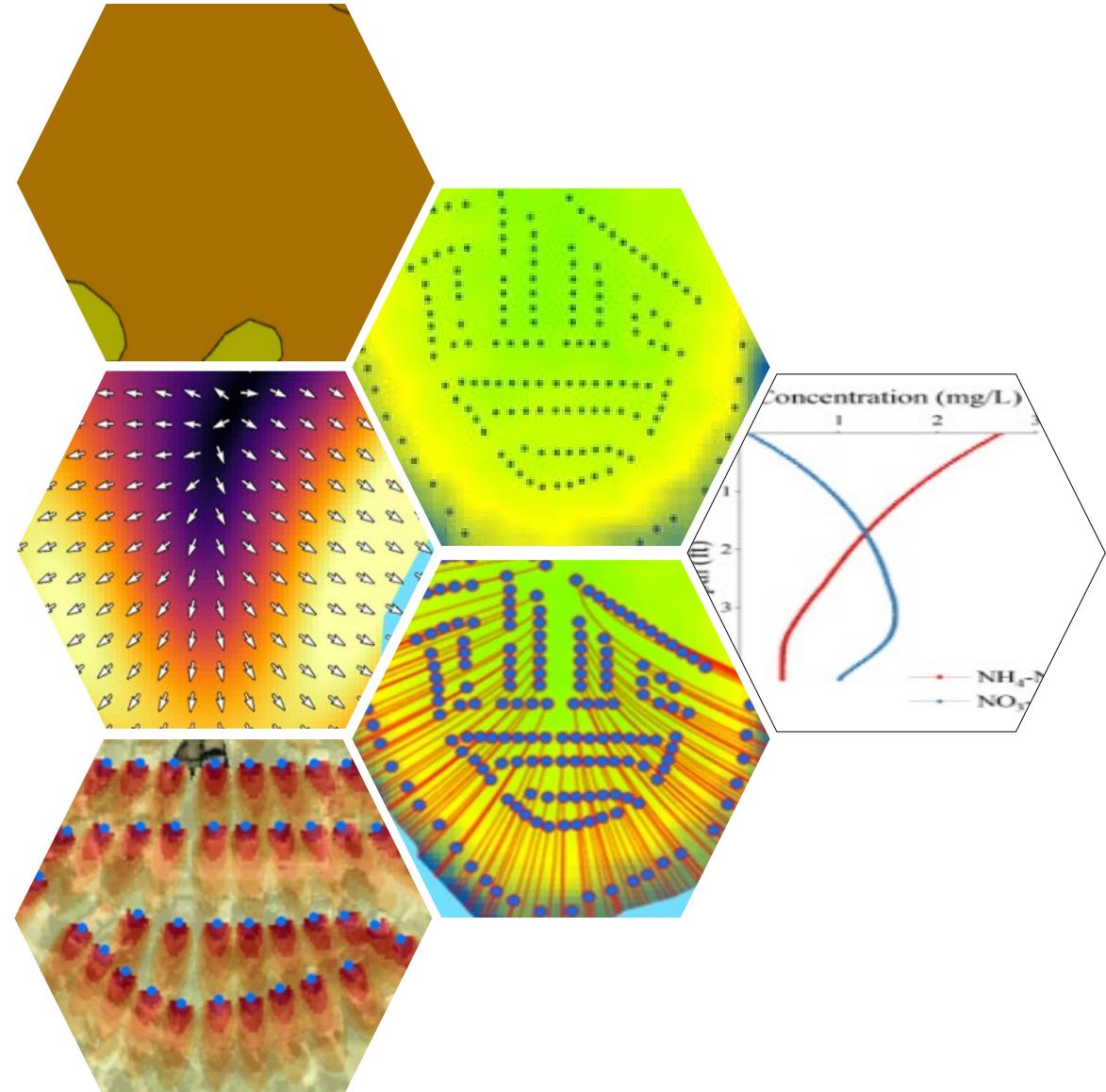
-  Introduction to the Model Application
-  Study Area
-  Data Preparation
-  Preprocessing Module
-  Groundwater Flow Module
-  Particle Tracking Module
-  VZMOD
-  Transport Module
-  Load Estimation Module
-  Conclusion and Q&A



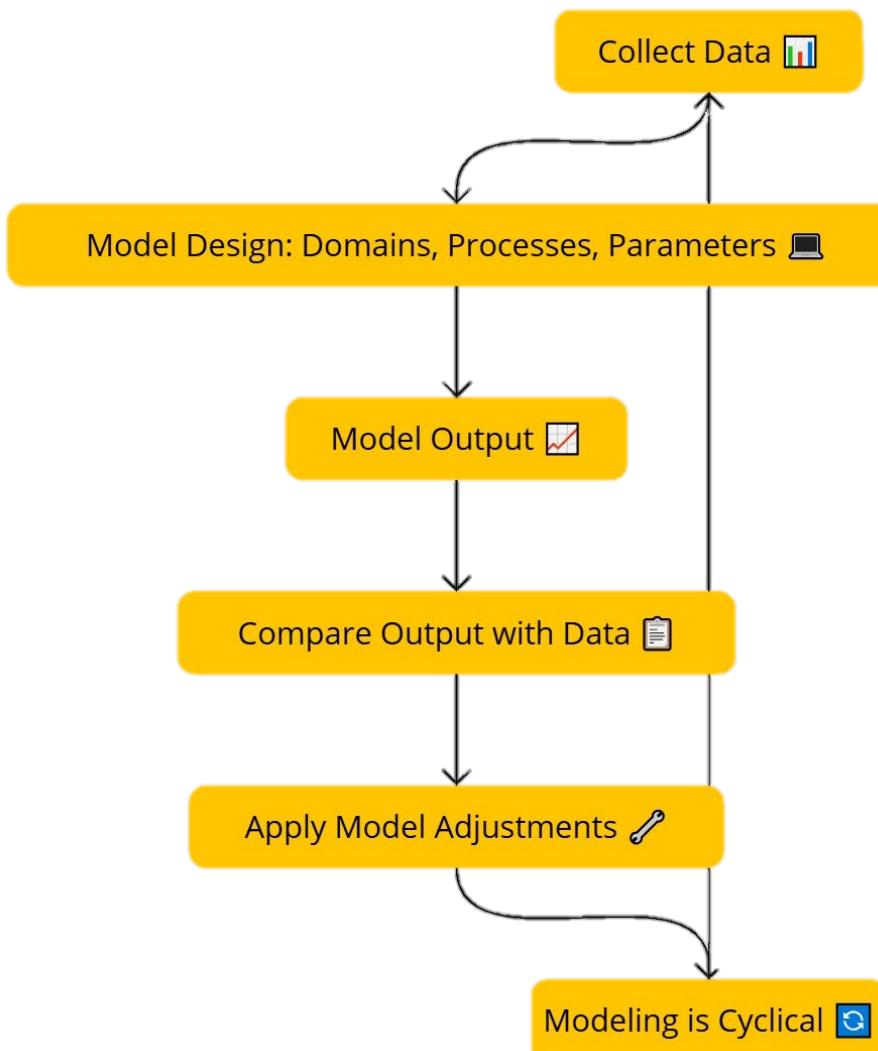
I. Introduction to the Calibration Manual

Introduction to ArcNLET-Py

- ArcNLET-Py Overview
 - ArcNLET-Py: **ArcGIS-based Nutrient Load Estimation Toolbox (Python version)**
 - Purpose: estimate nutrient loads (nitrogen and phosphorus) from onsite sewage treatment and disposal systems (OSTDS) to groundwater and surface water
 - Calibration training: designed for experienced users to deepen modeling and calibration skills



Introduction to Model Calibration



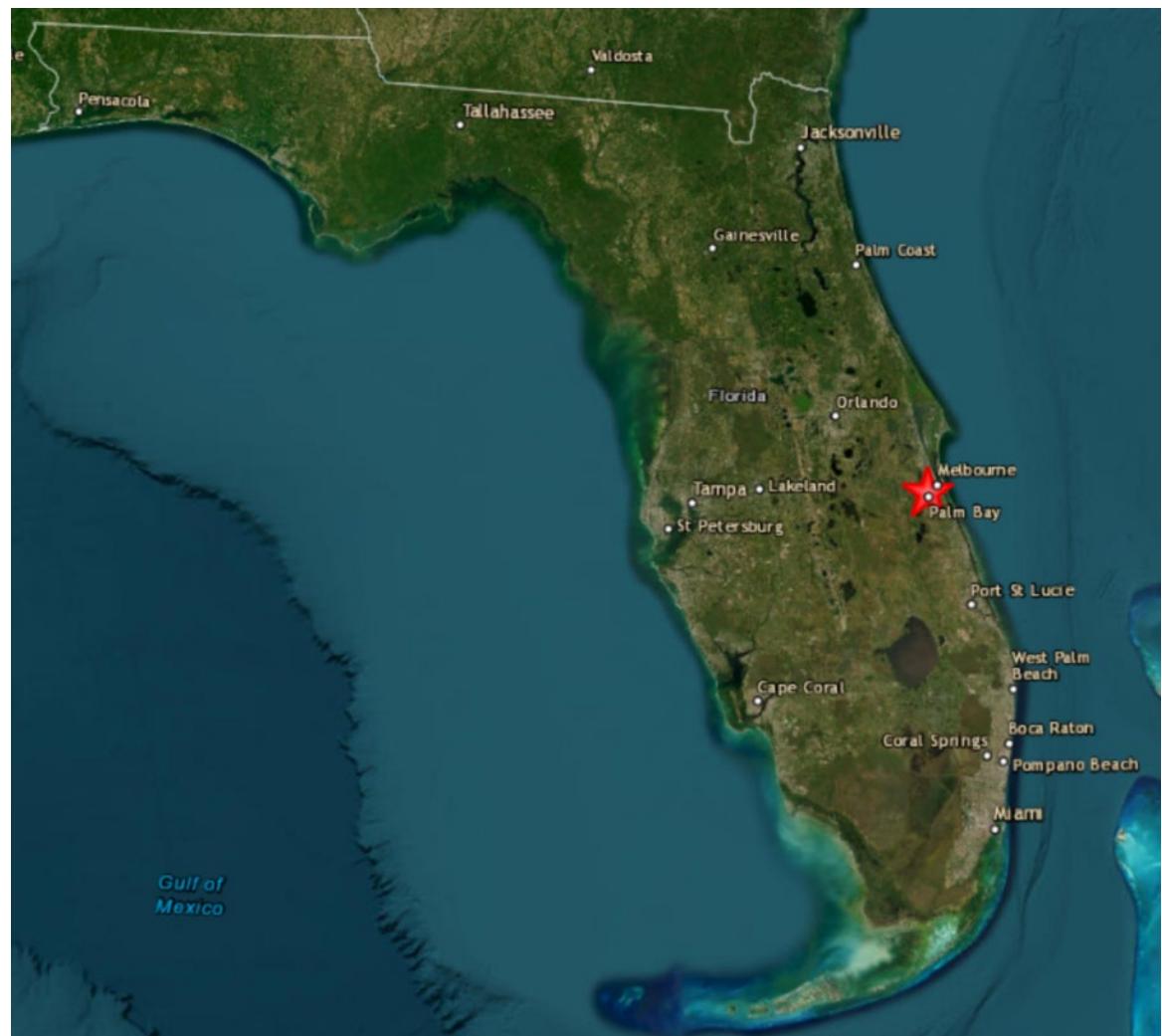
- Data Acquisition and Verification
 - Collect and check field data (e.g., monitoring wells, OSTDS measurements)
 - Review literature and reports for additional data
- Model Design
 - Define accurate study area and domains
 - Select processes and set initial parameters (e.g., nitrification rates, soil properties)
- Model Execution
 - Run ArcNLET-Py modules sequentially
- Compare Outputs with Data
 - Evaluate model results against observed data
 - Identify discrepancies and areas needing improvement
- Model Adjustment
 - Adjust parameters (e.g., smoothing factors, denitrification rates)
 - Refine model based on comparison findings
- Repeat the Cycle
 - Iterate the process until satisfactory alignment is achieved
 - Recognize modeling is an iterative and cyclical process



2. Study Area

Study Area: Turkey Creek Sub-Basin

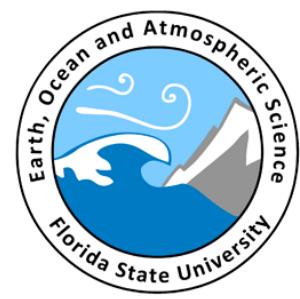
- Location and Significance
 - Central Florida, part of the Indian River Lagoon
 - High concentration of OSTDS
 - Monitoring data available from Ayres Associates (1993)
- Focus on Groseclose and Jones Residences
 - Detailed field data for model calibration
 - Measurements of greywater and blackwater effluent
 - Calibration targets for the VZMOD and Transport Modules



Essential Resources for ArcNLET-Py Modeling

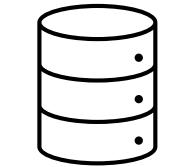
- ArcNLET-Py Toolbox
 - Available on GitHub: <https://github.com/ArcNLET-Py/ArcNLET-Py>
 - Contains all modules needed for nutrient load estimation
- ArcGIS Pro Software
 - Required platform for running ArcNLET-Py modules
- Datasets Required
 - OSTDS Locations obtained from Florida Department of Health (FDOH)
<https://www.floridahealth.gov/environmental-health/drinking-water/flwmi/index.html>
 - Digital Elevation Models (DEM) 1/9 arc-second DEM from USGS TNM Download (v2.0)
 - Waterbody shapefiles from the National Hydrography Dataset (NHD) reference materials from USGS TNM Download (v2.0)
 - <https://apps.nationalmap.gov/downloader/>
 - Shapefile of the study area
- Advanced User Manual (this presentation's source)
- Field Data and Literature
 - Studies referenced by Dr. Gao
https://floridadep.gov/sites/default/files/plume%20studies_ada_20221011.pdf



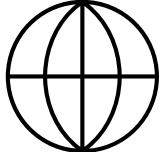


3. Data Preparation

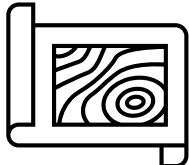
Data Preparation Overview



- Data Requirements



- All data must be in shapefile format (no geodatabases)



- Consistent projected coordinate system (PCS) in meters (e.g., NAD 1983 UTM Zone 17N)



- DEM cell size and vertical measurements in meters

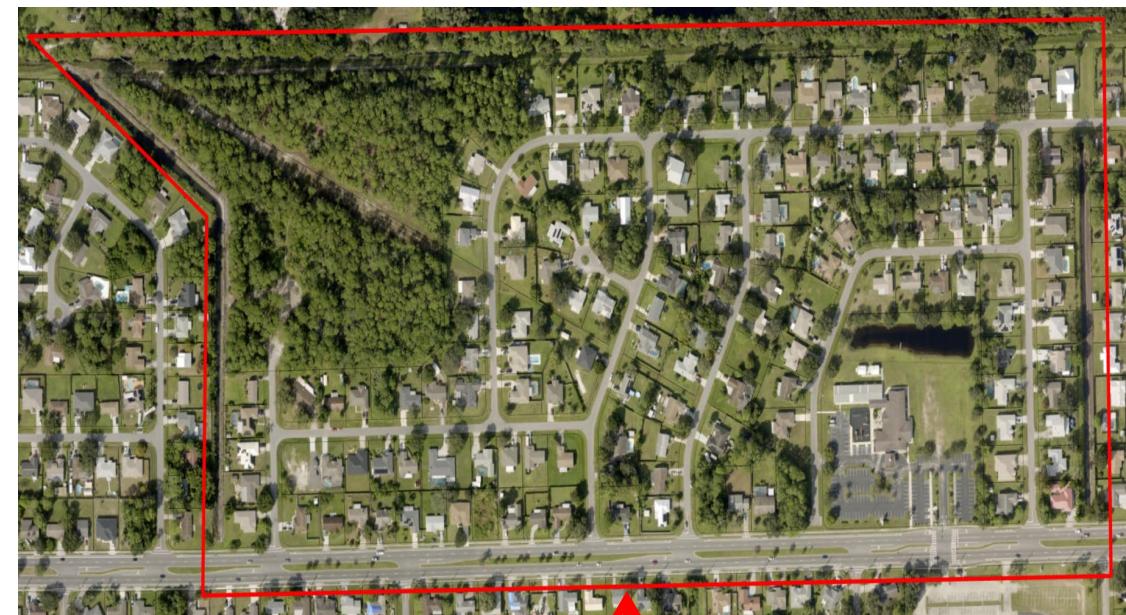


- Importance



- Accurate data preparation is critical for successful model calibration and results

Defining the Study Area Polygon

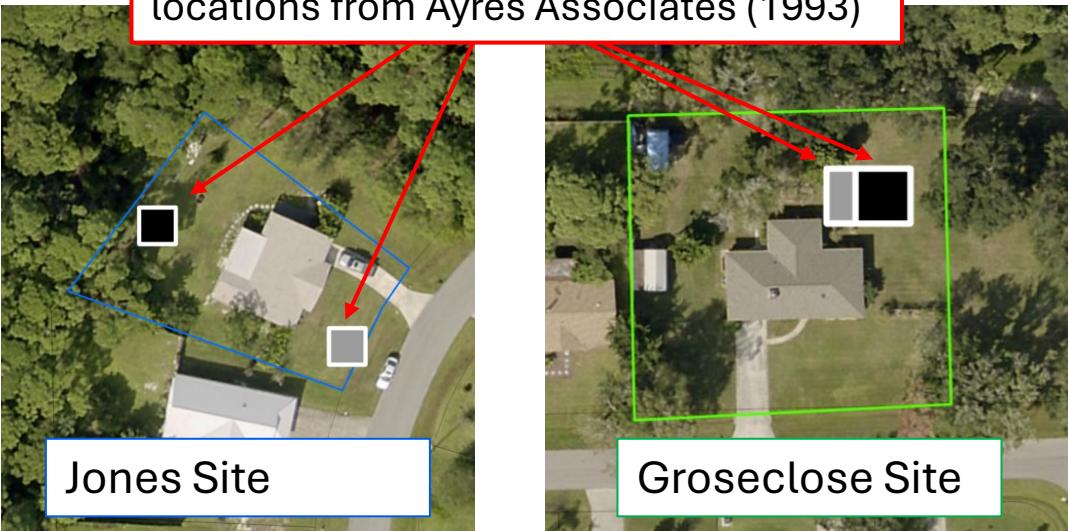


Study area shapefile
boundary

- Boundary Considerations
 - Align with natural (e.g., canals and ditches) and manmade features (roads)
 - Include all relevant waterbodies and OSTDS
- Sizing Guidelines
 - Create a buffer around OSTDS points
 - Buffer distance: at least 10% of the maximum distance between OSTDS
 - Ensures complete simulation of particle paths and nutrient plumes
 - Projection: Use NAD 1983 UTM Zone 17N
- Example: Turkey Creek Sub-basin
 - Northern, western, and eastern boundaries: canals or ditches
 - Southern boundary: major road
- Proper study area definition is crucial for the ArcNLET-Py modules to correctly extract essential data, ensuring all relevant OSTDS, waterbodies, and flow paths are included for precise nutrient load estimation.

Preparing OSTDS Points

Graywater & blackwater OSTDS locations from Ayres Associates (1993)



Jones Site

Groseclose Site

“WW” field for parcels with known, likely, or somewhat likely OSTDS from FDOH Florida Water Management Inventory

- Data Source
 - Florida Department of Health (FDOH) parcel data [Florida Water Management Inventory Project | Florida Department of Health \(floridahealth.gov\)](#)
 - Selection Criteria
 - Parcels with known, likely, or somewhat likely OSTDS (from the "WW" field)
 - Processing Steps
 - Use the "Feature to Point" tool to generate centroid points representing OSTDS locations
 - For precise locations, use actual OSTDS coordinates if available (e.g., Groseclose and Jones sites)
 - Projection
 - Project data using NAD 1983 UTM Zone 17N

Waterbody Polygons



The NHD flowline features that have been converted to polygons are shown in blue. Features with no width will be stepped over by the Particle Tracking Module. These types of errors in the data must be fixed

- Importance
 - Accurate representation of waterbodies is critical for flow path and nutrient transport simulations
- Data Issues
 - Watercourses represented by flowlines are incompatible with ArcNLET-Py because line features have no width. Therefore, the particles cannot terminate into the flowlines
 - Canals or streams in the National Hydrography Dataset (NHD), represented as flowlines, i.e., the canals in blue along the northern, eastern, and western boundaries of the study area

Waterbody Polygons



- Solution
 - Use Google Earth and DEMs to identify missing water features
 - Manually add missing canals and streams as polygon features
 - Convert flowlines (polylines) to polygons to include width
 - Ensure the waterbody shapefile uses NAD 1983 UTM Zone 17N
- Final Dataset
 - Comprehensive waterbody polygon shapefile including all lakes, ponds, canals, and other features
- Calibration Aspect
 - Creating accurate waterbody representations is essential for accurate particle tracking and load estimation

Digital Elevation Model (DEM)



- Clip a Larger Area
 - Ensure the DEM covers an area larger than your study area to avoid boundary effects
- Data Sources
 - USGS TNM Download (v2.0)
<https://apps.nationalmap.gov/downloader/>
- Choose Appropriate Resolution
 - 3-meter DEM is recommended (e.g., 3m × 3m)
 - Avoid coarse resolutions 10m × 10m is too coarse for small surface waterbodies
 - Avoid overly fine resolutions 1m × 1m may introduce unnecessary complexity
 - Requires excessive smoothing or resampling

Digital Elevation Model (DEM)



- Key Considerations
 - Ensure DEM uses the same projection and units as other datasets (NAD 1983 UTM Zone 17N)
- Data Verification
 - Even though Turkey Creek lacks tall buildings or parking lots, it's crucial to verify DEM accuracy
- Potential Issues
 - DEMs may contain errors or anomalies even in areas without significant urban structures
 - Small features like canals or ditches might be misrepresented
- Adjustments
 - If anomalies are found, manually correct the DEM
 - Modify elevations where necessary



4. Preprocessing Module

Preprocessing Module

- Purpose
 - Extract soil properties (hydraulic conductivity, porosity, soil type) for the modeling domain from SSURGO database
 - [Soil Survey Geographic Database \(SSURGO\) | Natural Resources Conservation Service \(usda.gov\)](#)
 - Prepares inputs for the Groundwater Flow and VZMOD modules.
- Inputs
 - Study area polygon shapefile
 - Correct projected coordinate system (PCS)
 - Specific soil depth ranges (e.g., 79 cm to 201 cm (Ayres Associates 1993))
 - Select extraction method (e.g., Harmonic Mean for Ks)
 - The raster cell size must match the DEM cell size
- Outputs
 - Raster files for hydraulic conductivity, porosity, and soil type
- Calibration Aspect
 - Accurate soil properties (e.g., depths and types) are foundational for subsequent module calibrations



Geoprocessing

0-Preprocessing

Parameters Environments

Study Area (polygon)
StudyAreaJonesGroseclose

Projected Coordinate System [m]
NAD_1983_UTM_Zone_17N

Top Depth [cm] 79

Bottom Depth [cm] 201

Extraction Method
Harmonic mean for Ks

Raster Cell Size [m] 3

Output Hydraulic Conductivity [m/d] (Raster)
hcond

Output Porosity (Raster)
porosity

(Optional) Output Soil type (VZMOD required)
type

(Optional) Output Spatial SSURGO Data (Shapefile)
spatial

Web Soil Survey



5. Groundwater Flow Module

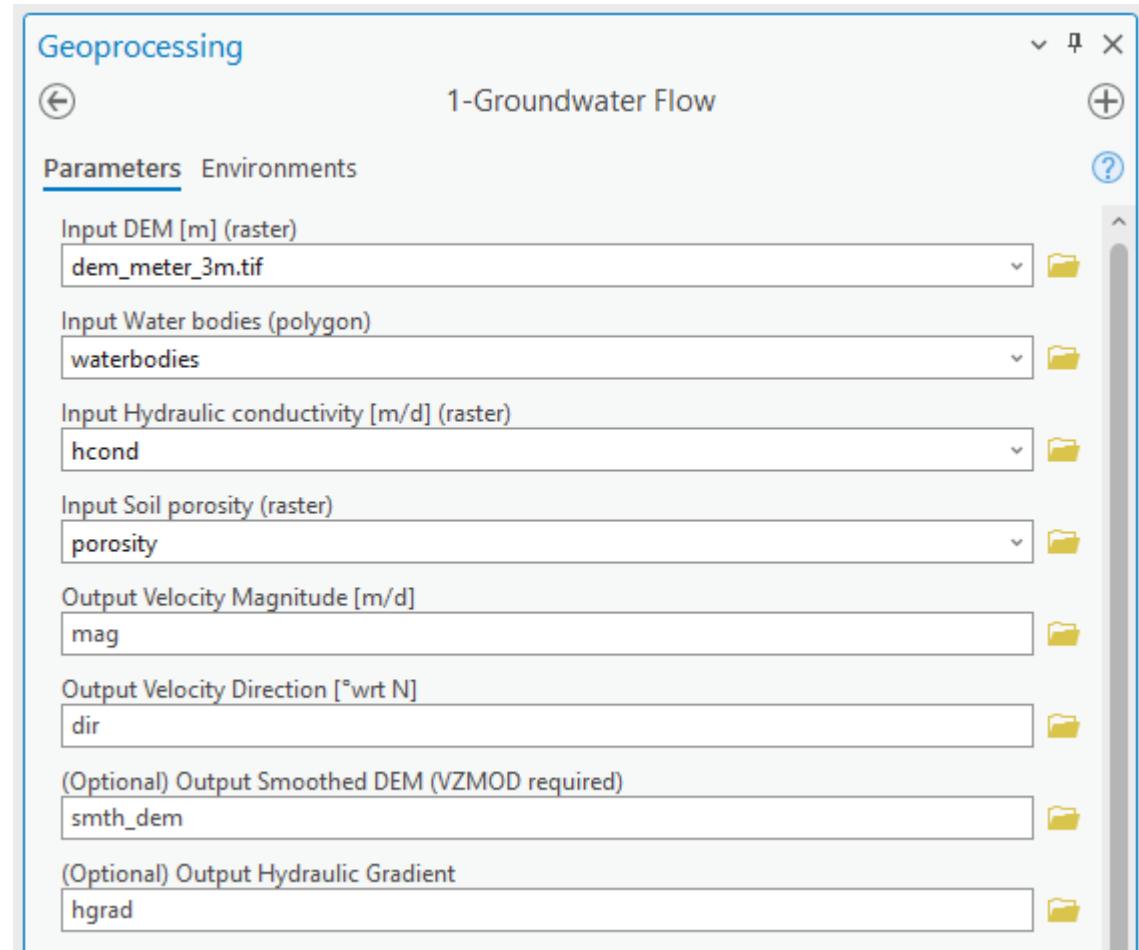
Groundwater Flow Module

➤ Objective

- Estimate groundwater velocity (magnitude and direction) using a smoothed DEM
- Accurate groundwater velocity is essential for simulating particle paths and nutrient transport

➤ Calibration Process

- Adjust the smoothing factor (the degree of smoothing) and smoothing cell size (neighborhood size)
- Merge waterbody elevations back into the smoothed DEM to preserve features like canals and lakes
- Apply multiple smoothing iterations to gradually refine the DEM while preserving waterbody features



Groundwater Flow Module

➤ Key Parameters

- Initial **smoothing factor** (i.e., 10), with **smoothing cell size** (i.e., 31)
- **Smoothing factors after merging:** multiple iterations with decreasing smoothing factors (i.e., 10 and 5)
- Adjust the neighborhood **smoothing cell sizes after merging** (i.e., 27 and 21) to incorporate natural flow gradients near waterbodies, which allows particle paths to flow accurately.
- **Merge waterbody elevations** back into the smoothed DEM

➤ Calibration Goal

- Ensure particle paths flow naturally into waterbodies
- Adjust parameters until particle paths are reasonable
- The groundwater elevations of the smoothed DEM can be checked through hydraulic head records
- Avoid over-smoothing (losing important features) or under-smoothing (retaining unnecessary details)

➤ Troubleshooting

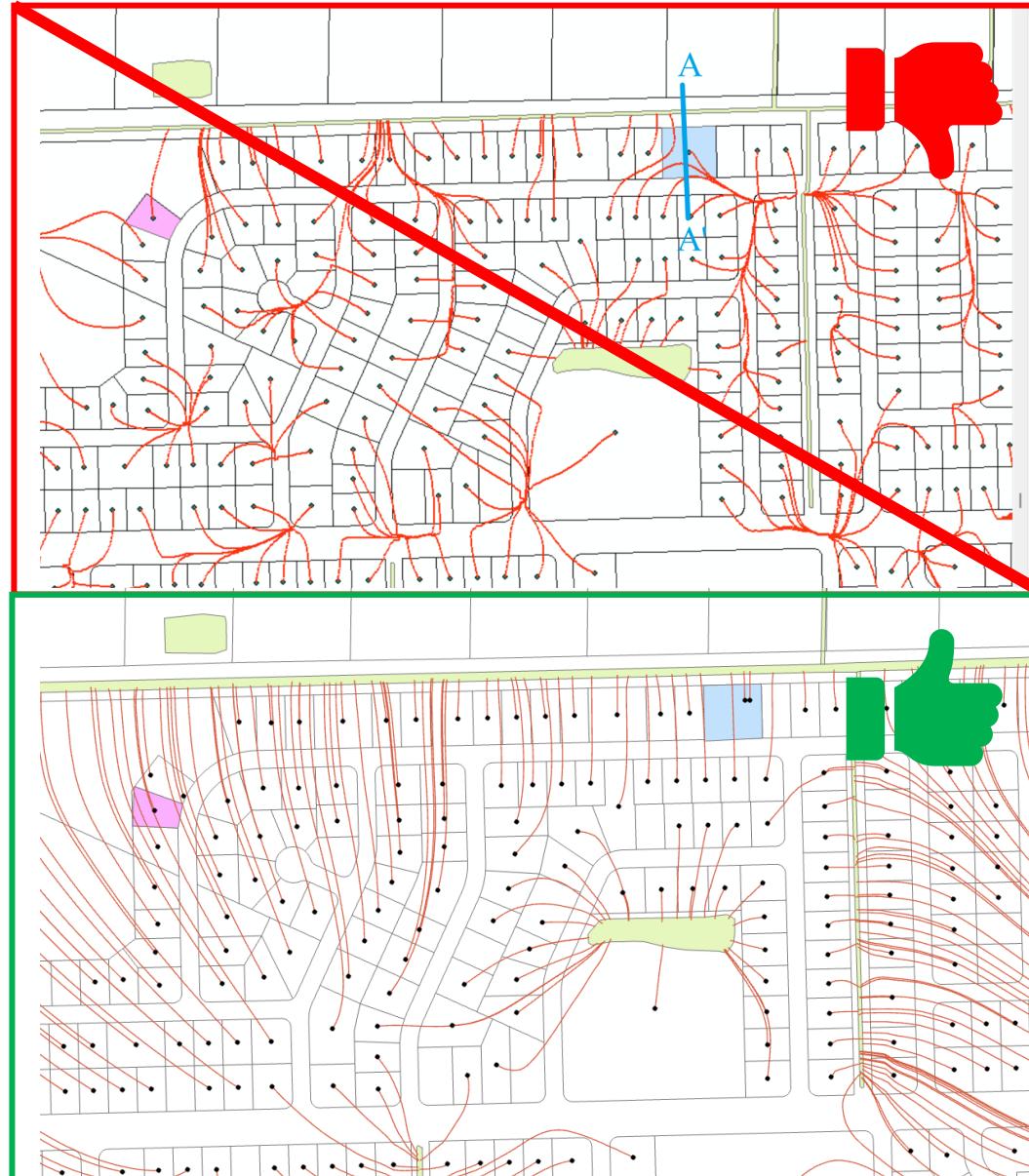
- Revisit the module if particle paths are trapped or inaccurate

The screenshot shows the 'Parameters' section of the Groundwater Flow Module. It includes fields for Smoothing Factor (10), Smoothing Cell (31), and Merge Waterbodies (checked). Below these are two sections for 'Smoothing Factor after Merging' and 'Smoothing Cell after Merging', each with four entries. The 'Smoothing Factor after Merging' section is highlighted with a red border and contains values 10, 10, 5, and 2. The 'Smoothing Cell after Merging' section is highlighted with a green border and contains values 27, 21, 15, and 7. There are 'Add another' buttons for each section. At the bottom are fields for Z-Factor (1) and Maximum number of continuous smoothing (50).

Parameters	
Smoothing Factor	10
Smoothing Cell	31
<input type="checkbox"/> Fill Sinks	
<input checked="" type="checkbox"/> Merge Waterbodies	
Smoothing Factor after Merging	
10	x
10	
5	
2	
(+) Add another	
Smoothing Cell after Merging	
27	x
21	
15	
7	
(+) Add another	
Z-Factor	1
Maximum number of continuous smoothing	50

Visual Inspection and Calibration

- Check Vertical Profiles
 - Ensure canals and ditches are correctly preserved in the smoothed DEM
- Verify Particle Paths
 - Trapped and unreasonable flow paths indicate an issue with the Groundwater Flow Module outputs.
 - Run the Particle Tracking Module to confirm flow paths lead into waterbodies



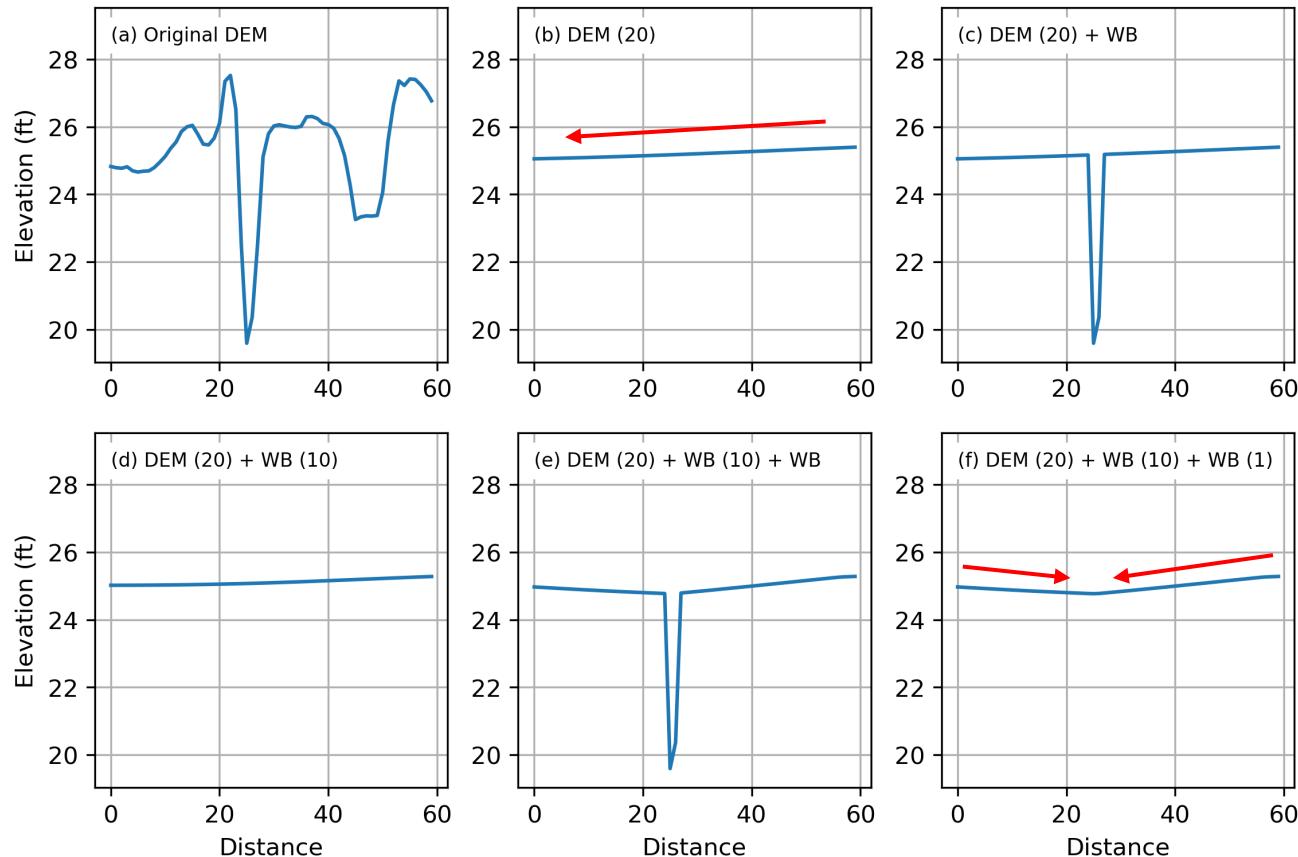
Visual Inspection and Calibration

➤ Importance of Merging Waterbodies During Smoothing

- Without Merging: Smoothing can elevate waterbody areas, causing them to disappear in the DEM
 - Leads to inaccurate flow paths, as particles may not enter waterbodies
- With Merging: Preserves elevations of canals and lakes
 - Maintains accurate representation of surface features
 - Essential for realistic groundwater flow modeling

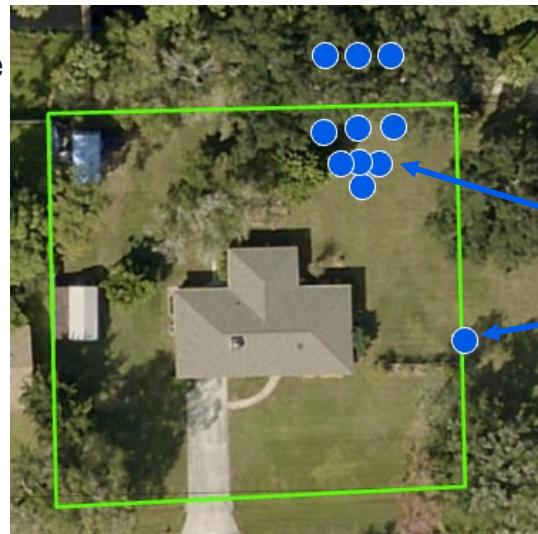
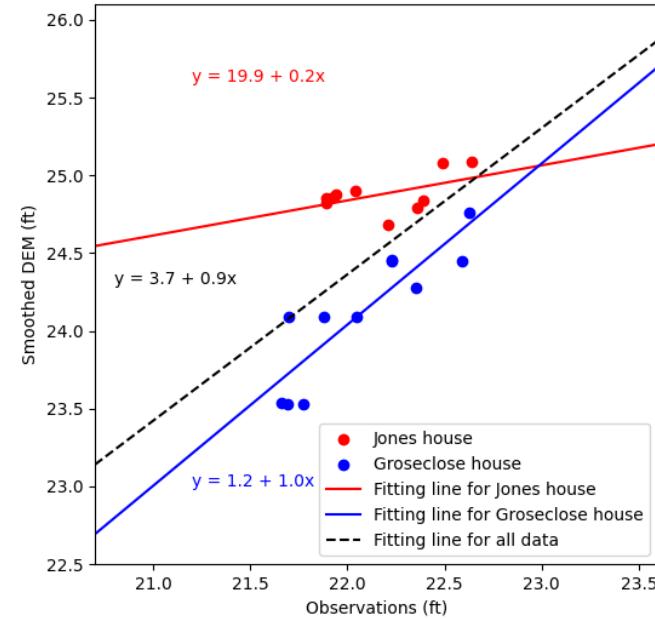
➤ Illustration

- Original DEM: Contains detailed topography, including waterbodies
- After Initial Smoothing: Waterbodies may disappear without merging
- After Merging and Additional Smoothing:
 - Waterbodies are preserved
 - DEM gradients direct flow naturally into waterbodies



Visual Inspection and Calibration

- Comparison with Observed Water Levels
 - Calibration Goal: Achieve a straight-line relationship (slope ~1) between smoothed DEM and observed groundwater levels
 - Use monitoring well data from Groseclose and Jones sites
- Adjusting Smoothing Parameters
 - If discrepancies exist: Fine-tune smoothing factors and cell sizes
 - Re-merge waterbodies as needed
 - Visual Inspection: Check DEM profiles to ensure waterbodies are maintained
 - Verify particle paths lead naturally into waterbodies
- Example Results
 - Groseclose Site: Good fit with slope ~1.04
 - Jones Site: Local discrepancies due to specific well data

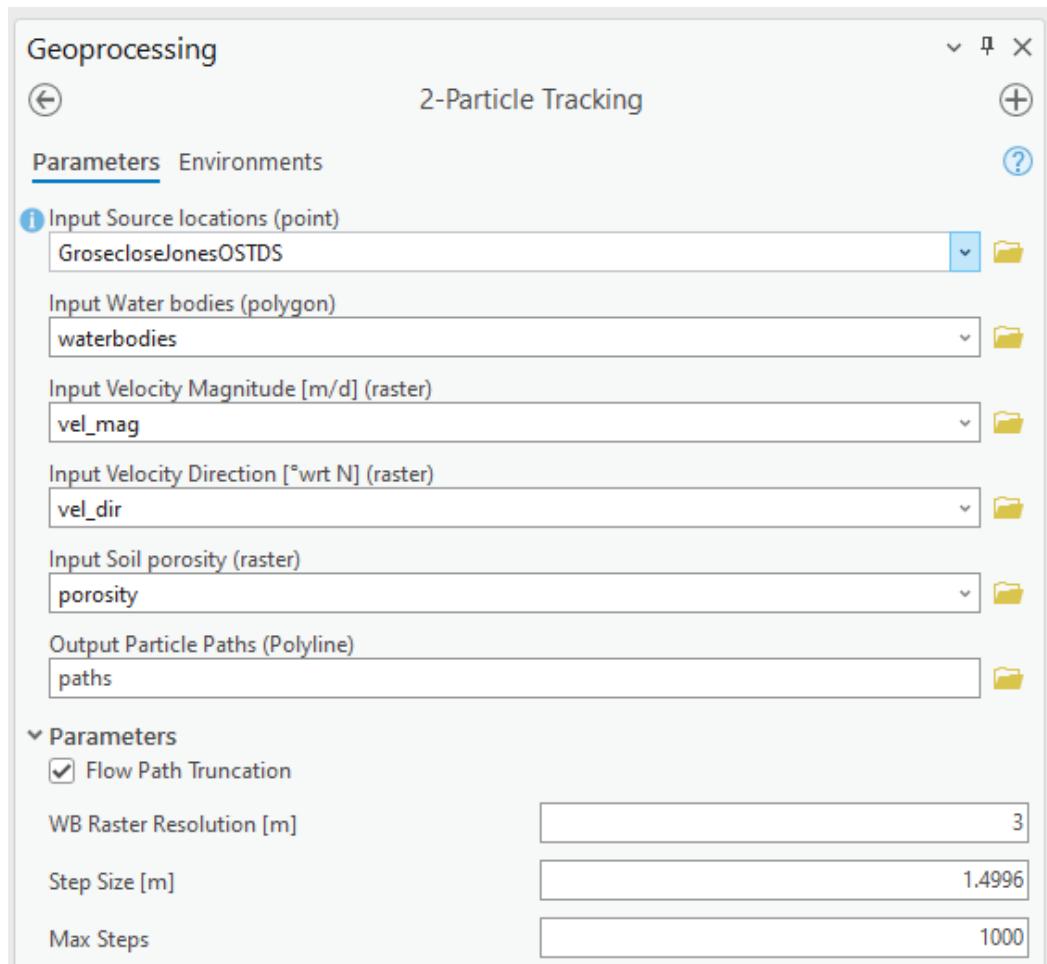


Monitoring wells with hydraulic head data reported in Ayres Associates (1993)



6. Particle Tracking Module

Particle Tracking Module



- Purpose
 - Simulate groundwater flow paths along which nutrients travel
- Calibration Dependency
 - Relies on an accurate waterbody data source that accounts for missing canals and drainage ditches
 - The outputs from the calibrated Groundwater Flow Module are needed
 - If particle paths are not reasonable: revisit and adjust Groundwater Flow Module parameters and the waterbody shapefile
 - Refine DEM smoothing and waterbody merging
- Best Practices:
 - Verify all inputs are in the correct formats (folder-based shapefiles and rasters)
 - Keep file paths and names within character limits to avoid errors
- Verification:
 - Ensure particle paths correspond with expected groundwater flow directions

Applying the Particle Tracking Module to the Domain



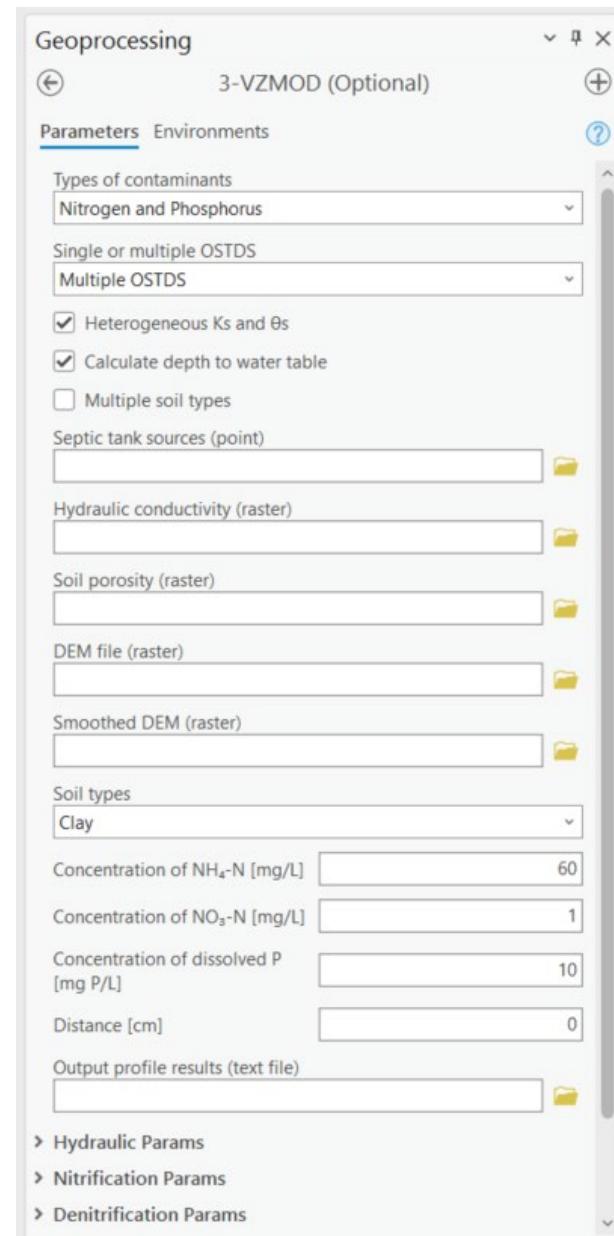
The particle paths are shown in **light coral** lines, the OSTDS are **black** dots, the study sites with data are **pink** and **blue**, and the water features are **yellow**

- Use Calibrated Groundwater Flow results
 - Apply Particle Tracking Module using the calibrated groundwater velocity field from the Groundwater Flow Module.
- Application Process
 - Run Particle Tracking Module for all OSTDS in the study area
 - Input Data: use the OSTDS point shapefile containing all OSTDS locations in the domain and the calibrated smoothed DEM
 - Flow Field: utilize the calibrated groundwater flow field to simulate accurate flow paths
- Data Format Considerations
 - Use folder-based shapefiles and raster files
 - Avoid geodatabases to prevent NoneType errors
- Result
 - Simulated Flow Paths for all OSTDS across the entire domain
 - Provides essential inputs for the VZMOD and Transport Modules



7.VZMOD

- Objective
 - Simulate transport and transformation of $\text{NH}_4\text{-N}$, $\text{NO}_3\text{-N}$, and $\text{PO}_4\text{-P}$ in the unsaturated zone
 - Estimates nutrient attenuation through processes like nitrification and denitrification
- Calibration Process
 - Use field measurements from Groseclose and Jones residences
 - Adjust key parameters to match observed concentrations
- Parameters to Adjust
 - Nitrification Rate (K_{nit}): Rate at which $\text{NH}_4\text{-N}$ converts to $\text{NO}_3\text{-N}$
 - Denitrification Rate (K_{dnt}): Rate at which $\text{NO}_3\text{-N}$ is reduced to nitrogen gas
 - Phosphate Precipitation Rate (R_{precip}): Rate of $\text{PO}_4\text{-P}$ precipitation
 - Sorption Coefficients (K): For phosphorus adsorption modeling
- Calibration Goal
 - Predicts nutrient concentrations reaching the groundwater table
 - Provides inputs for the Transport Module



Measured Effluent Concentrations at Groseclose Residence

- Initial Nitrogen and Phosphorus Concentrations

- NO₃-N Concentrations

- Graywater: 0.06 mg/L
 - Blackwater: 0.02 mg/L

- Total Kjeldahl Nitrogen (TKN)

- Graywater: 3.8 mg/L
 - NH₄-N (73% of TKN): 2.76 mg/L
 - Blackwater: 110 mg/L
 - NH₄-N (73% of TKN): 80 mg/L

- PO₄-P Concentrations

- Graywater: 1.14 mg/L
 - Blackwater: 18.0 mg/L

- Note

- Graywater: wastewater from showers, sinks, etc.
 - Blackwater: wastewater from toilets

Table 8. Septic Tank Effluent Characteristics, Groseclose Residence (mg/L)

PARAMETER	Graywater			AVERAGE Graywater	BLACK WATER		AVERAGE BLACK WATER
	11/20/91	2/12/92	4/19/92		2/12/92	4/9/92	
COD	350	160	280	263	340	460	400
BOD	100	117	113	110	229	176	202.5
TSS	44	20	35	33	37	80	58.5
TDS	478	442	456	459	598	562	580
NO ₃ -N	0.13	0.02	0.02	0.06	<0.01	0.03	<0.02
TKN	3.6	3.3	4.6	3.8	120	100	110
TP	2	0.56	0.87	1.14	19	17	18
CL ⁻	160	120	150	143	150	170	160
FOAMING AGENTS	58	19	32	36	4.8	7.8	6.3
OIL & GREASE	19	38	30	29	13	23	18
FECAL COLI	49,000	24,000	1,300	24,767	150,000	130,000	140,000
FECAL STREP	<10	<10	<10	<10	48,000	51,000	49,500

Ayres Associates (1993)

HLR, Knit, Kdnt, and Rprecip Parameters for Groseclose

➤ Soil Properties

- Soil Type: Loamy Sand

➤ Effluent Parameters

➤ Blackwater

- NH₄-N (C_0): 80 mg/L
- NO₃-N (C_0): 0.02 mg/L
- PO₄-P (C_0): 18.0 mg/L

➤ Calibrated Reaction Rates

- Nitrification Rate (Knit): 0.275 1/d
- Denitrification Rate (Kdnt): 0.585 1/d
- Phosphate Precipitation Rate (Rprecip): 0.0011 1/d
- Phosphate Langmuir Coefficient (K): 0.2 L/mg
- Maximum Sorption Capacity (Qmax): 700 mg/kg

➤ Hydraulic Parameters

- Hydraulic Loading Rate (HLR)
 - Blackwater: 2.893 cm/d

The screenshot shows the 3-VZMOD software interface with various parameter settings. A yellow box highlights the 'Soil types' dropdown set to 'Loamy Sand'. A purple box highlights the 'Nitrification Parameters' section with 'Knit [1/d]' set to 0.275. A red box highlights the 'Phosphorus Parameters' section with 'Rprecip [mg/kg 1/day]' set to 0.0011. To the right, a table summarizes soil test results for NO₃-N, TKN, and TP.

Geoprocessing
3-VZMOD (Optional)

Parameters Environments

Types of contaminants: Nitrogen and Phosphorus
Single or multiple OSTDS: Single OSTDS
Soil types: Loamy Sand

Concentration of NH₄-N [mg/L]: 80
Concentration of NO₃-N [mg/L]: 0.02
Concentration of PO₄-P [mg/L]: 18
Depth to water table [cm]: 150

Output profile results (text file): C:\Users\mcore\OneDrive - Florida State University\ArcNLET\GitHub\GitHub

Hydraulic Parameters

	NO ₃ -N	TKN	TP	<0.01	0.03	<0.02
NO ₃ -N	0.13	3.6	2	0.06	120	110
TKN	0.02	3.3	0.56	4.6	100	110
TP	0.02	4.6	0.87	0.06	19	17
	<0.01	3.8	1.14	<0.01	18	<0.02

Concentration of NH₄-N [mg/L]: 2.893
α [-]: 0.035
K_s [cm/d]: 105.12
θ_r [-]: 0.049
θ_s [-]: 0.39
n [-]: 1.747

Nitrification Parameters

	Topt-nit [°C]	βnit [-]	ε2 [-]	ε3 [-]	fwp [-]	Swp [-]	SI [-]	Sh [-]
Knit [1/d]	25	0.347	2.267	1.104	0	0	0.665	0.809
Topt-nit [°C]	25	0.347	2.267	1.104	0	0	0.665	0.809
βnit [-]	0.347	2.267	1.104	0	0	0	0.665	0.809
ε2 [-]	2.267	1.104	0	0	0	0	0.665	0.809
ε3 [-]	1.104	0	0	0	0	0	0.665	0.809
fwp [-]	0	0	0	0	0	0	0.665	0.809
Swp [-]	0	0	0	0	0	0	0.665	0.809
SI [-]	0.665	0	0	0	0	0	0.665	0.809
Sh [-]	0.809	0	0	0	0	0	0.665	0.809

Denitrification Parameters

	Kdnt [1/d]	Topt-dnt [°C]	βdnt [-]	ε1 [-]	Sdnt [-]
Kdnt [1/d]	0.585	26	0.347	3.774	0
Topt-dnt [°C]	26	26	0.347	3.774	0
βdnt [-]	0.347	26	0.347	3.774	0
ε1 [-]	3.774	26	0.347	3.774	0
Sdnt [-]	0	26	0.347	3.774	0

NH₄-N Adsorption Parameters

	k _d for NH ₄ -N [cm ³ /g]
k _d for NH ₄ -N [cm ³ /g]	1.46

Dispersion, Bulk Density and Temperature

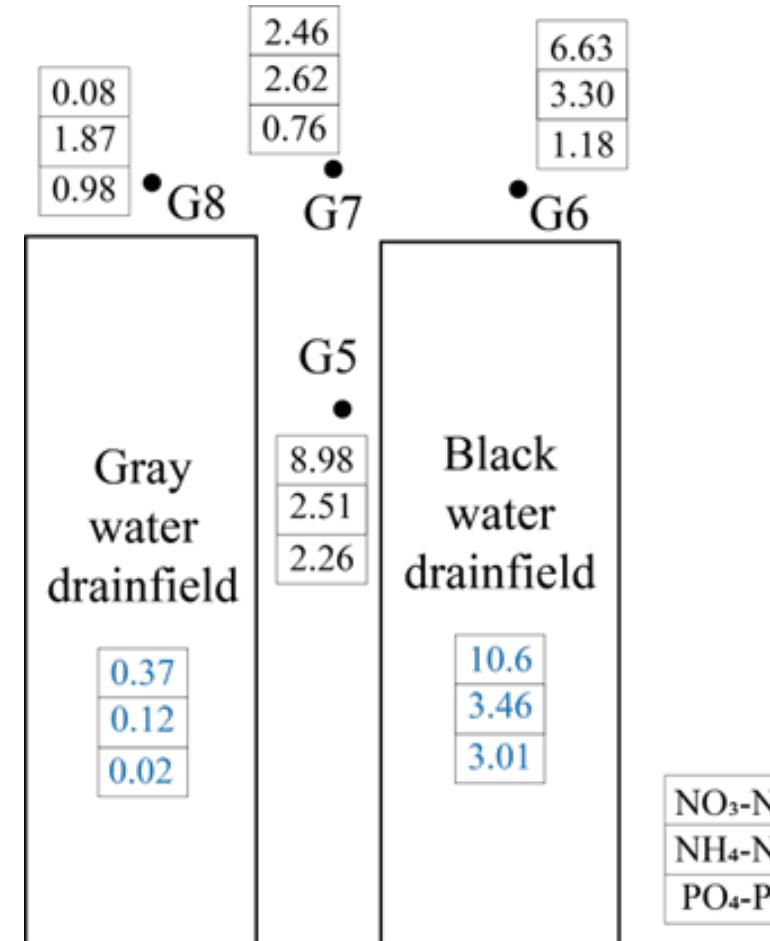
	Dispersion coefficient [cm ² /d]	Bulk Density ρ [g/cm ³]	Temperature [°C]
Dispersion coefficient [cm ² /d]	4.32	1.5	25.5
Bulk Density ρ [g/cm ³]	1.5	1.5	25.5
Temperature [°C]	25.5	1.5	25.5

Phosphorus Parameters

	Rprecip [mg/kg 1/day]	Sorption isotherm	Langmuir coefficient [L/mg]	Maximum sorption capacity [mg P / kg]
Rprecip [mg/kg 1/day]	0.0011	Langmuir	0.2	700
Sorption isotherm	Langmuir	Langmuir	0.2	700
Langmuir coefficient [L/mg]	0.2	0.2	0.2	700
Maximum sorption capacity [mg P / kg]	700	700	700	700

VZMOD Calibration Results for Groseclose Site

- Simulated vs. Measured Concentrations
 - NH₄-N
 - Simulated concentrations decrease due to nitrification
 - Align with observed data at the groundwater table
 - NO₃-N
 - Simulated concentrations increase initially (from nitrification) and then decrease due to denitrification
 - Good match with measured concentrations
 - PO₄-P
 - Attenuated through sorption and precipitation
 - Simulated values closely match observed data
- Outcome
 - Successful Calibration
 - Simulated concentrations at the water table align with field measurements
 - Provides Accurate Inputs for the Transport Module



VZMOD-simulated concentrations (in blue) of NO₃-N, NH₄-N, and PO₄-P at the water table and measured concentrations (black) in groundwater monitoring wells at the Groseclose site.

VZMOD Parameters for Jones Site

- Soil and Hydraulic Properties
 - Soil Type: Loamy Sand
 - Hydraulic Loading Rate (HLR): 1.79 cm/d
- Effluent Concentrations
 - NH₄-N
 - Blackwater: 77.1 mg/L
 - NO₃-N
 - Blackwater: 0.019 mg/L
 - PO₄-P
 - Blackwater: 17.35 mg/L
- Calibrated Reaction Rates
 - Nitrification Rate (Knit): 0.048 1/d
 - Denitrification Rate (Kdnt): 0.122 1/d
 - Phosphate Precipitation Rate (Rprecip): 0.00015 1/d

The screenshot shows the VZMOD software interface with various parameters set for the Jones Site. The parameters are categorized into several groups:

- Geoprocessing**:
 - Types of contaminants: Nitrogen and Phosphorus
 - Single or multiple OSTDS: Single OSTDS
 - Soil types: Loamy Sand
 - Concentration of NH₄-N [mg/L]: 77.1
 - Concentration of NO₃-N [mg/L]: 0.019
 - Concentration of PO₄-P [mg/L]: 17.35
 - Depth to water table [cm]: 150
 - * Output profile results (text file): [empty input field]
- Nitrification Parameters**:
 - Knit [1/d]: 0.048
 - Topt-nit [°C]: 25
 - βnit [-]: 0.347
 - e2 [-]: 2.267
 - e3 [-]: 1.104
 - fs [-]: 0
 - fwp [-]: 0
 - Swp [-]: 0.154
 - SI [-]: 0.665
 - Sh [-]: 0.809
- Denitrification Parameters**:
 - Kdnt [1/d]: 0.122
 - Topt-dnt [°C]: 26
 - βdnt [-]: 0.347
 - e1 [-]: 2.865
 - Sdnt [-]: 0
- NH₄-N Adsorption Parameters**:
 - Dispersion, Bulk Density and Temperature
 - Dispersion coefficient [cm²/d]: 4.32
 - Bulk Density ρ [g/cm³]: 1.5
 - Temperature [°C]: 25.5
- Phosphorus Parameters**:
 - Rprecip [mg/kg 1/day]: 0.00015
 - Sorption isotherm:
 - Langmuir
 - Langmuir coefficient [L/mg]: 0.2
 - Maximum sorption capacity [mg P / kg]: 700

VZMOD Calibration Results for Jones Site

- Simulated vs. Measured Concentrations

- NH₄-N

- Simulated decrease due to nitrification

- Matches observed groundwater concentrations

- NO₃-N

- Simulated concentrations reflect the balance of nitrification and denitrification

- Align with field measurements

- PO₄-P

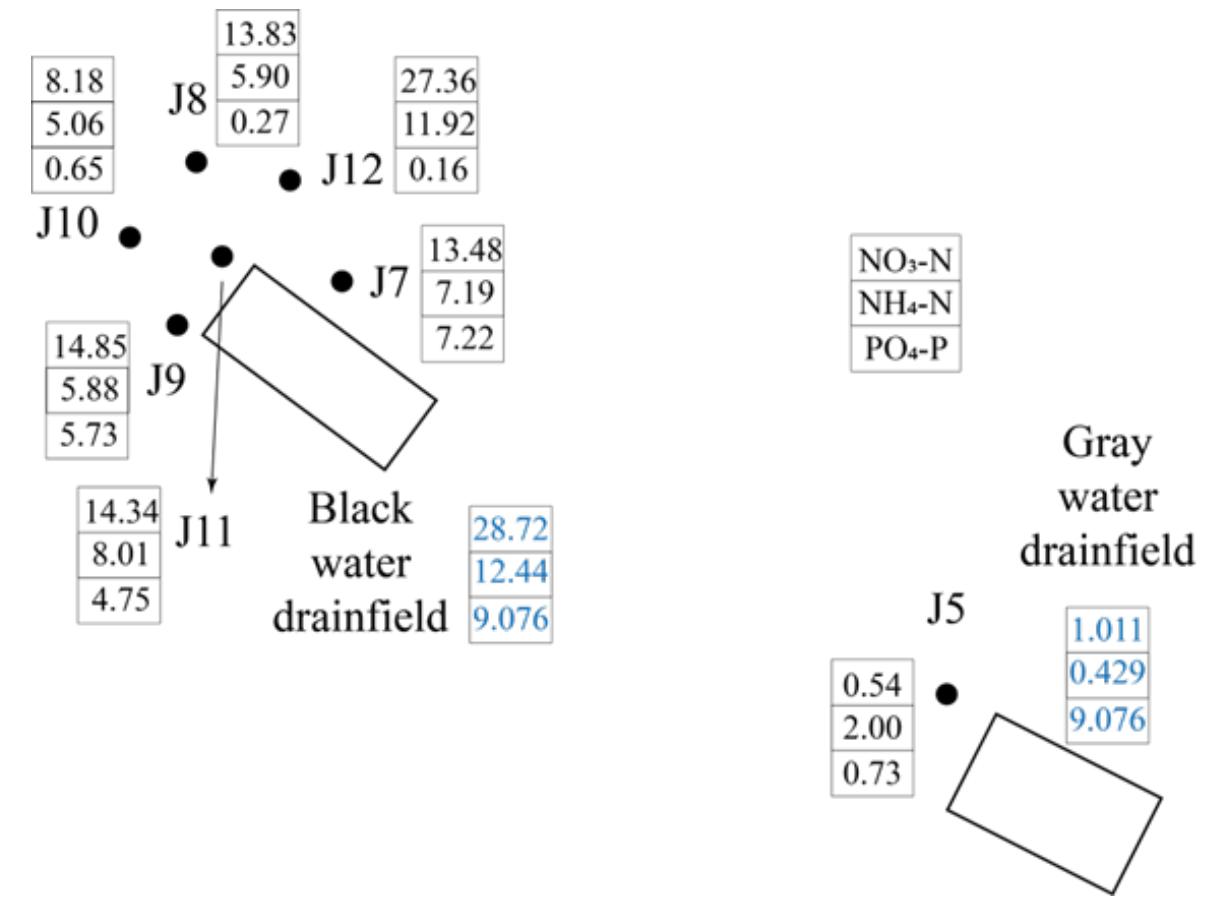
- Attenuation through sorption and precipitation

- Simulated values correspond with observed data

- Outcome

- Adjusted Parameters reflect local soil and vadose zone conditions

- Calibration ensures the model represents real-world nutrient transport



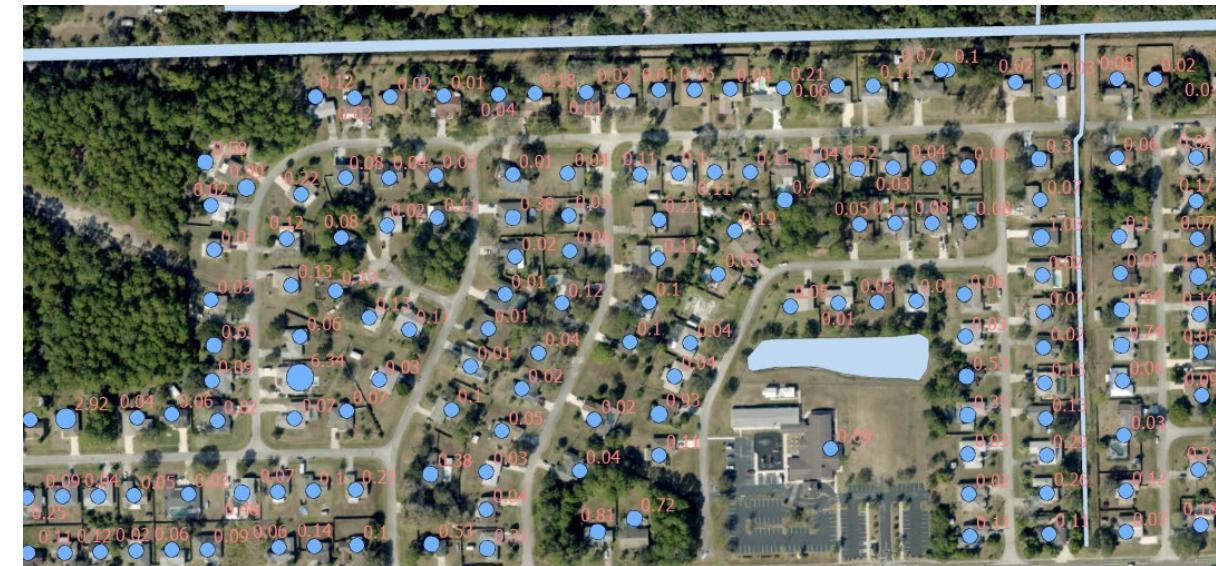
VZMOD-simulated concentrations (in blue) of NO₃-N, NH₄-N, and PO₄-P at the water table and measured concentrations (black) in groundwater monitoring wells at the Jones site.

Applying VZMOD to the Entire Study Area

- Use Calibrated Parameters from Groseclose and Jones sites: apply to all OSTDS across the study area
- Adjusted Parameters for the Study Area
 - Soil Types: Loamy sand, sand, sandy clay loam, sandy loam
 - Obtained from the Preprocessing Module
 - Hydraulic Loading Rate (HLR): 2.342 cm/d
 - Effluent Concentrations:
 - NH₄-N: 40 mg/L
 - NO₃-N: 0.04 mg/L
 - PO₄-P: 9.5 mg/L
 - Calibrated Reaction Rates:
 - Nitrification Rate (Knit): 0.162 1/d
 - Denitrification Rate (Kdnt): 0.354 1/d
- Phosphate Precipitation Rate (Rprecip): 0.000625 1/d
- Phosphate Sorption Parameters:
 - Langmuir Coefficient (K): 0.2 L/mg
 - Maximum Sorption Capacity (Qmax): 700 mg/kg
- Result
 - Simulated Vertical Attenuation of nutrients to the water table across the entire domain
 - Provides inputs for the Transport Module to simulate horizontal transport



VZMOD-simulated NO₃-N concentrations entering groundwater around the Groseclose and Jones homes.



VZMOD-simulated PO₄-P concentrations entering groundwater around the Groseclose and Jones homes.



8. Transport Module

Transport Module

- Purpose: simulate horizontal reactive transport of nutrients in groundwater to surface waterbodies
- Calibration Process: use VZMOD outputs as source concentrations
 - Parameters to Adjust
 - Source Plane Parameters
 - Domenico Bdy: Specified Z
 - Source Dimension Y: 6 m
 - Longitudinal Dispersivity (α_L): controls solute spreading along the flow direction
 - NO₃-N:
 - Before Calibration: 2.113 m
 - After Calibration: 4.226 m
 - Horizontal Transverse Dispersivity (α_H): controls spreading perpendicular to flow
 - NO₃-N:
 - Before Calibration: 0.234 m
 - After Calibration: 0.468 m
 - NH₄-N:
 - Before Calibration: 0.234 m
 - After Calibration: 0.194 m
 - PO₄-P:
 - Calibrated Value: 0.234 m
 - Calibration Goal: match simulated nutrient concentrations with monitoring well data
 - Iteration: adjust parameters and rerun simulations as needed

Solution Options

Solution type: DomenicoRobbinsSSDecay2D

Plume warping control point spacing [Cells]: 48

Plume warping method: Spline

Threshold Concentration [mg/l]: 0.000001

Postprocessing: Medium

Domenico Bdy: Specified Z

Maximum plumes of continuous calculation for one time: 400

Source Plane Parameters

Source Dimension Y [m]: 6

Source Dimension Z [m]: 1.5

Plume cell size [m]: 0.4

Volume Conversion Factor: 1000

Bulk Density [g/cm³]: 1.42

Nitrogen Parameters

Concentration of NO₃-N [mg/l]: 40

NO₃-N Dispersivity α_L [m]: 4.226

NO₃-N Dispersivity α_H [m]: 0.468

Denitrification Decay Rate [1/d]: 0.008

Concentration of NH₄-N [mg/l]: 10

NH₄-N Dispersivity α_L [m]: 2.113

NH₄-N Dispersivity α_H [m]: 0.194

Nitrification Decay Rate [1/d]: 0.0001

kd for NH₄-N [cm³/g]: 2

Phosphorus Parameters

Concentration of PO₄-P [mg/l]: 2

PO₄-P Dispersivity α_L [m]: 2.113

PO₄-P Dispersivity α_H [m]: 0.234

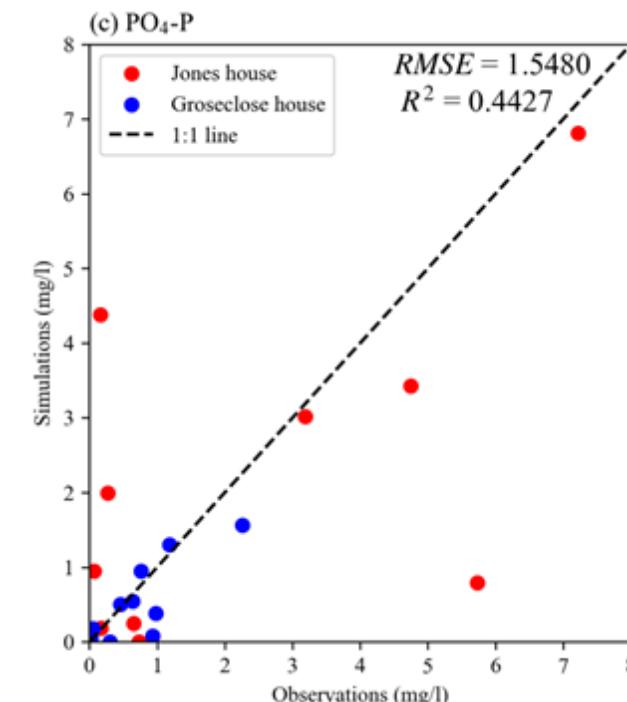
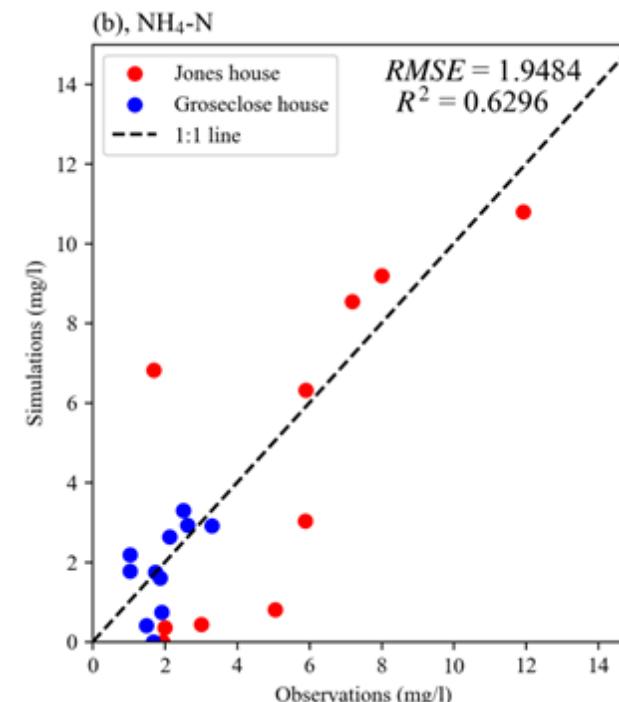
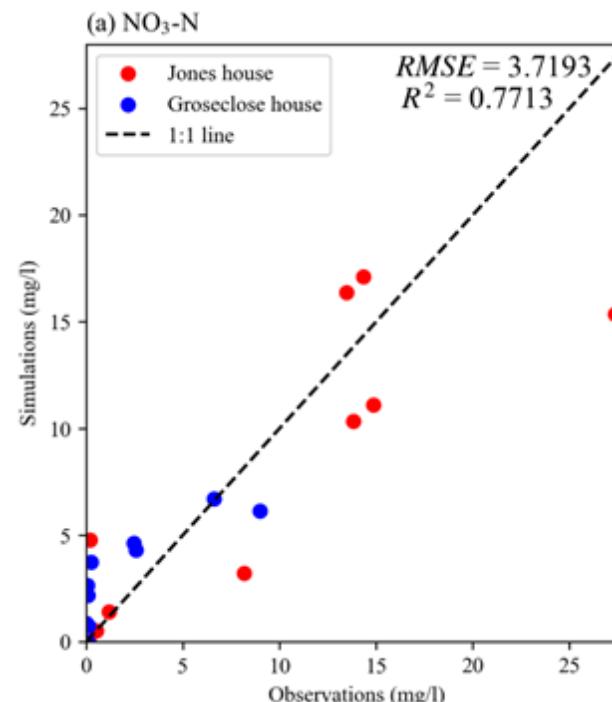
Rprecip [mg/kg 1/day]: 0.002

Sorption isotherm: Linear

Linear distribution coefficient [L/kg]: 15.1

Calibration Using Monitoring Well Data

- Monitoring Wells
 - Data from wells near Groseclose and Jones residences
- Process
 - Compare simulated concentrations of $\text{NH}_4\text{-N}$, $\text{NO}_3\text{-N}$, and $\text{PO}_4\text{-P}$ with observed values
 - Identify discrepancies and adjust transport parameters
- Adjustment Examples
 - Increase dispersivity to reflect greater solute spreading
- Modify reaction rates if attenuation is over- or underestimated
- Outcome
 - Calibrated Transport Module results ready for load estimation



Optimizing Dispersivity Using RMSE Matrices

- When Initial Dispersivity Values Don't Fit
 - Challenge: difficulty in finding correct longitudinal and horizontal dispersivity values
 - Solution: systematically test combinations using RMSE (Root Mean Square Error) matrices
- Creating an RMSE Matrix in Excel
 - Set Up Dispersivity Ranges
 - Longitudinal Dispersivity (α_L) values along the top row (X-axis)
 - Horizontal Transverse Dispersivity (α_{TH}) values along the first column (Y-axis)
 - Example α_L values: 2, 2.5, 3, 3.5, 4, 4.5, 5, 5.5, 6 meters
 - Example α_{TH} values: 0.2, 0.25, 0.3, 0.35, 0.4, 0.45, 0.5 meters
 - Run Simulations for Each Pair
 - Use ArcNLET-Py to simulate nutrient transport for each α_L and α_{TH} combination

NO₃-N RMSE for
Groseclose

α_{TH} combination

- Calculate the RMSE between simulated and observed concentrations
- Populate the Matrix with RMSE Values
 - Enter the RMSE results into the corresponding cells in Excel
 - Each cell represents an α_L and α_{TH} pair
- Example: in the matrix, the lowest RMSE is 1.68 at $\alpha_L = 2$ m and $\alpha_{TH} = 0.4$ m
- Apply Color Coding to RMSE values
 - Green: lowest RMSE (best fit)
 - Red: highest RMSE (poorest fit)
 - Gradient: shades of yellow for intermediate values

		α_L									
		2	2.5	3	3.5	4	4.5	5	5.5	6	
α_{TH}	0.2	1.87	1.90	1.93	1.95	1.97	1.95	1.90	2.00	2.02	
	0.25	1.73	1.75	1.78	1.80	1.82	1.83	1.85	1.87	1.89	
	0.3	1.95	1.98	2.00	2.02	2.04	2.06	2.08	2.10	2.11	
	0.35	1.89	1.91	1.93	1.93	1.97	1.98	2.00	2.01	2.03	
	0.4	1.68	1.70	1.71	1.73	1.75	1.76	1.78	1.79	1.81	
	0.45	1.81	1.71	1.73	1.74	1.76	1.77	1.78	1.80	1.81	
	0.5	1.78	1.79	1.81	1.82	1.83	1.85	1.86	1.87	1.88	
		0.55	1.83								

Optimizing Dispersivity Using RMSE Matrices

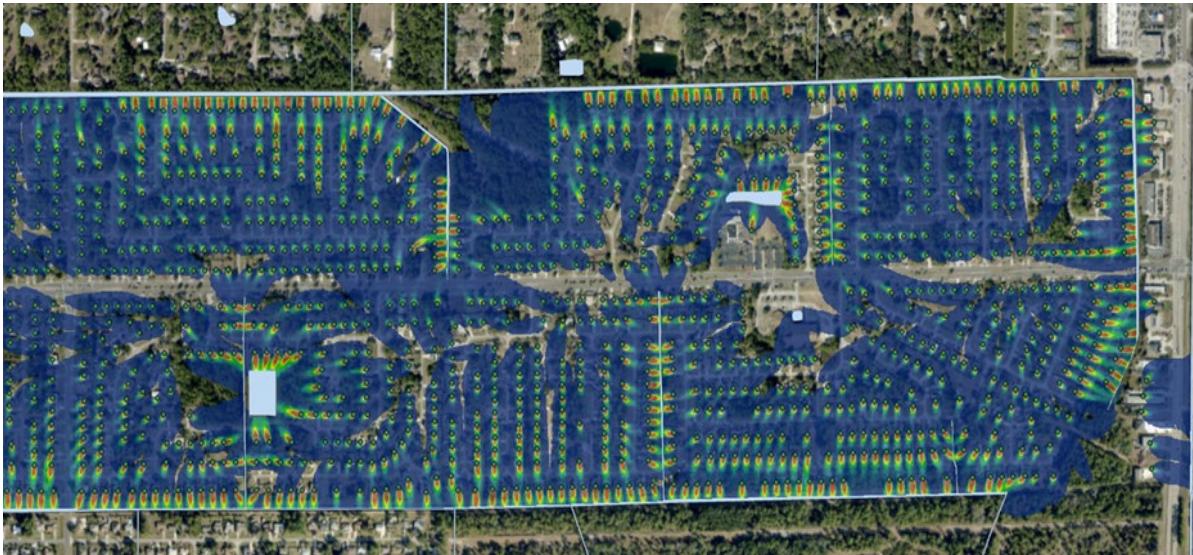
- Visual Aid: easily identify the optimal dispersivity pair with the lowest RMSE
- Repeating the Process for Other Nutrients
 - NH₄-N and PO₄-P
 - Create similar RMSE matrices
 - Adjust α_L and α_H values based on nutrient behavior
 - Combined Sites Analysis
 - Aggregate data from Groseclose and Jones residences
- Benefits of This Approach
 - Systematic Exploration: identifies the combination of dispersivity values that minimize RMSE
 - Data-Driven Calibration: improves model accuracy by aligning simulations with observed data
- If you need help adjusting the VZMOD to real-world data, plotting RMSE can aid in adjusting the VZMOD parameters for Knit and Kdnit
- Next Steps
 - Select Optimal Dispersivity Values: use the combination with the lowest RMSE for final simulations
 - Validate Model Performance: ensure that adjusted parameters produce realistic nutrient transport behavior
 - Document the Process: maintain records of all tested combinations and results for transparency

NO₃-N RMSE for combined Jones and Groseclose

		α_L									
		2	2.5	3	3.5	4	4.5	5	5.5	6	
α_T	0.2	5.09	5.02	5.15	5.10	5.02	4.98	4.71	4.83	4.80	
	0.25	4.88	5.08	4.70	4.89	4.95	4.80	4.79	4.77	4.61	
	0.3	5.11	4.92	4.95	4.80	4.79	4.75	4.80	4.61	4.72	
	0.35	5.01	4.90	4.94	4.94	4.62	4.76	4.69	4.66	4.86	
	0.4	4.94	4.82	4.75	4.90	4.80	4.98	4.93	4.78	4.87	
	0.45	5.26	4.99	5.07	5.07	4.95	4.94	4.82	4.75	4.86	
	0.5	5.27	5.14	5.04	4.96	5.04	4.87	4.88	4.90	4.73	
	0.55	5.09									

Applying the Transport Module to the Entire Study Area

- Use Calibrated Parameters from Groseclose and Jones Sites
 - Extend Application to all OSTDS across the study area
 - Ensure Consistent Parameters for reliable modeling
- Adjusted Parameters for the Study Area
 - Source Plane Concentrations (C_0)
 - Derived from VZMOD outputs for each OSTDS
- Dispersivity Parameters
 - Longitudinal Dispersivity (α_L)
 - $\text{NO}_3\text{-N}$: 4.226 m
 - Horizontal Transverse Dispersivity (α_{TH})
 - $\text{NO}_3\text{-N}$: 0.468 m
 - $\text{NH}_4\text{-N}$: 0.194 m
 - $\text{PO}_4\text{-P}$: 0.234 m



Transport Module-simulated $\text{NO}_3\text{-N}$ concentrations in the groundwater around the Groseclose and Jones homes.

- Application Process
 - Run Transport Module for all OSTDS
 - Use VZMOD outputs as source concentrations
 - Utilize flow paths from the Particle Tracking Module
- Manage Computational Resources
 - Divide Study Area if necessary (large datasets)
 - Adjust the 'Maximum plumes of continuous calculations' parameter
 - Default is 400; reduce if memory issues occur
- Result
 - Simulated Horizontal Transport of nutrients across the entire domain
 - Provides Inputs for the Load Estimation Module



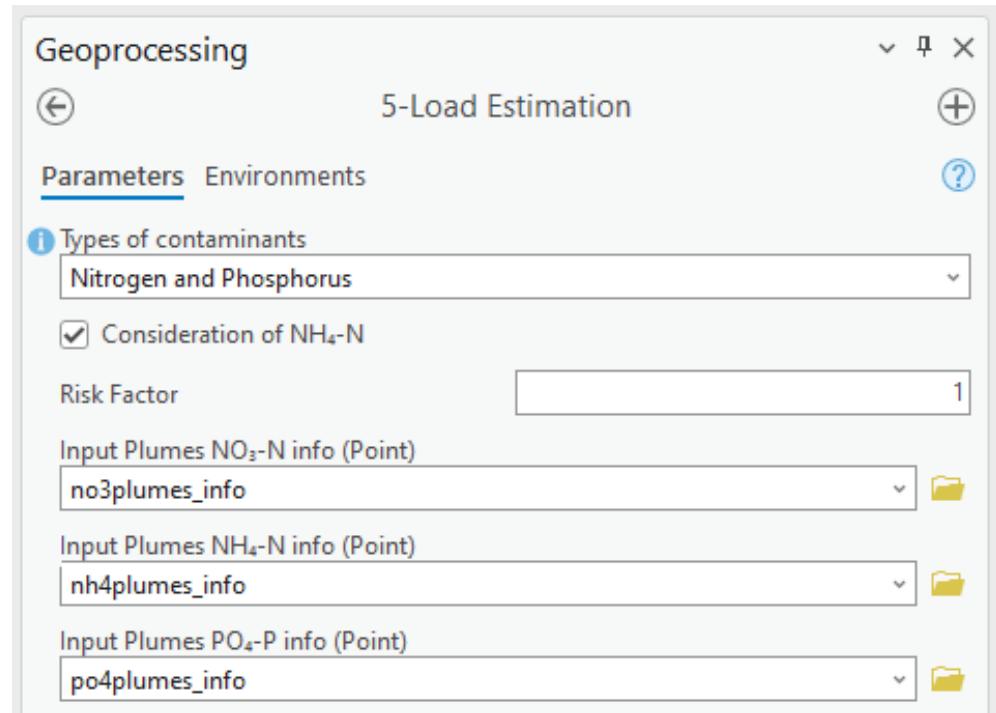
Transport Module-simulated $\text{PO}_4\text{-P}$ concentrations in the groundwater around the Groseclose and Jones homes.



9. Load Estimation Module

Load Estimation Module

- Function
 - Estimate nutrient loads from OSTDS reaching surface waterbodies
- Inputs
 - Calibrated outputs from the Transport Module
- Process
 - Calculate nutrient loads using the mass balance approach
 - Account for removal processes (e.g., denitrification, adsorption)
- Calibration Aspect
 - Ensure estimated loads are consistent with field measurements and expectations
 - Note that PO₄-P is “N/A” because the plumes did not reach the water
- Final Step
 - Once calibration is satisfactory, proceed to simulate the entire domain



	NH ₄ -N	NO ₃ -N	PO ₄ -P
Mass Output Load (mg/d)	72.71	721.49	N/A
Mass Input Load (mg/d)	118.30	4916.38	N/A
Mass Removal Rate (mg/d)	45.59	4194.90	N/A

Simulated loading for NO₃-N, NH₄-N, and PO₄-P entering surface waterbodies.



I0. Conclusion and Q&A

Overall Modeling Workflow

- Data Preparation
 - Gather Essential Datasets
 - Study Area Shapefile
 - OSTDS Locations
 - Waterbody Polygons
 - Digital Elevation Model (DEM)
 - Ensure Data Consistency
 - Same projection (NAD 1983 UTM Zone 17N)
 - Uniform units (meters) and formats (.shp) and (raster)
- Model Calibration at Groseclose and Jones Sites
 - Calibration Step 1: Groundwater Movement
 - Objective: Match simulated groundwater levels with measured water table elevations
 - Process:
 - Adjust smoothing factors and cell sizes in the Groundwater Flow Module
 - Merge waterbody elevations to preserve features
 - Compare smoothed DEM with observed groundwater levels
 - Outcome: Calibrated groundwater flow model reflecting actual subsurface conditions
 - Calibration Step 2: Reactive Nutrient Transport
 - Objective: Align simulated nutrient concentrations with observed concentrations in monitoring wells
 - Process:
 - Use the VZMOD Module for vertical nutrient attenuation
 - Adjust nitrification, denitrification, and phosphorus parameters
 - Utilize Transport Module for horizontal nutrient transport
 - Optimize dispersivity values using RMSE matrices
 - Outcome: The calibrated transport model accurately simulates nutrient movement



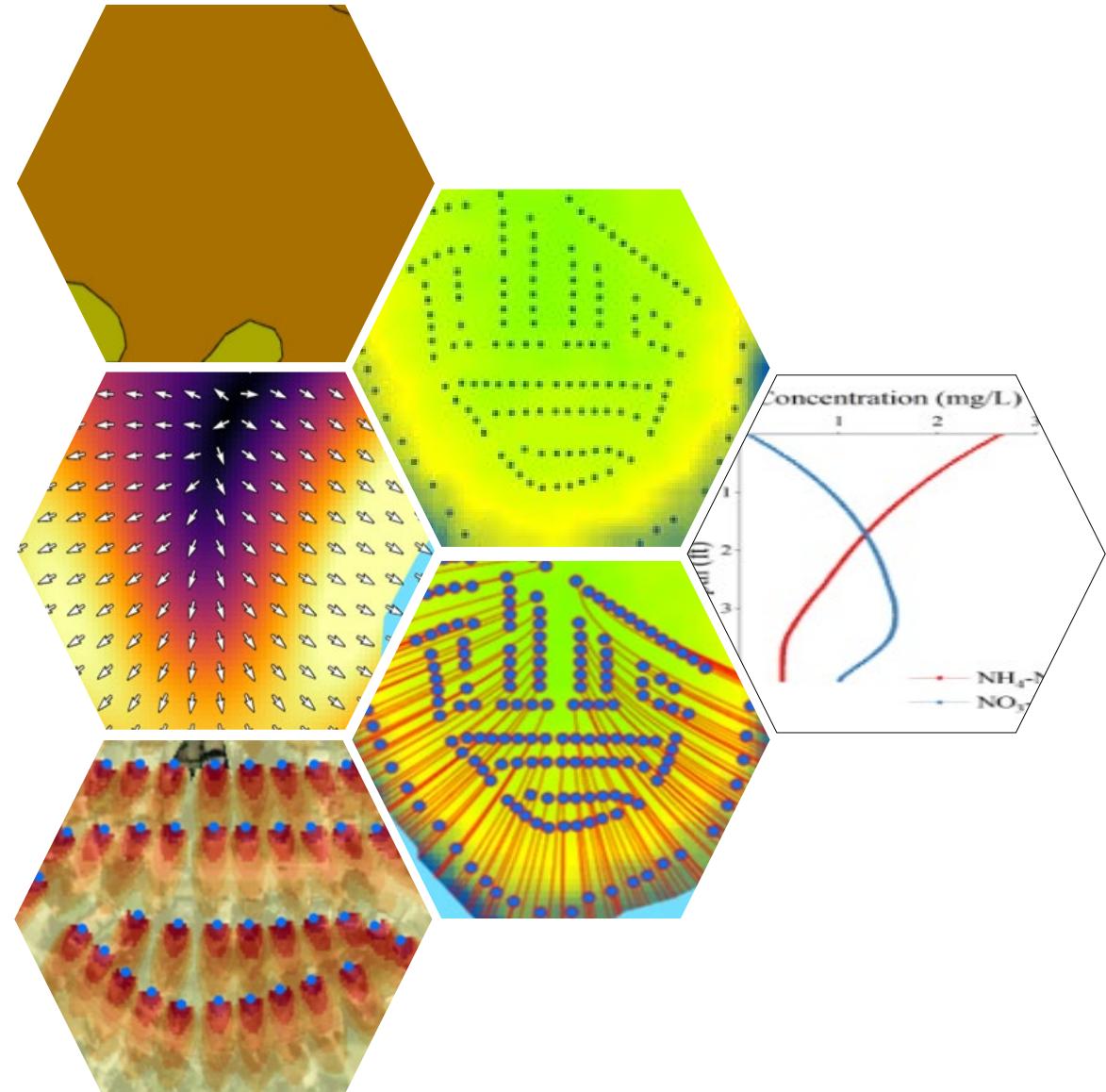
Overall Modeling Workflow

- Application to the Entire Study Area
 - Run Calibrated Models across all OSTDS in the study area
 - Apply calibrated parameters uniformly or adjust for local conditions
 - Manage computational resources (divide area if necessary)
 - Generate Spatial Outputs
 - Simulated concentrations of NH₄-N, NO₃-N, PO₄-P across the domain
- Nutrient Load Estimation
 - Use the Load Estimation Module
 - Calculate nutrient loads from OSTDS to surface waterbodies
 - Outputs: Quantitative load estimates (e.g., grams per day)
- Key Takeaways
 - Structured Workflow ensures systematic modeling and calibration
 - Calibration at Specific Sites enhances overall model accuracy
 - Application to Entire Domain provides comprehensive nutrient load estimations
 - Final Outputs inform strategies to protect water quality in communities using OSTDS



Conclusion

- Summary
 - Detailed calibration steps are essential for accurate ArcNLET-Py modeling
 - Each module requires careful adjustment of parameters based on field data
- Calibration Steps Recap
 - Preprocessing Module: accurate study area, PCS, soil depths
 - Groundwater Flow Module: adjust smoothing factors, smoothing cells, and merge waterbodies
 - Particle Tracking Module: verify flow paths; revisit Groundwater Flow Module if necessary
 - VZMOD: calibrate using field measurements; adjust nitrification, denitrification, and phosphorus parameters
 - Transport Module: adjust dispersivities; calibrate with monitoring well data
 - Load Estimation Module: use calibrated results for accurate load calculations
- Benefits:
 - Provides reliable estimates of nutrient loads
 - Supports the development of science-based solutions for water quality protection

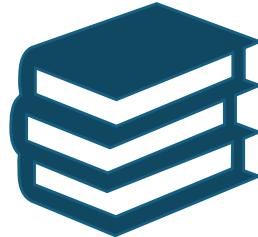


Common Issues and Troubleshooting

- Particle Tracking Module Errors
 - NoneType Errors
 - Caused by using geodatabase formats
 - Solution: use folder-based shapefiles and raster files
 - Ensure all inputs are shapefiles, not feature classes
- File Path Considerations
 - Keep file paths and names short
 - ArcGIS Pro limits
 - Raster filenames: max 13 characters
 - Total path length: max 128 characters
 - Avoid spaces and special characters in file names
- Memory Limitations
 - For large study areas
 - Divide the domain into smaller sections
 - Adjust 'Maximum plumes of continuous calculations' in the Transport Module
 - Monitor computational resources to prevent crashes
 - Improving Flow Paths
 - If particle paths are trapped or inaccurate: revisit the Groundwater Flow Module
 - Adjust smoothing factors, cell sizes, and waterbody merging

ArcNLET-Py Resources

- Source code on GitHub and online User's manual
 - <https://github.com/ArcNLET-Py/ArcNLET-Py>
- Training videos on YouTube
 - <https://www.youtube.com/@mingye9168/videos>
- FSU Website
 - <https://atmos.eoas.fsu.edu/~mye/ArcNLET/>
- USGS The National Map (TNM) Download (v2.0)
 - DEM and waterbodies data source
 - <https://apps.nationalmap.gov/downloader/>
- FDOH, Florida Water Management Inventory Project (FLWMI)
 - Parcels with known septic tank data source
 - <https://www.floridahealth.gov/environmental-health/drinking-water/flwmi/index.html>
 - Florida OSTDS plume studies
 - https://floridadep.gov/sites/default/files/plume%20studies_ada_20221011.pdf



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Thank you!