

# **Phase 7 WSM Development – Water Quality Calibration (~October 2024 version)**

Modeling Workgroup Quarterly Meeting – October 2024

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# Presentation Outline

## Phase 7 Dynamic Watershed Model (DWM)

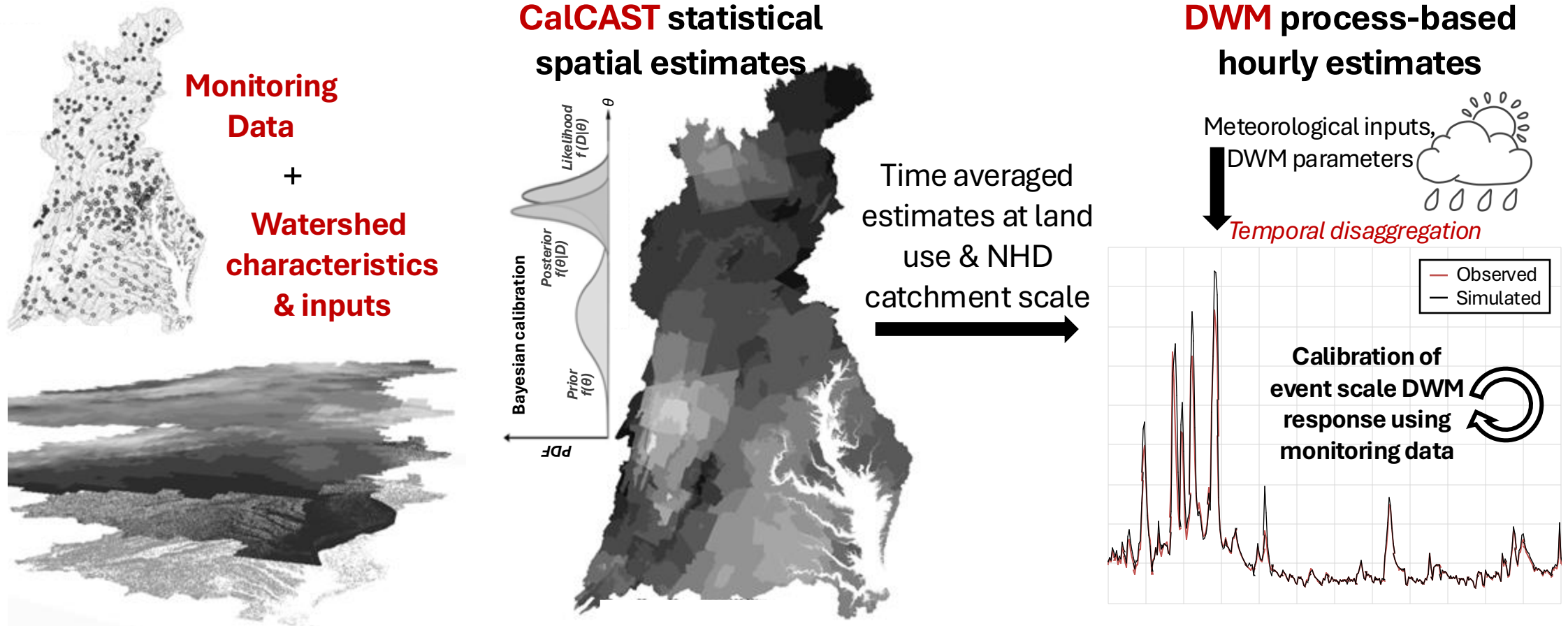
- 1. Dynamic Watershed Model Overview**
- 2. Review of prior model development progress**
- 3. Water quality calibration**
  - Revisions to streamflow simulations
  - Implementations of water temperature module
  - Water quality calibration approaches
  - Review of October 2024 version of the model
- 4. Summary and next steps**

# Purpose

## **NHD Scale Dynamic Watershed Model (DWM)**

- Inputs for the estuarine models (MBM/MTMs)
- Watershed model calibration and scenario applications
- Support research and collaboration activities

# Framework: Statistical Model (CalCAST) → Dynamic Watershed Model (DWM)



- Data-driven CalCAST informs DWM parameters and responses.
- NHD-scale DWM prototype is now using CalCAST *average annual* (a) total flow, (b) stormflow, (c) sediment erosion and delivery factors, and (d) total nitrogen and total phosphorus loads and delivery factors.



# Dynamic Watershed Model (DWM) Development

- **Year 2022:** NHD-scale model structure and prototypes for hydrology, sediment, and nutrients.
  - Operational prototypes with reasonable runtime and on the graph paper model results.
- **Year 2023:** Incremental refinements of model prototypes in terms of model segmentation, CalCAST→DWM linkage, and simulation of the small streams.

## Development Milestones (2022)

100K NHD	NHD-scale model structure; Hydrology prototype; Expanded simulation period 1985 to 2020; <sup>[1][2]</sup>
HYDROLOGY	Hydrology calibration (CalCAST→DWM) method updates; initial testing of numerical simplifications for flow routing; <sup>[3]</sup>
SEDIMENT	Sediment model; Hydrology model calibration updates with respect to stormflow; <sup>[4]</sup>
NUTRIENTS	Nutrient (Nitrogen and Phosphorus) model; Updated sediment model; <sup>[5]</sup>

[1] <https://d18evl0k5eia.cloudfront.net/chesapeakebay/documents/Progress-in-Phase-7-WSM-Development-1.4.2022-GopalBhatt-Penn-State.pdf>  
[2] <https://d18evl0k5eia.cloudfront.net/chesapeakebay/documents/Progress-in-Phase-7-WSM-Development-4.5.2022-GopalBhatt-Penn-State.pdf>  
[3] <https://d18evl0k5eia.cloudfront.net/chesapeakebay/documents/Progress-in-Phase-7-WSM-Development-7.12.22.pdf>  
[4] <https://d18evl0k5eia.cloudfront.net/chesapeakebay/documents/Progress-in-Phase-7-WSM-Development-GopalBhatt-Penn-State-10.4.22-v2.pdf>  
[5] <https://d18evl0k5eia.cloudfront.net/chesapeakebay/documents/Progress-in-Phase-7-WSM-Development-GopalBhatt-Penn-State-1.10.2023.pdf>

## ... incremental improvements during 2023

Segmentation	We performed re-segmentation and tested the revised model. <ul style="list-style-type: none"><li>■ tidal percent attribute was updated using new shoreline layer</li><li>■ all databases (river mainstem, topology, etc.) were updated</li><li>■ segmentations in the tidal watershed were improved</li></ul>
Model	Improvements on overcoming the 'aggregation effect' in the simulation of river mainstems (CalCAST → DWM) <ul style="list-style-type: none"><li>➢ Non-iterative hydraulic routing for small 100K NHDplus streams</li><li>➢ WQ routing (TN) for small 100K NHDplus streams</li></ul>
Simulation	Testing on Amazon AWS and MS Azure cloud HPC environments with various node type and size configurations

[1] <https://d18evl0k5eia.cloudfront.net/chesapeakebay/documents/20230401-BHATT-Phase-7-WSM-Development-DynamicModelDevelopment2023Q1.pdf>  
[2] <https://d18evl0k5eia.cloudfront.net/chesapeakebay/documents/Progress-in-Phase-7-WSM-Development-GopalBhatt-Penn-State-6.20.2023.pdf>  
[3] <https://d18evl0k5eia.cloudfront.net/chesapeakebay/documents/Progress-in-Phase-7-WSM-Development-GopalBhatt-Penn-State-10.17.2023.pdf>  
[4] <https://d18evl0k5eia.cloudfront.net/chesapeakebay/documents/20240109-BHATT-Phase-7-WSM-Development-DynamicModelDevelopment2023Q4.pdf>

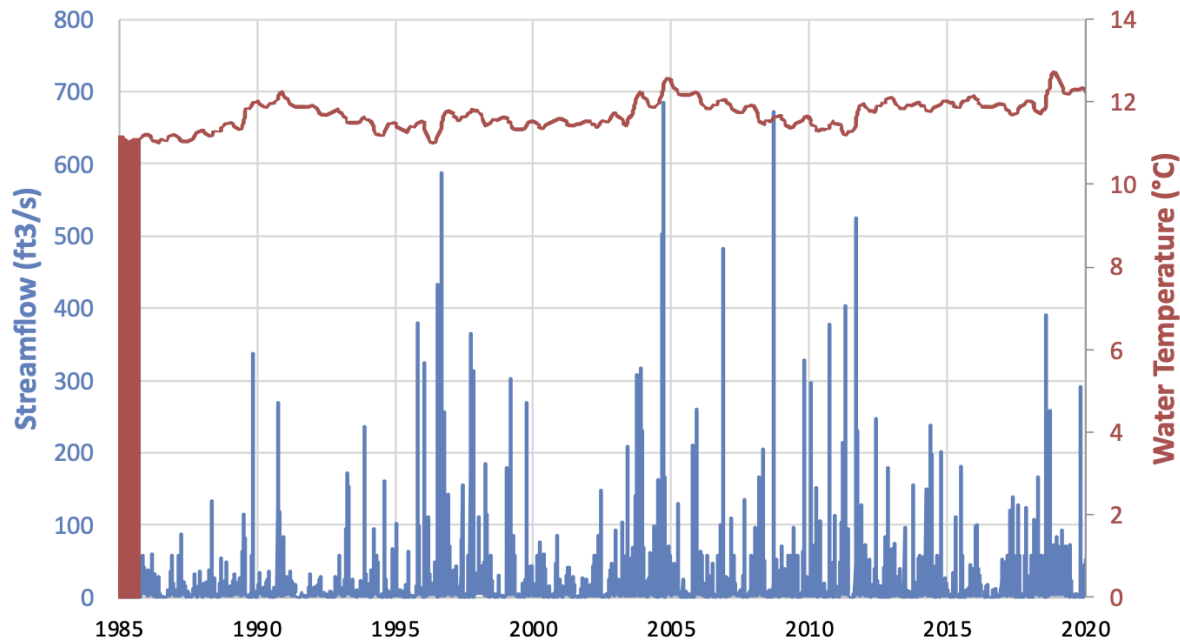
- **Year 2024: (Q1)** stream water quality routing based on  $\beta$  parameters; (Q2) mechanics of water quality calibrations (step 1 of 2)

[1] <https://d18evl0k5eia.cloudfront.net/chesapeakebay/documents/Progress-in-Phase-7-WSM-Development-GopalBhatt-Penn-State-CBPO-4.2.2024.pdf>  
[2] <https://d18evl0k5eia.cloudfront.net/chesapeakebay/documents/Phase-7-WSM-Development-Modeling-WG-July-2024.pdf>

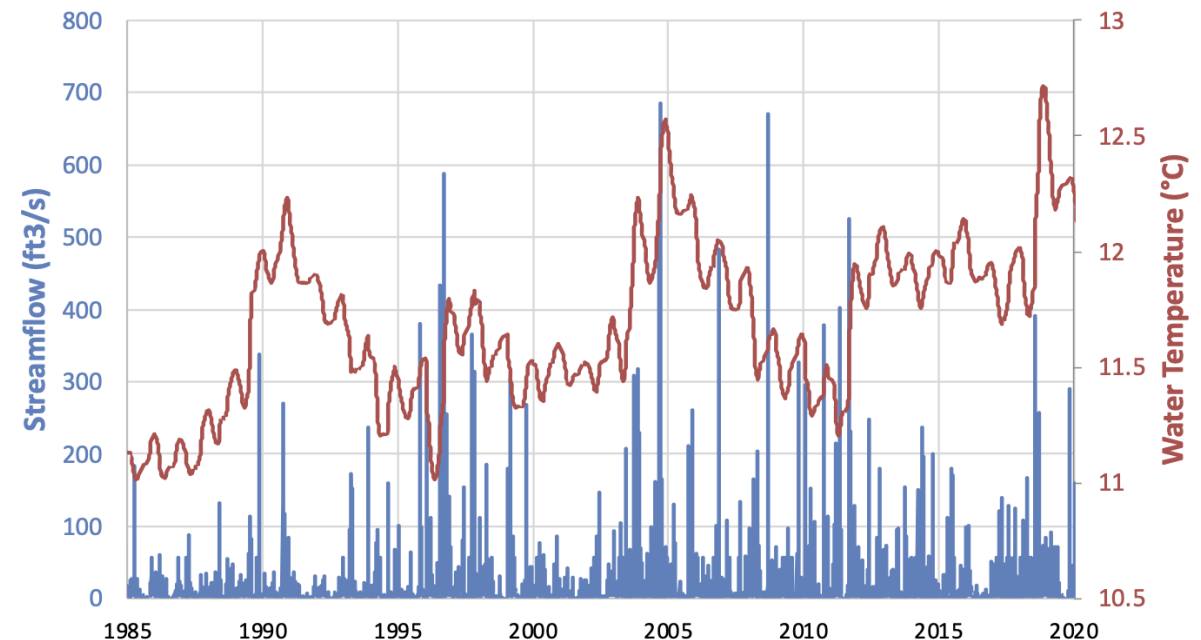
# Flow refinements

- We implemented changes for addressing instability issues
  - A constrain of slow  $\Delta$ storage when it is greater than the storage
  - A constrain for slow flow release after reaching a low volume threshold
  - A few bug fixes were made

July 2024

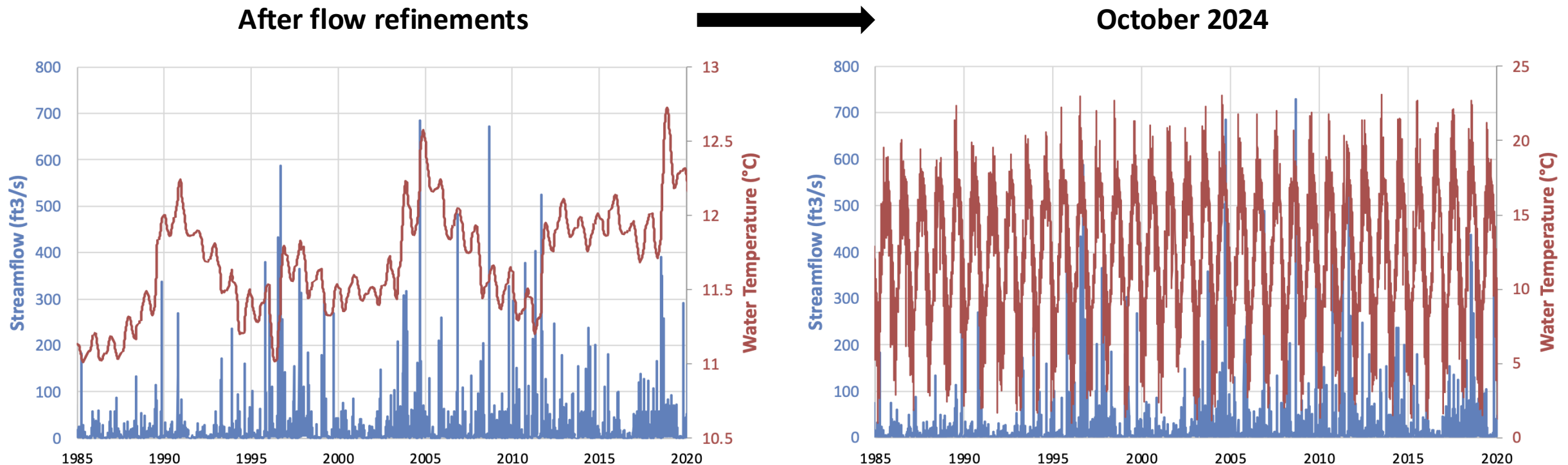


After flow refinements



# Water temperature

- We implemented a routing module while ensuring heat-balance
  - A constrain for idle water volume was added to overcome precision loss
  - A few bug fixes were made



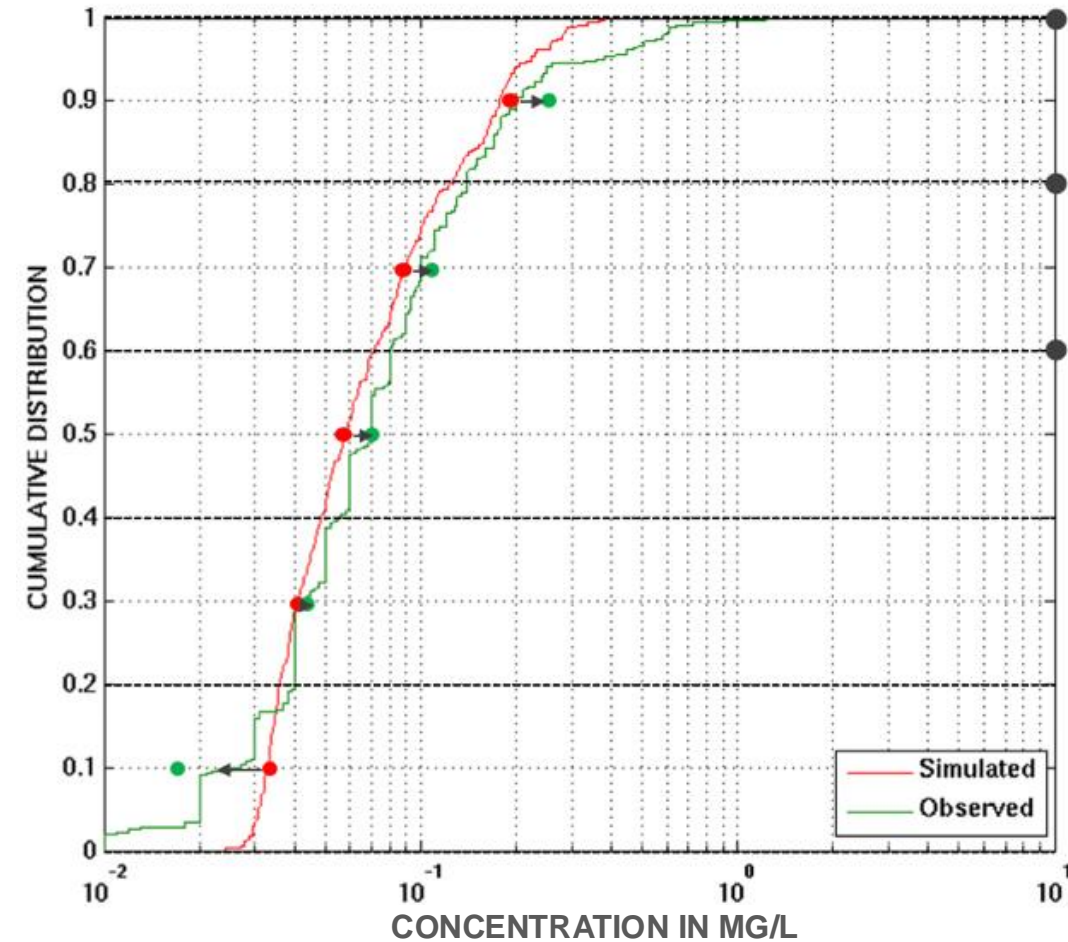
- (1) It offers potential for including emergent behavior of small streams processes, e.g., as a function of shading.  
(2) Groundwater temperature currently isn't sensitive to changes in future climate so that could be included in Phase 7 for completeness.

# Water quality calibration methods

Information available for the calibration dynamic model parameters:

- Observations of daily concentrations for nutrient species at monitoring stations
- Transport factors for TN, TP, and SS for each river mainstems (CalCAST)
- QC relationships (generalized  $\beta$  parameters for river mainstems)

Figure: Cumulative distribution of concentrations at a monitoring station

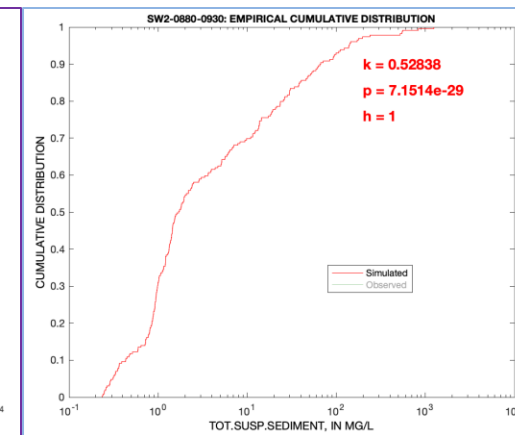
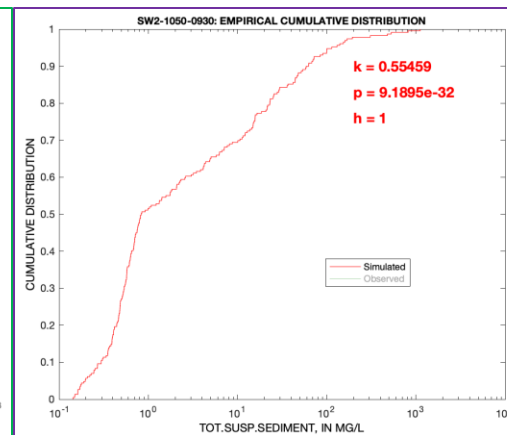
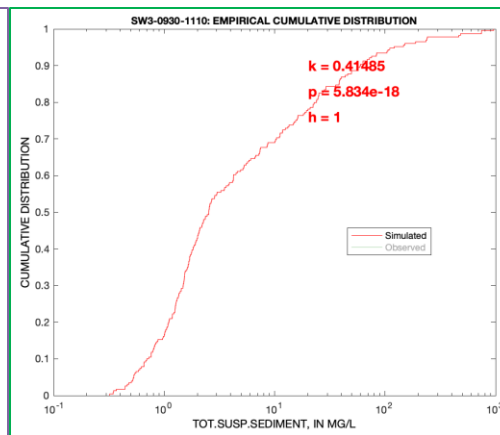
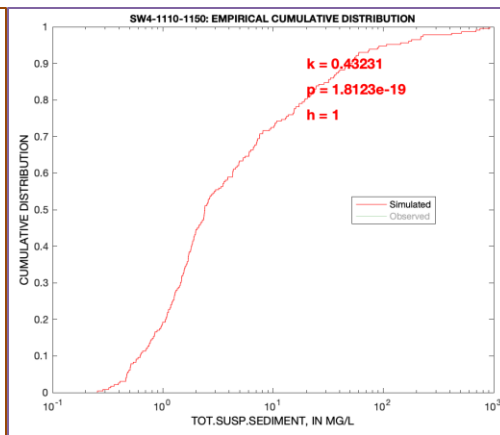
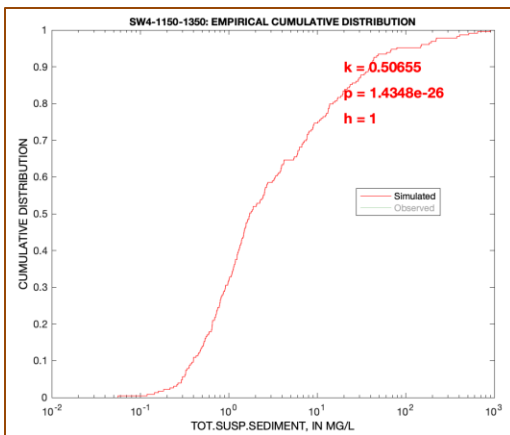
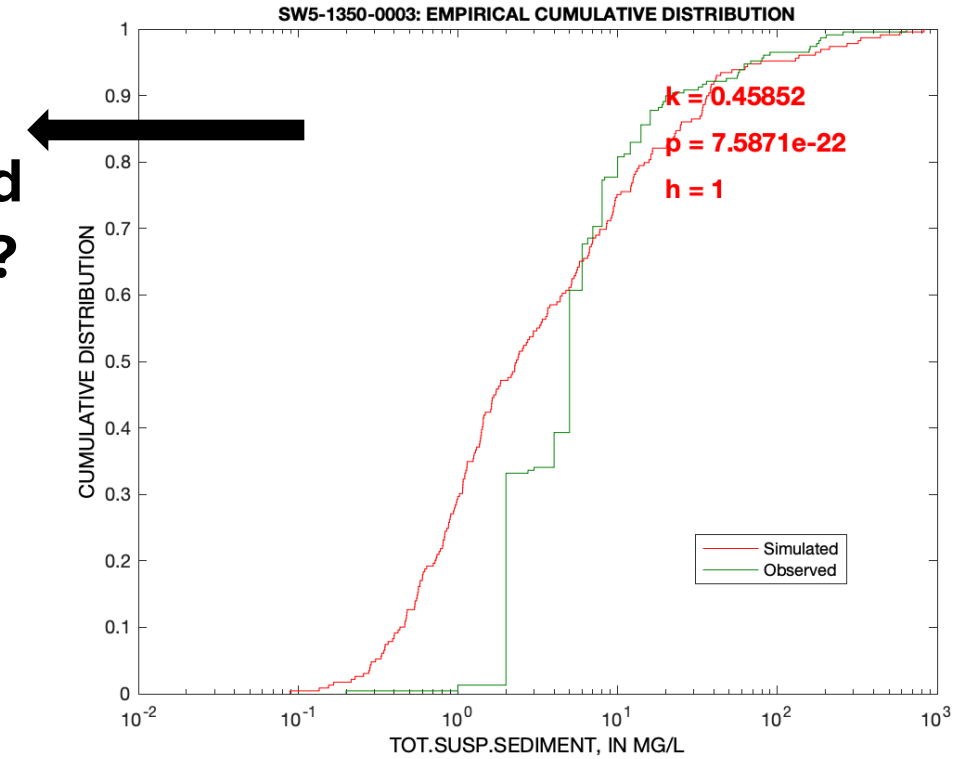
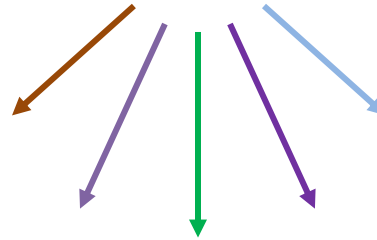


**We calibrate model parameters to improve agreement in cumulative frequency distribution (CFD) of observed and simulated concentrations**

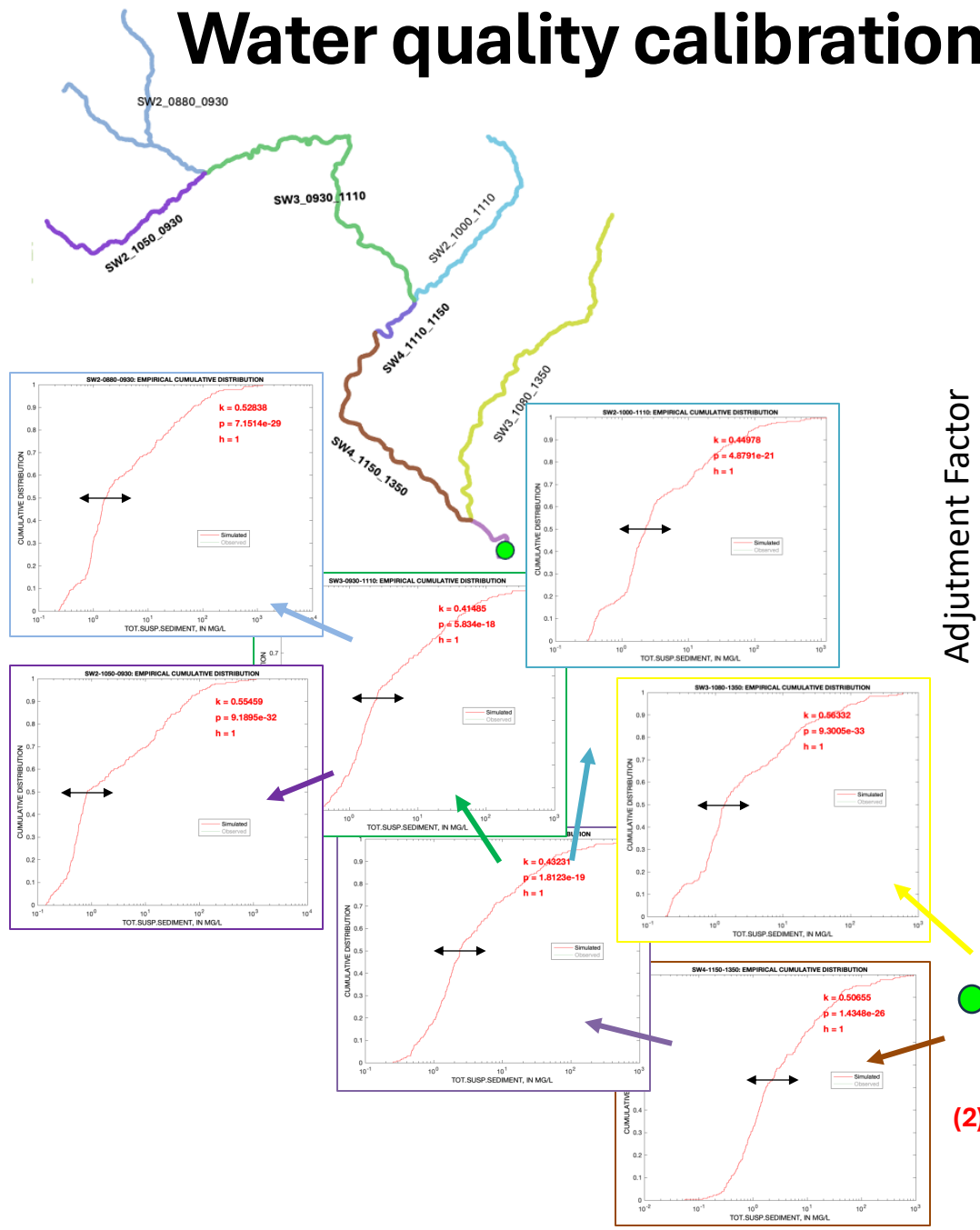
# Water quality calibration methods

Question: How should  
the CFDs of unmonitored  
segments be calibrated?

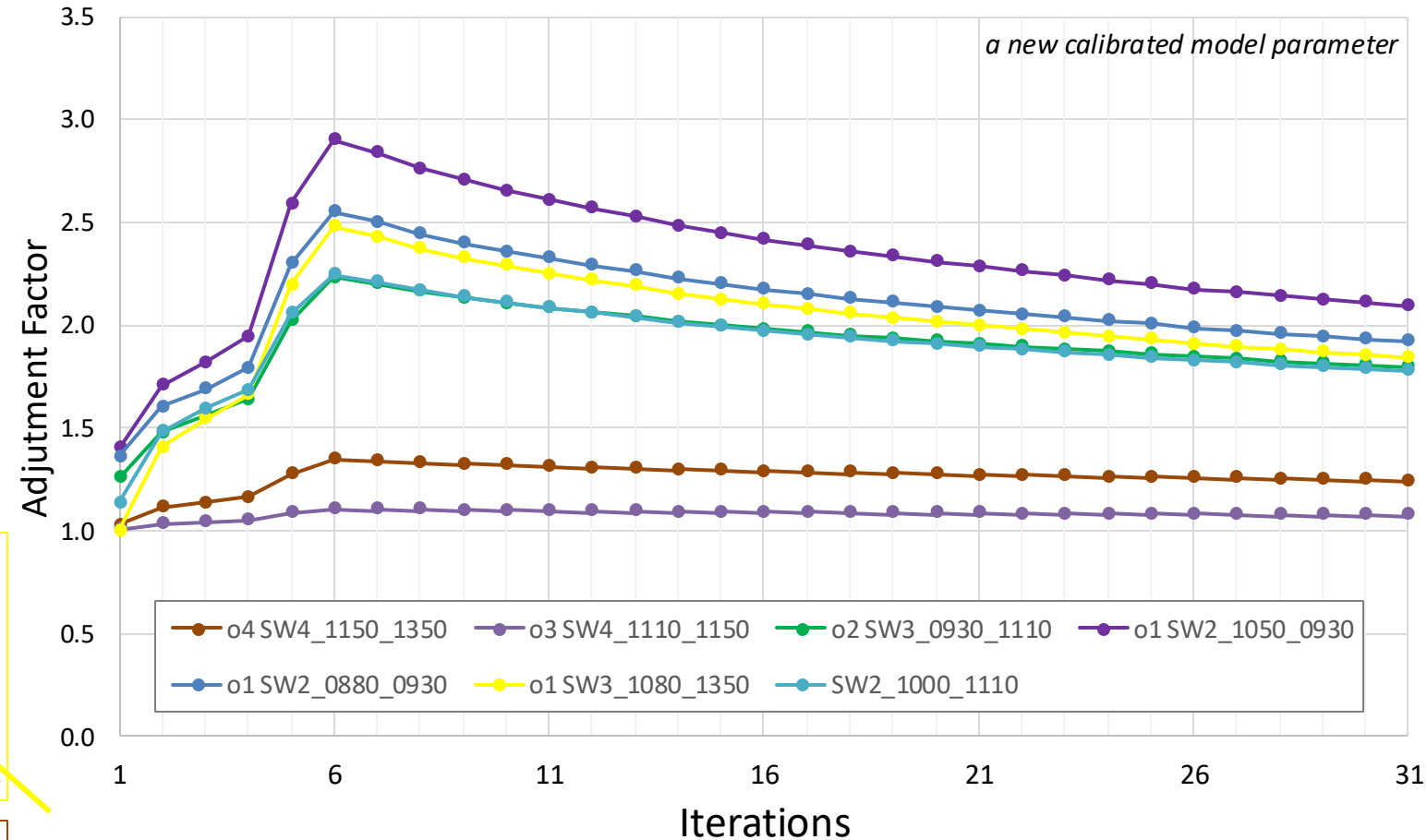
considering 3 options



# Water quality calibration methods



## Adjustment Factors for Sediment CFDs



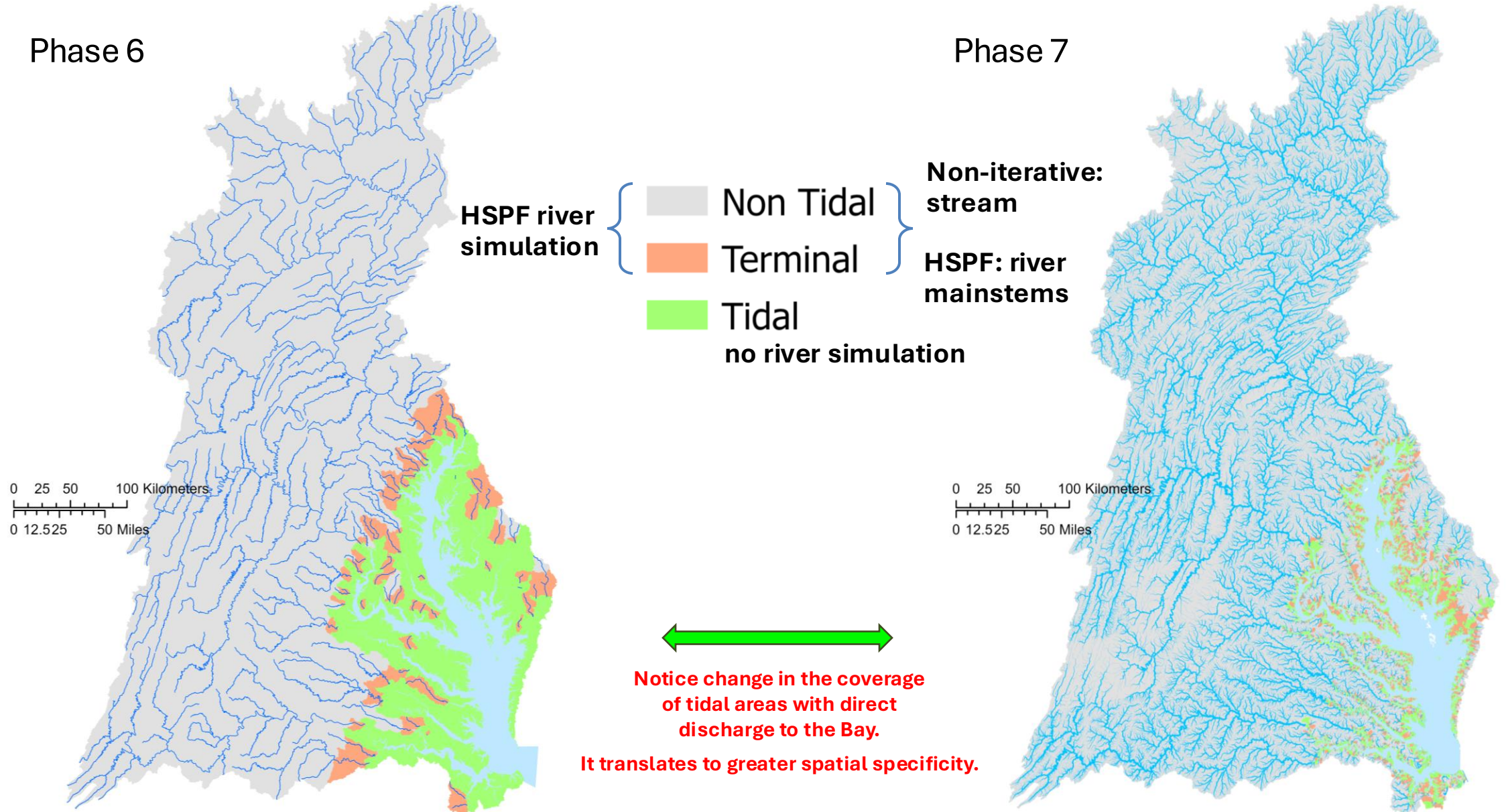
- (1) We propagate changes in parameters needed for improving agreement in the shape of the CFDs.
- (2) We shift TN|TP|SS CFDs for matching CalCAST average annual delivery potential or transport factors.



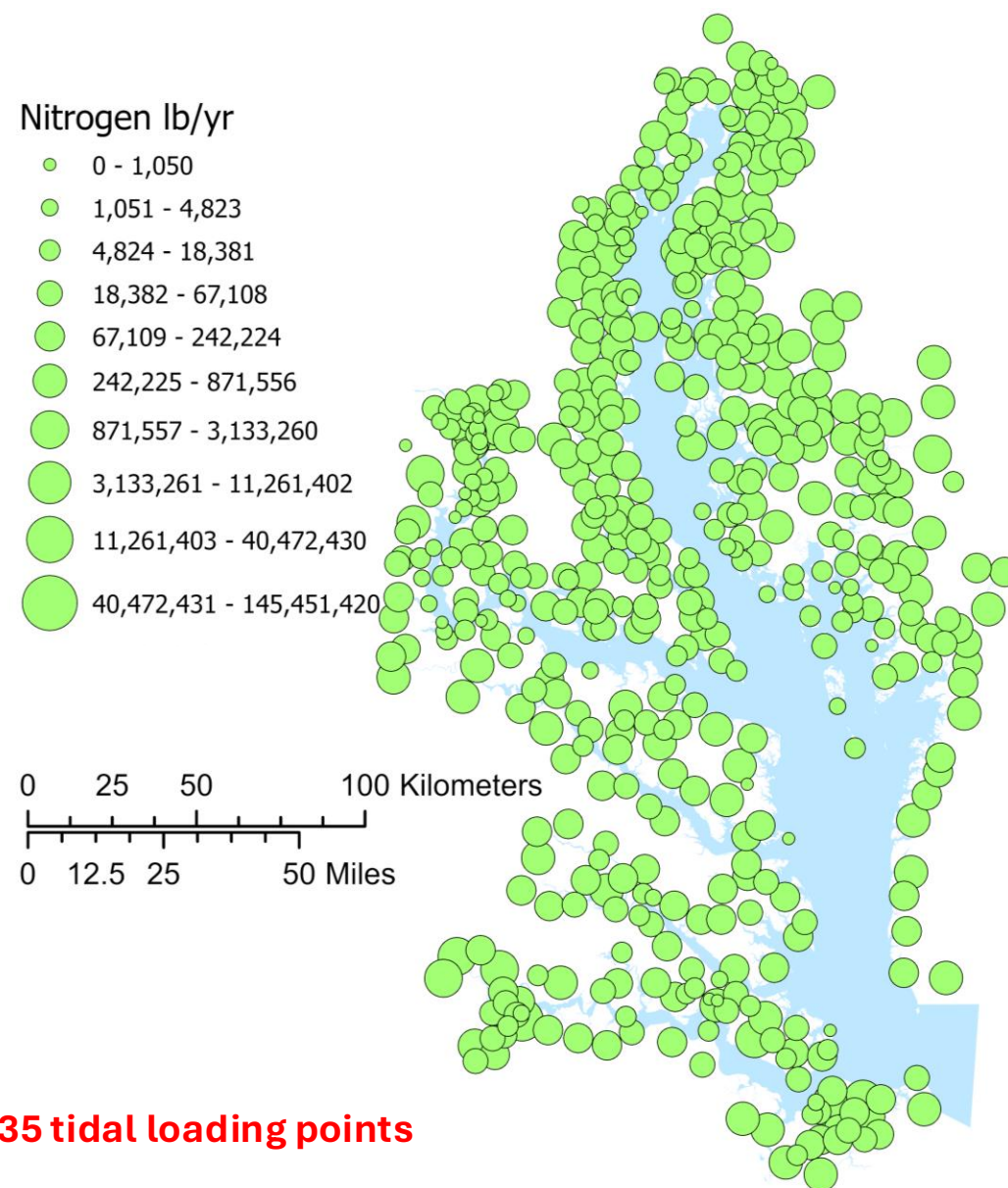
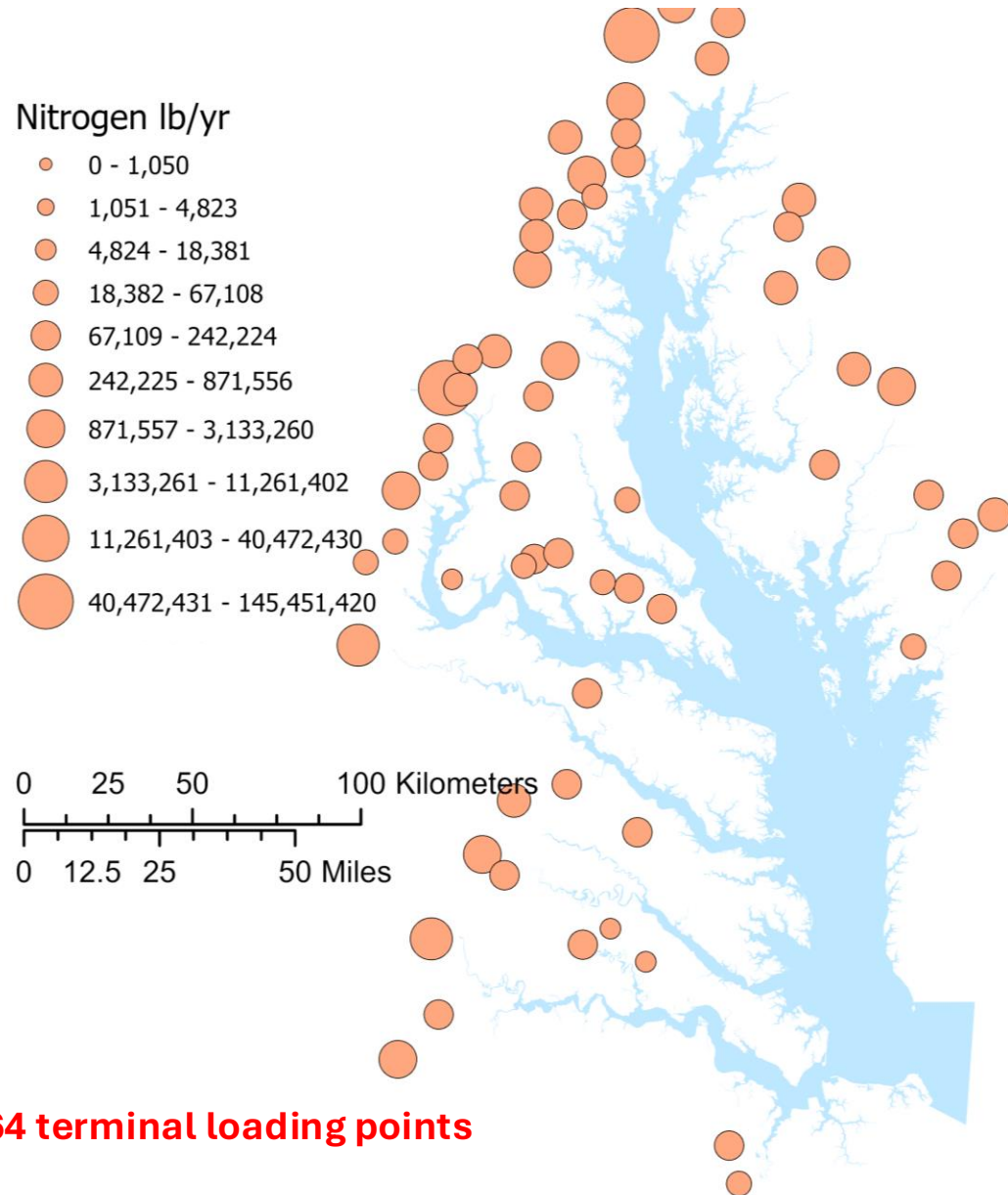
# Terminal and Tidal loadings

Phase 6

Phase 7



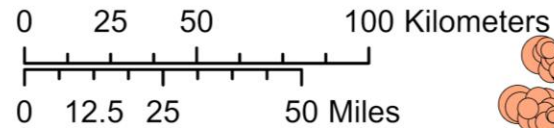
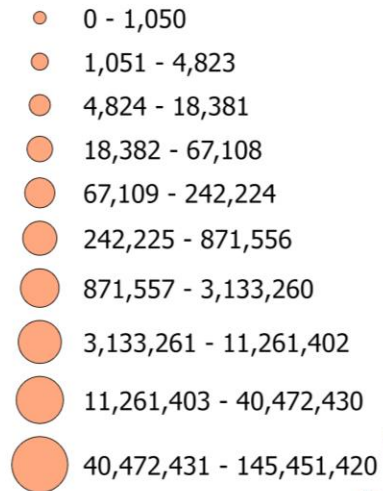
# Phase 6: Terminal and Tidal loadings





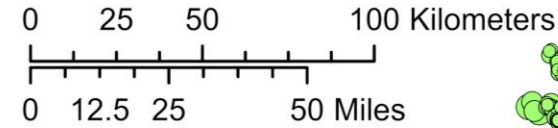
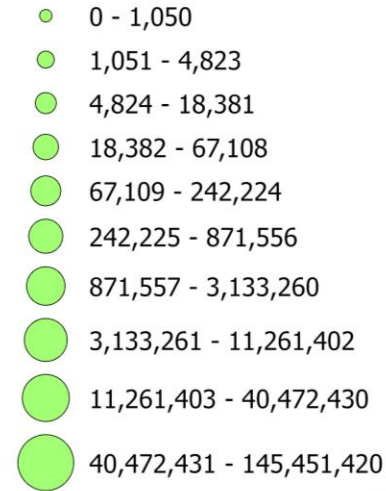
# Phase 7: Terminal and Tidal loadings

Nitrogen lb/yr



**2693 terminal loading points**

Nitrogen lb/yr

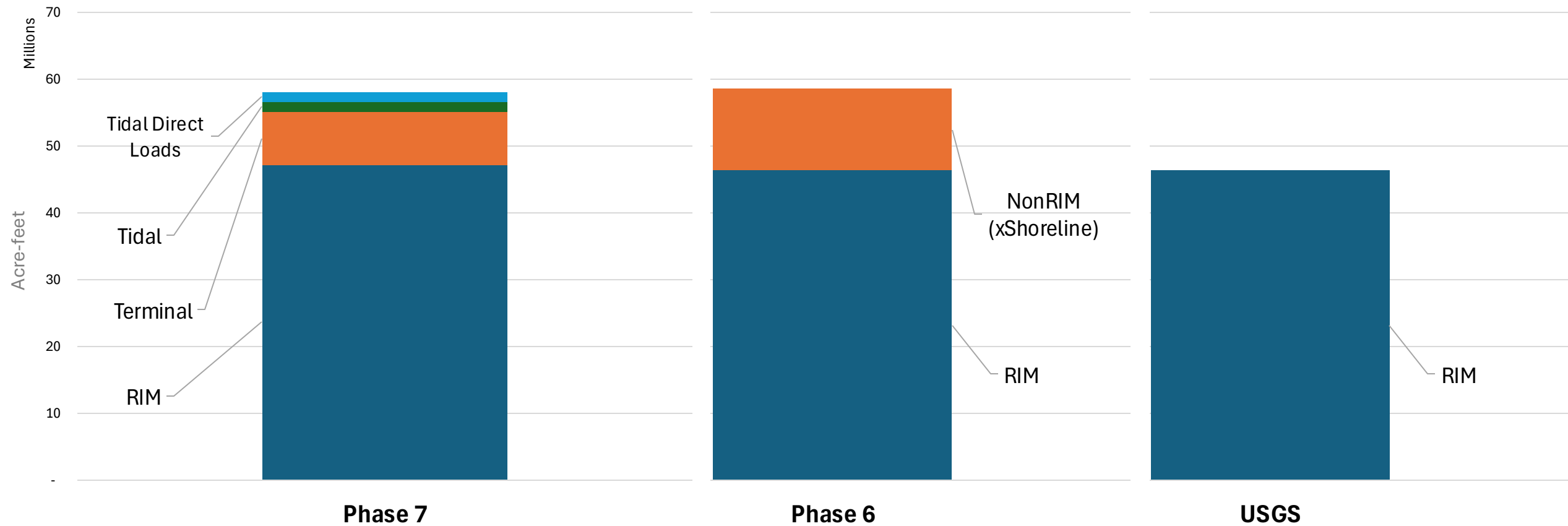


**7690 tidal loading points**

# Summary of Average Annual Loads

- We examined Phase 7 (October 2024 version) as compared to Phase 6 and WRTDS

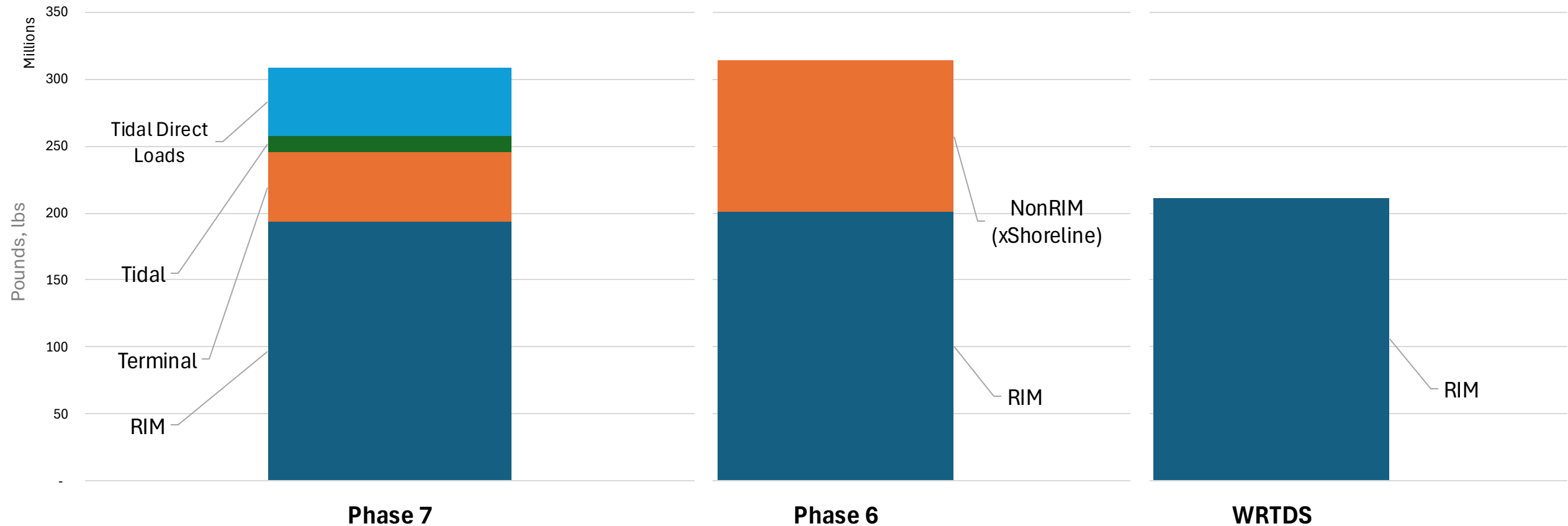
# Freshwater Delivery from the Watershed



*"Tidal Direct Loads" is currently not included in Phase 7 DWM*

*Δ total P7 vs. P6 = -1%*

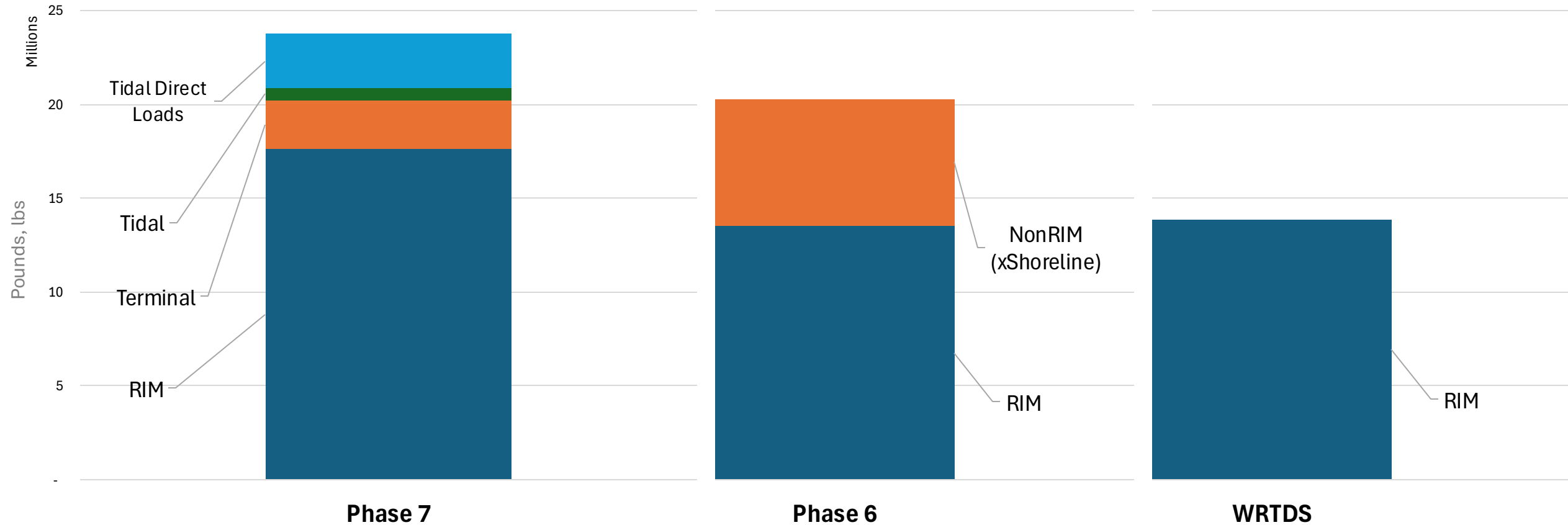
# Total Nitrogen Delivery from the Watershed



*"Tidal Direct Loads" is currently not included in Phase 7 DWM*

$\Delta$  total P7 vs. P6 = -2%

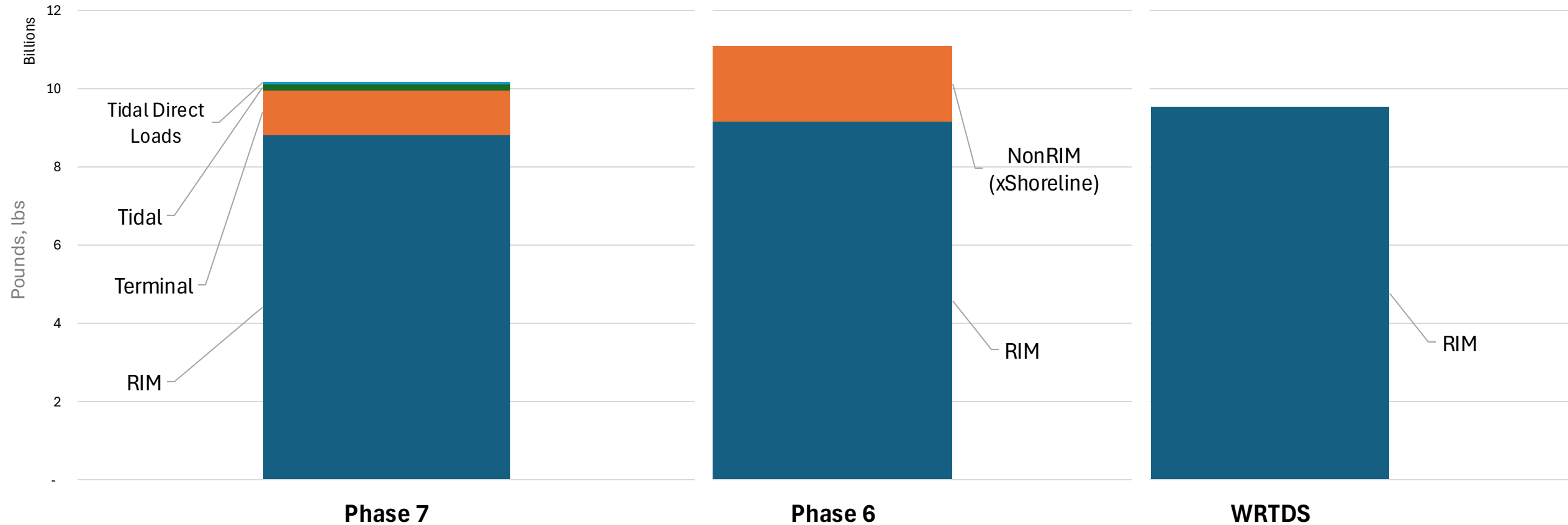
# Total Phosphorus Delivery from the Watershed



*"Tidal Direct Loads" is currently not included in Phase 7 DWM*

$\Delta$  total P7 vs. P6 = +17%

## Sediment Delivery from the Watershed



*"Tidal Direct Loads" is currently not included in Phase 7 DWM*

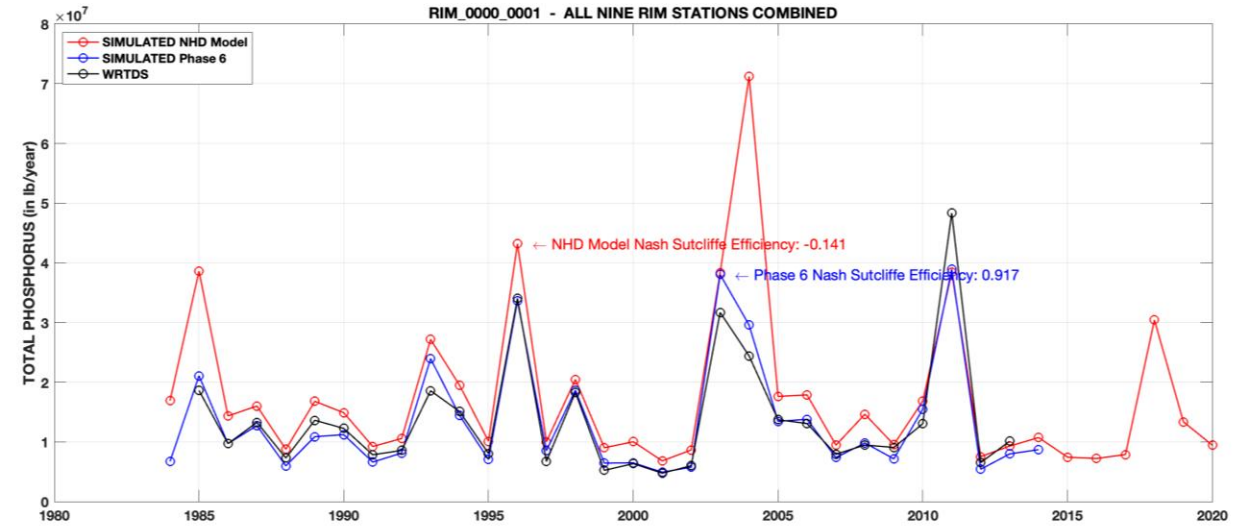
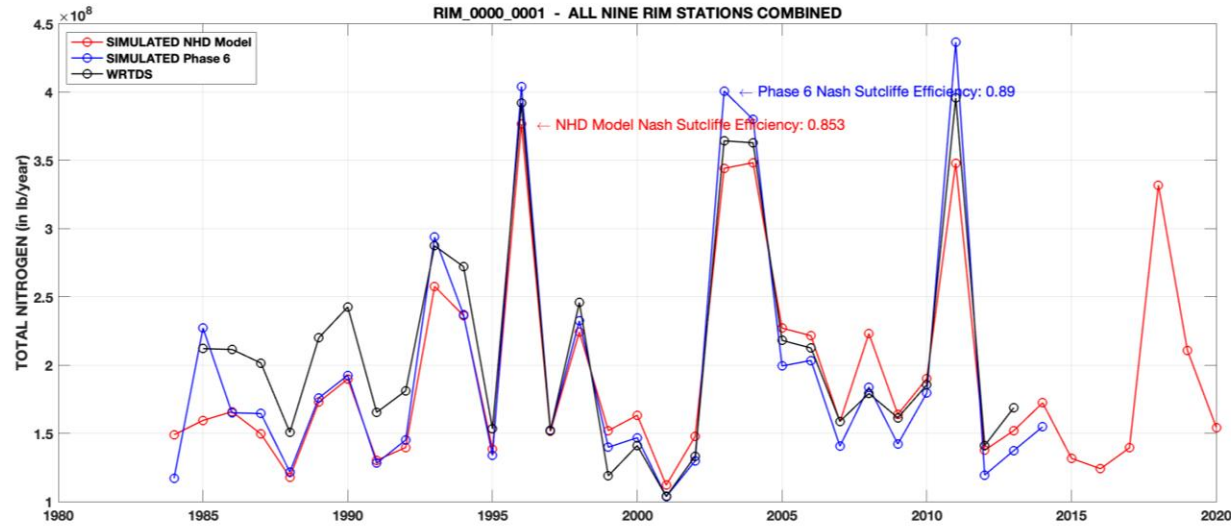
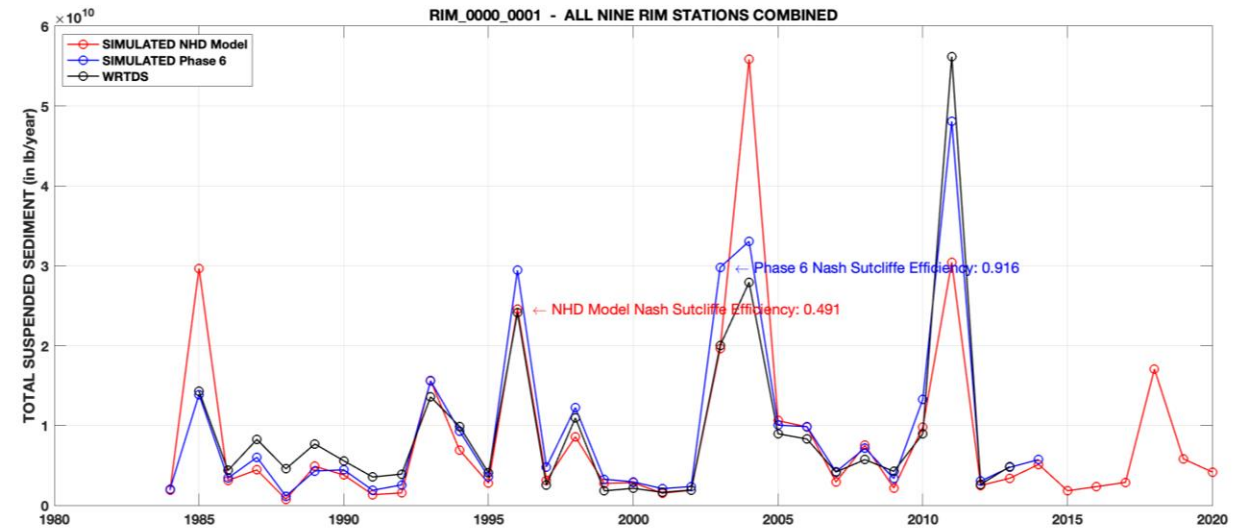
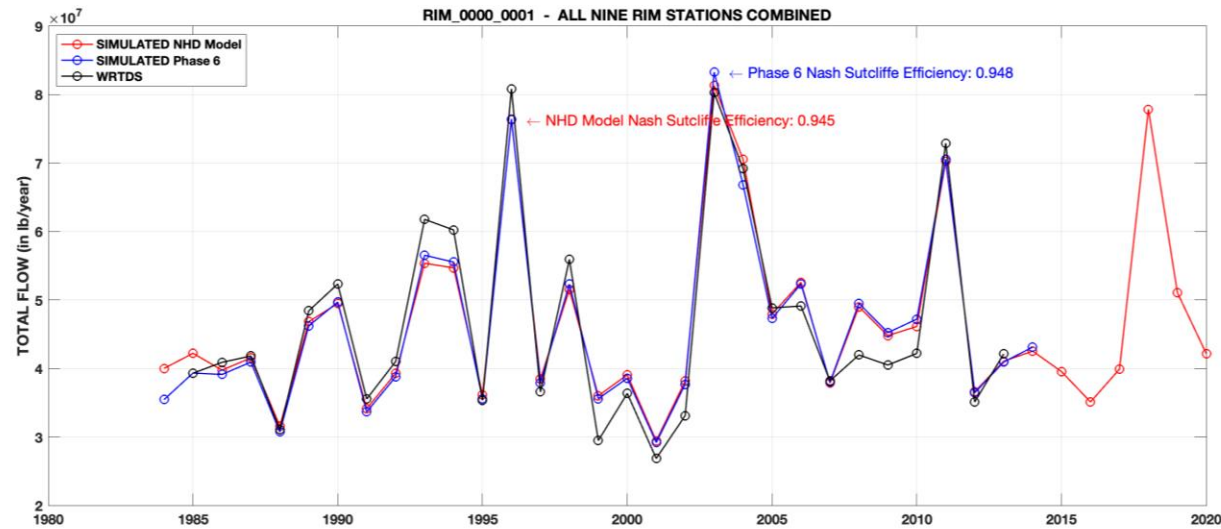
$\Delta$  total P7 vs. P6 = -8%

# Phase 7 (October 2024) RIM stations loads vs. WRTDS

(a) biases in 1985-2014 average loads as compared to WRTDS; (b) NSE of annual loads in parentheses;

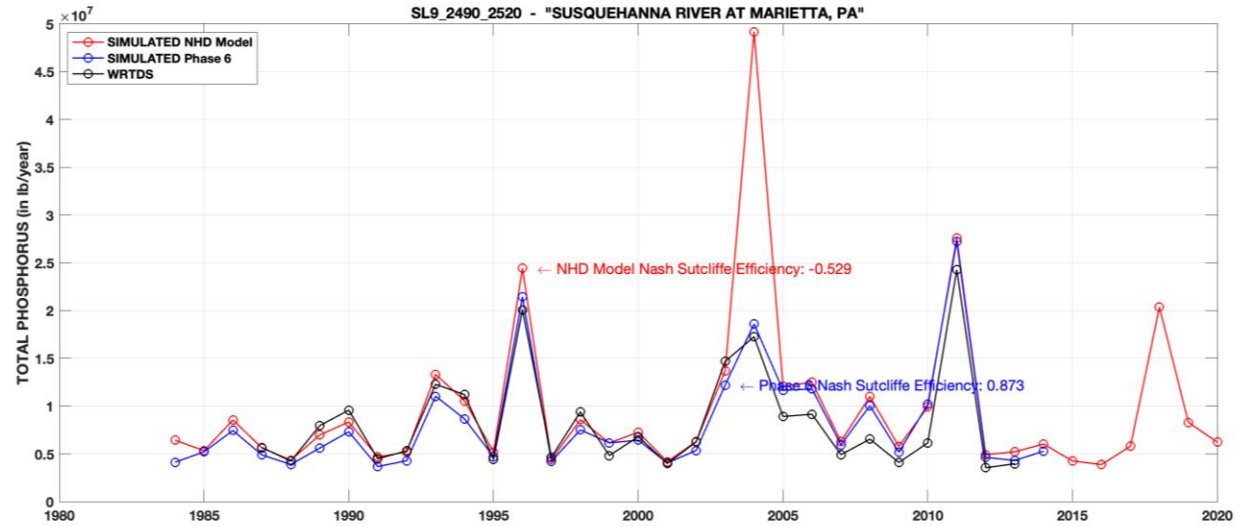
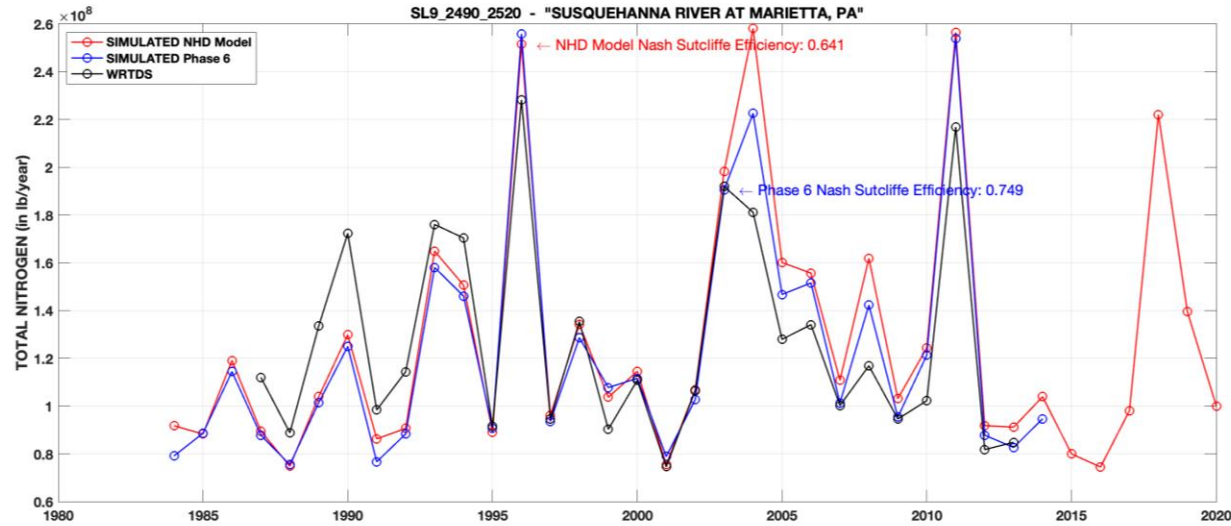
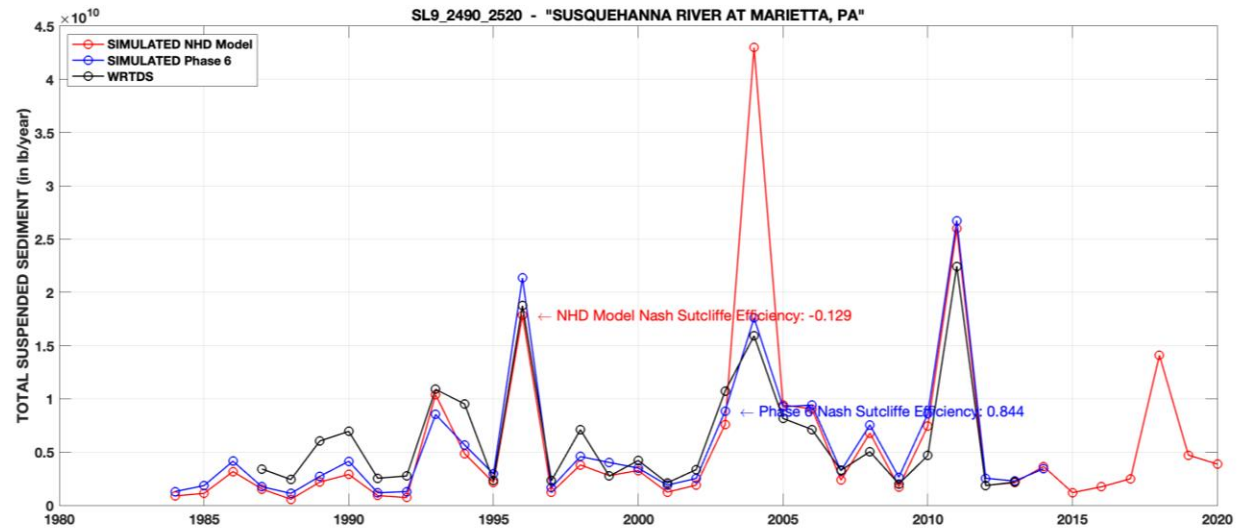
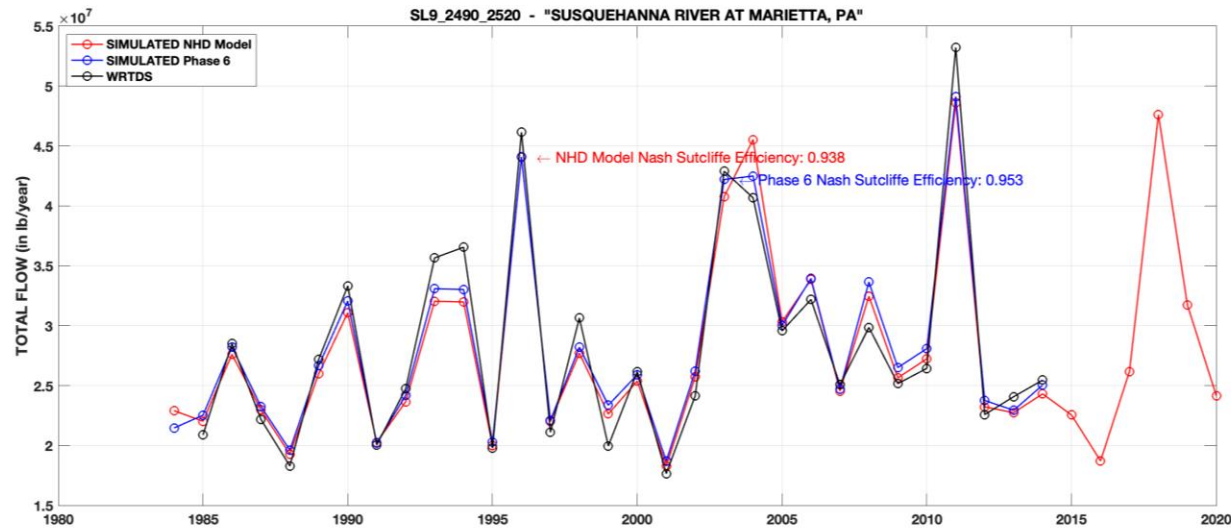
Rivers	Flow	Nitrogen	Phosphorus	Sediment
Susquehanna Conowingo MD	+00.0% (+0.946)	+05.1% (+0.773)	+68.1% (-0.954)	+18.1% (+0.452)
Susquehanna Marietta PA	-01.2% (+0.938)	+04.2% (+0.641)	+26.3% (-0.529)	+02.8% (-0.129)
Potomac Washington, DC	+00.3% (+0.885)	-35.2% (+0.228)	+24.3% (+0.262)	-08.5% (-0.461)
James Cartersville, VA	+03.7% (+0.891)	-39.1% (+0.219)	-06.2% (+0.800)	-36.0% (+0.625)
Rappa. Fredericksburg, VA	-01.3% (+0.903)	-19.0% (+0.673)	-13.8% (-2.679)	-41.9% (-0.737)
Appomattox Matoaca, VA	00.0% (+0.903)	-18.2% (+0.743)	-01.1% (+0.555)	-32.9% (+0.526)
Pamunkey Hanover, VA	+03.6% (+0.815)	-14.1% (+0.684)	-09.4% (+0.020)	-44.2% (+0.229)
Mattaponi Beulahville, VA	+11.0% (+0.714)	+61.6% (-2.501)	+01.8% (+0.272)	+101.7% (-10.449)
Patuxent Bowie, MD	+03.8% (+0.857)	+06.8% (+0.821)	-04.8% (+0.641)	+26.9% (+0.496)
Choptank Greensboro, MD	-05.4% (+0.730)	+103.2% (-6.738)	+11.0% (+0.562)	-19.3% (+0.106)

# All 9 RIM Stations Combined

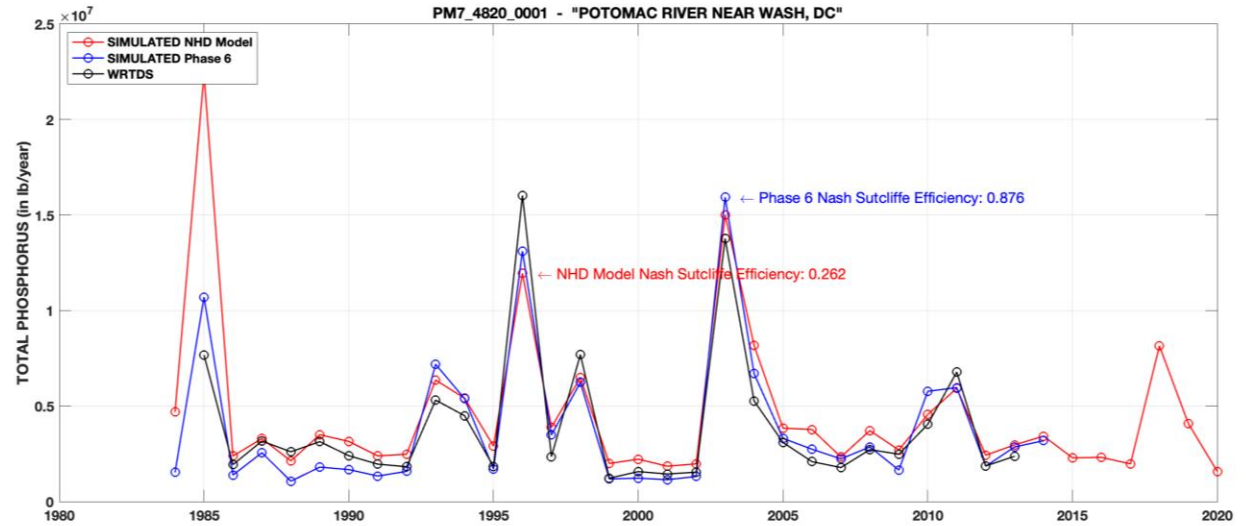
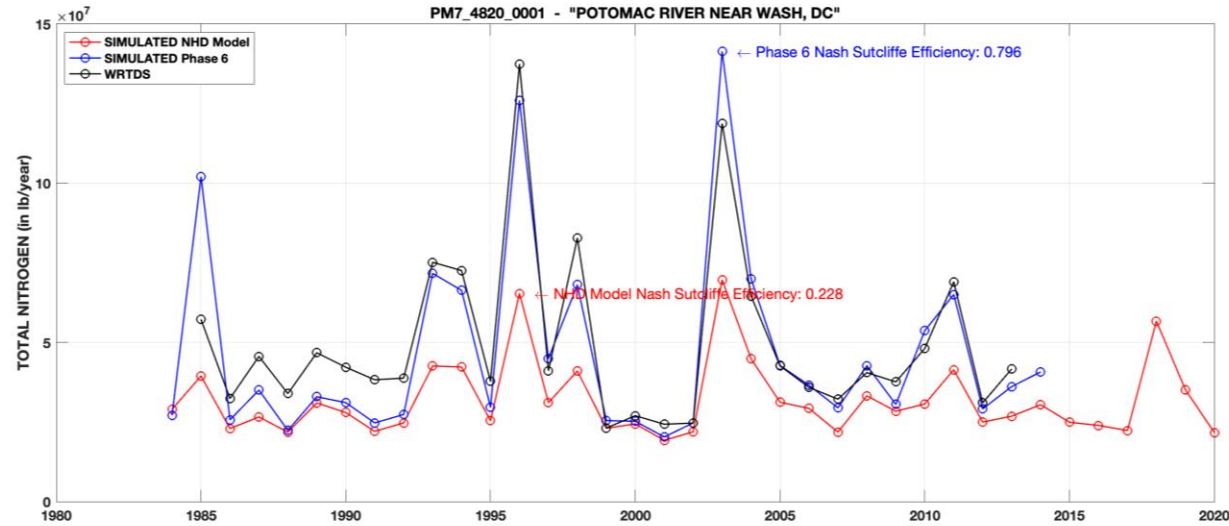
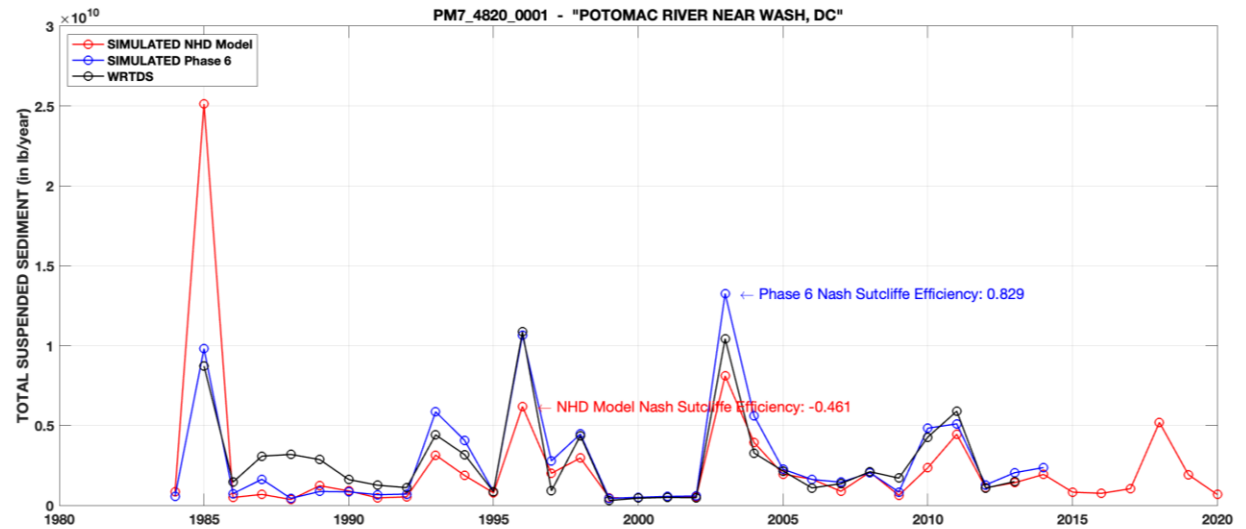
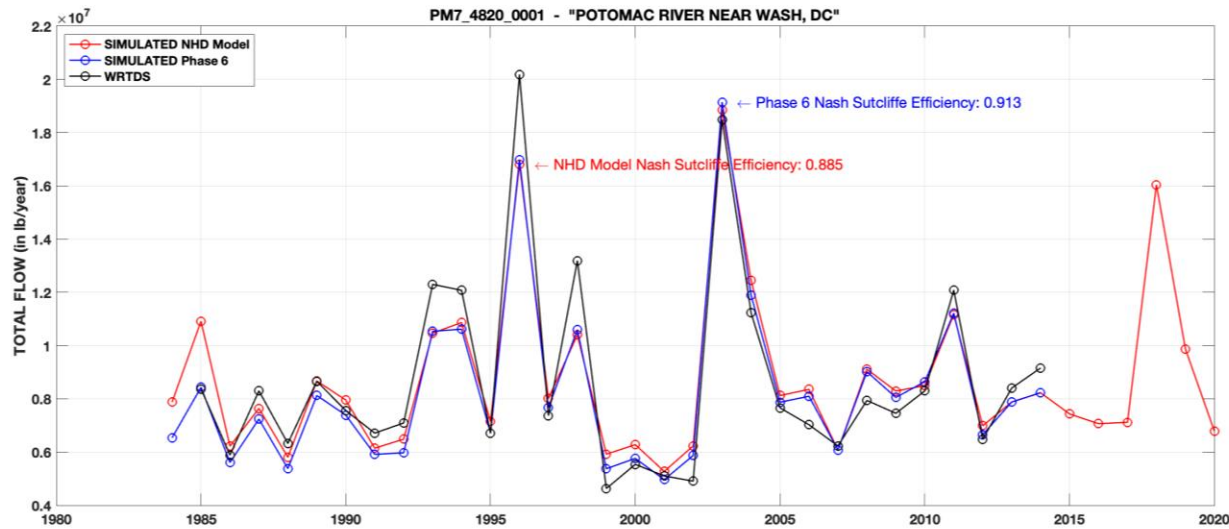




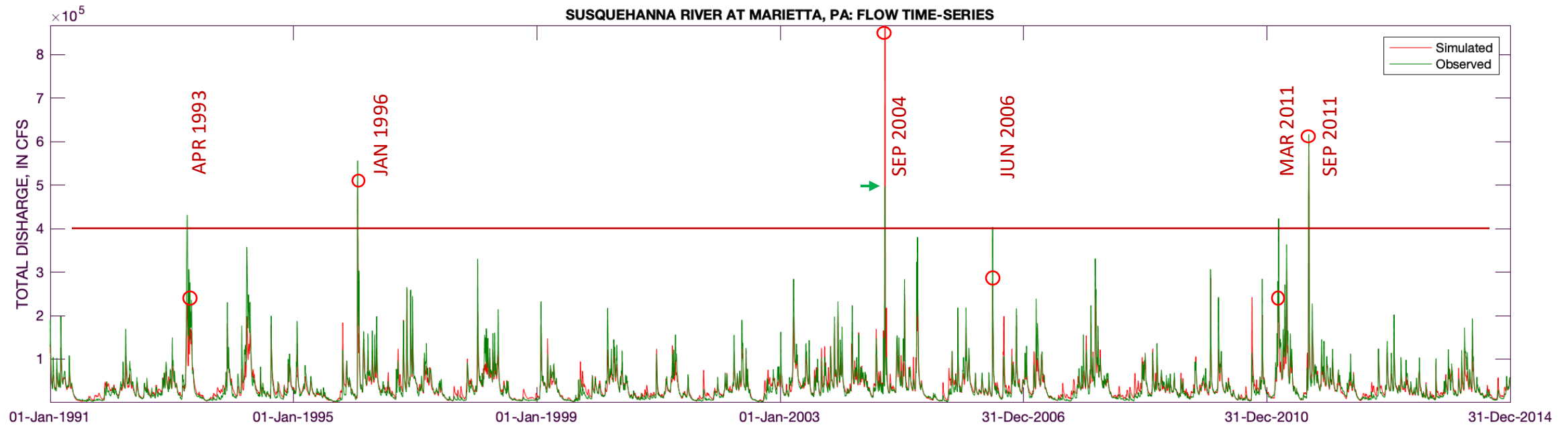
# Susquehanna River at Marietta, PA



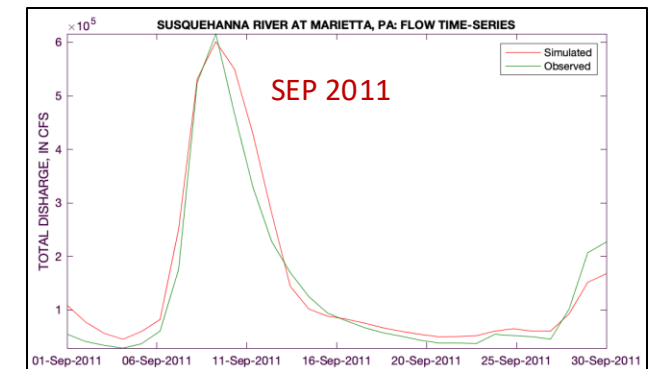
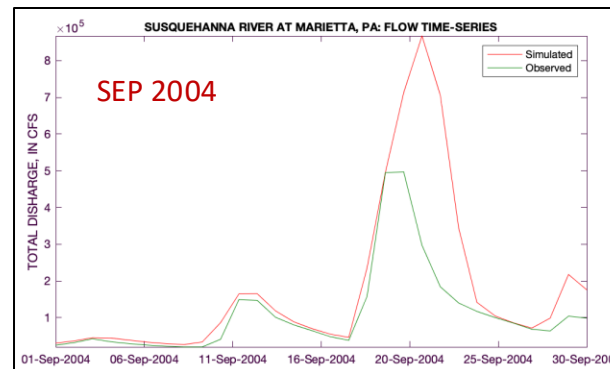
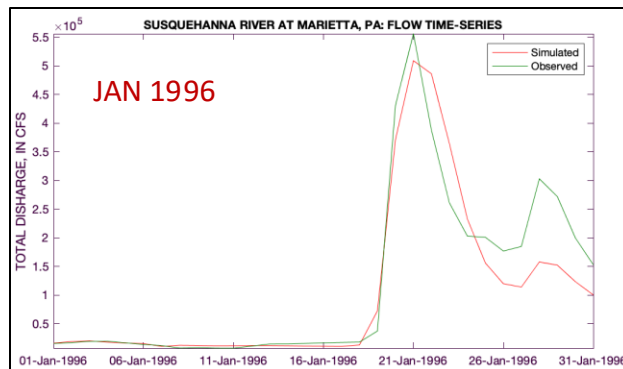
# Potomac River at Washington, DC



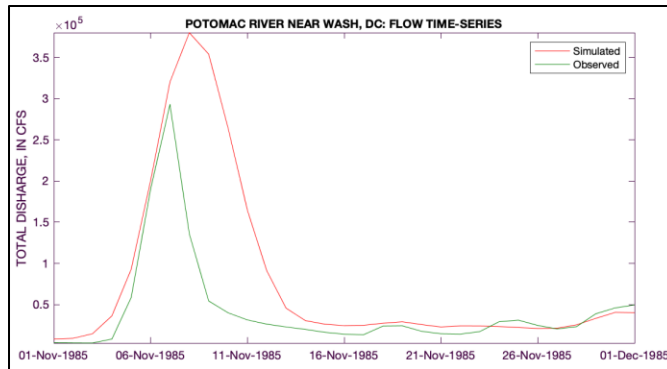
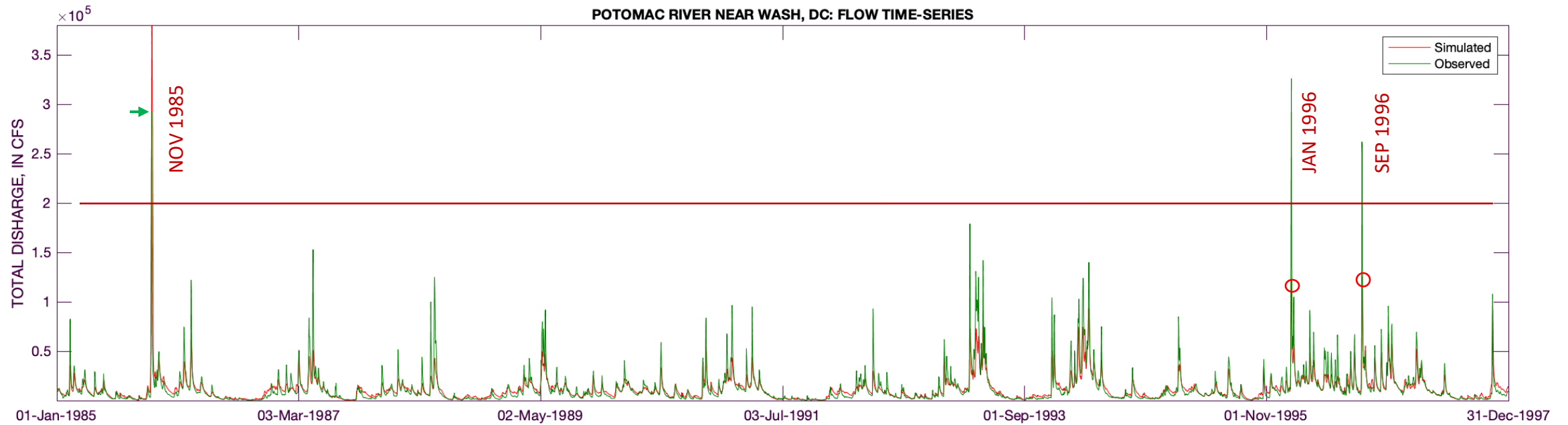
# Susquehanna River at Marietta, PA



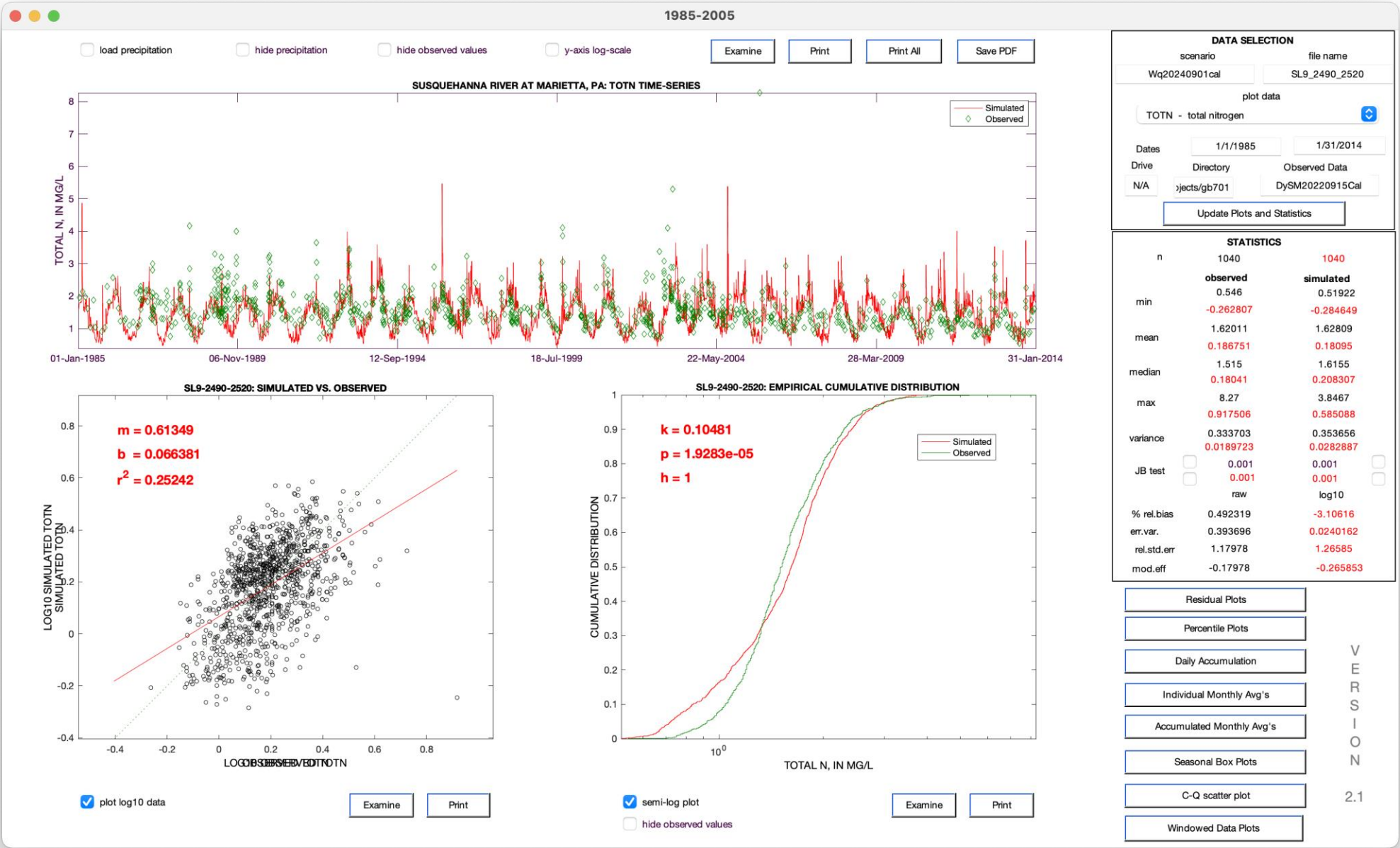
*There were 6 events when flow exceeded 400,000 cfs and most of them were under simulated, except for 2004*



# Potomac River near Washington, DC

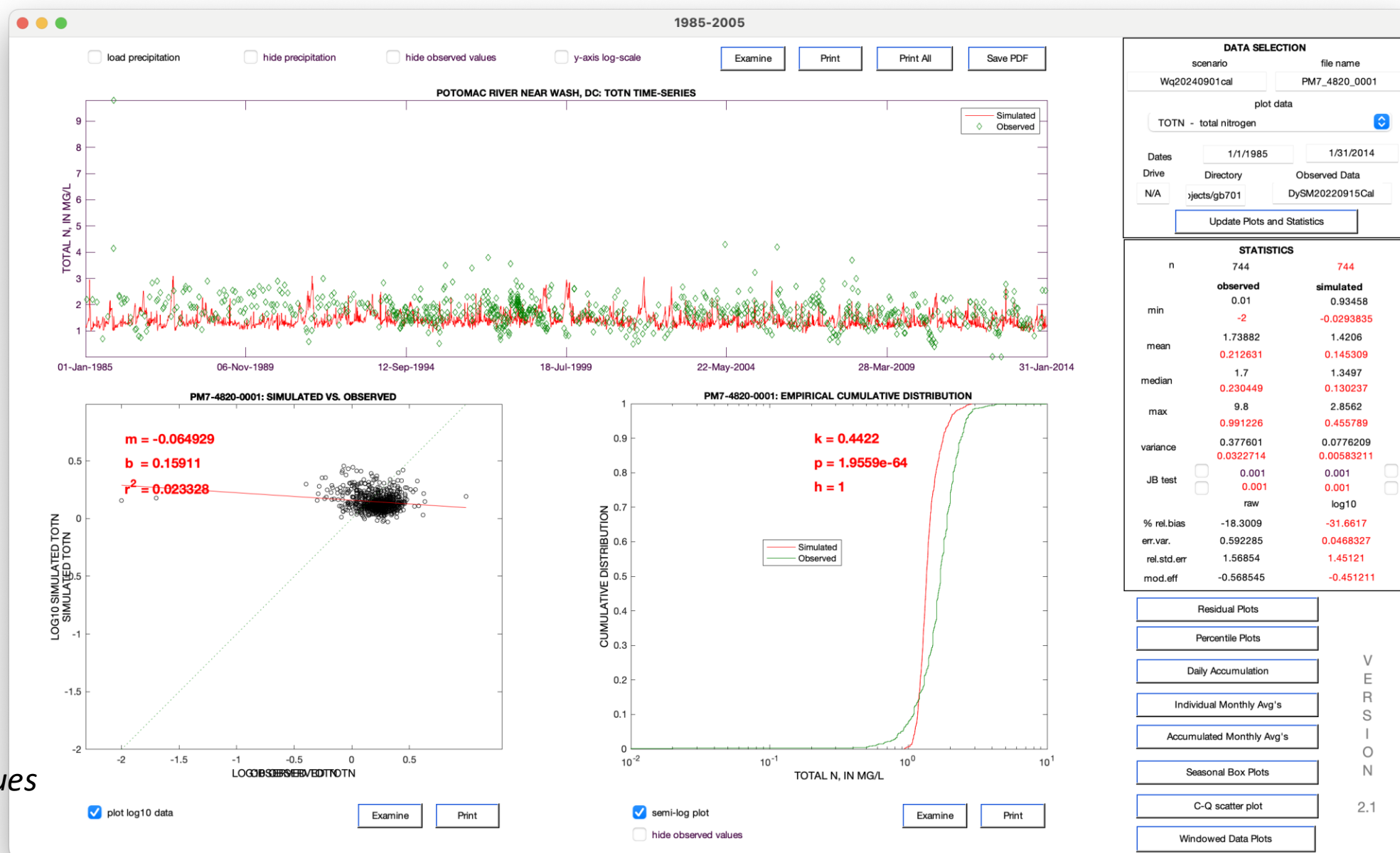


*There were 3 events when flow exceeded 200,000 cfs and two in 1996 were under simulated, but one in Nov 1985 is over simulated with flow exceeding 200,000 on 3 consecutive days rather than ~1*



$\Delta = +04.2\%$





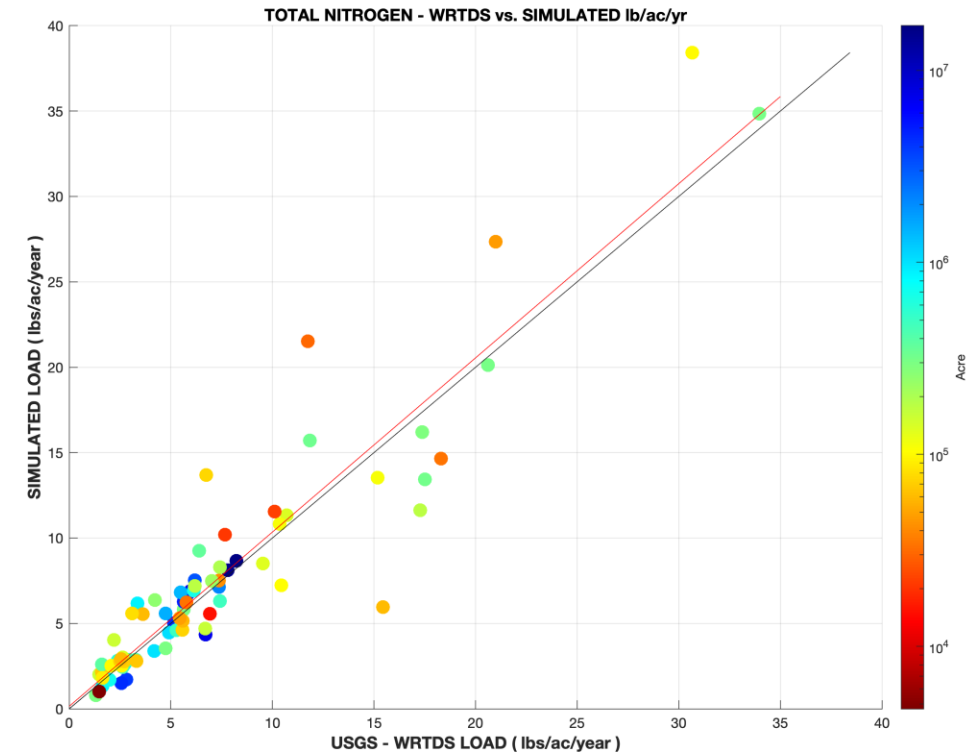
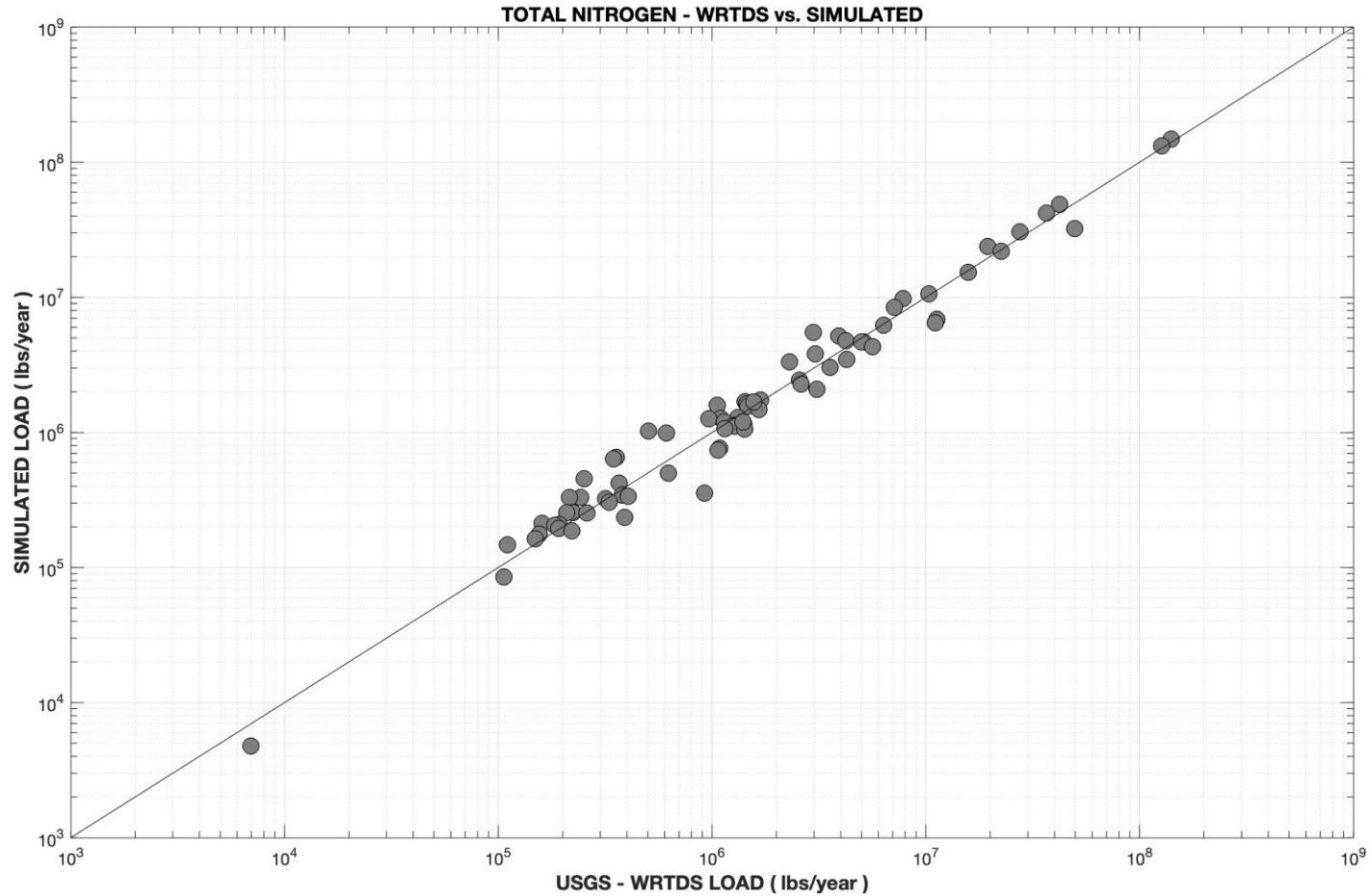
potential issues

$\Delta = -35.2\%$

Beta parameters

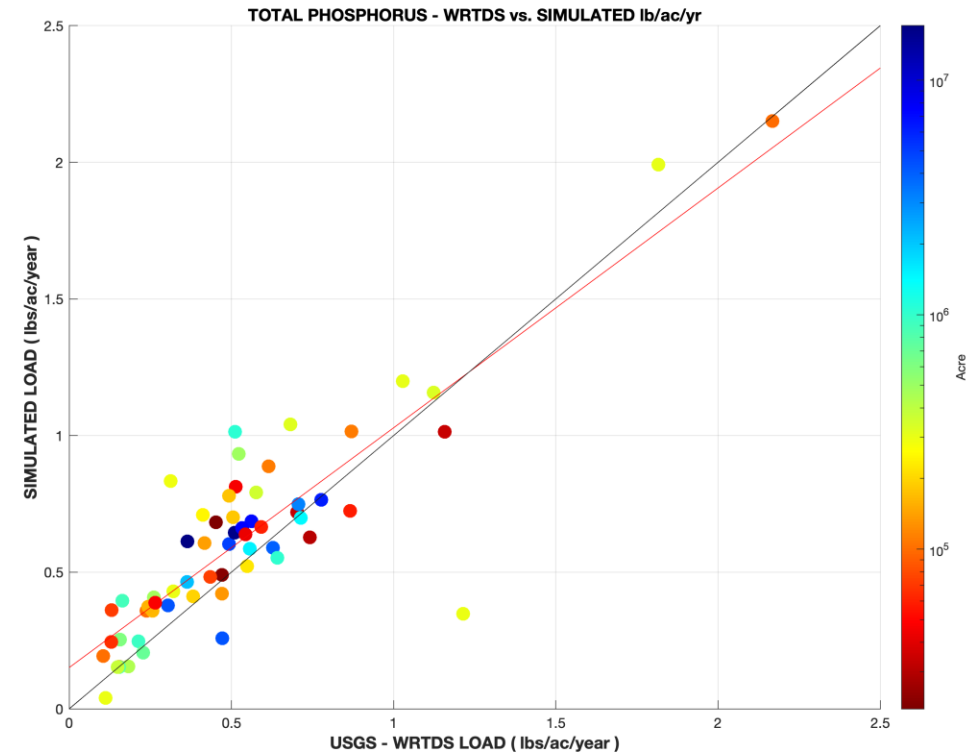
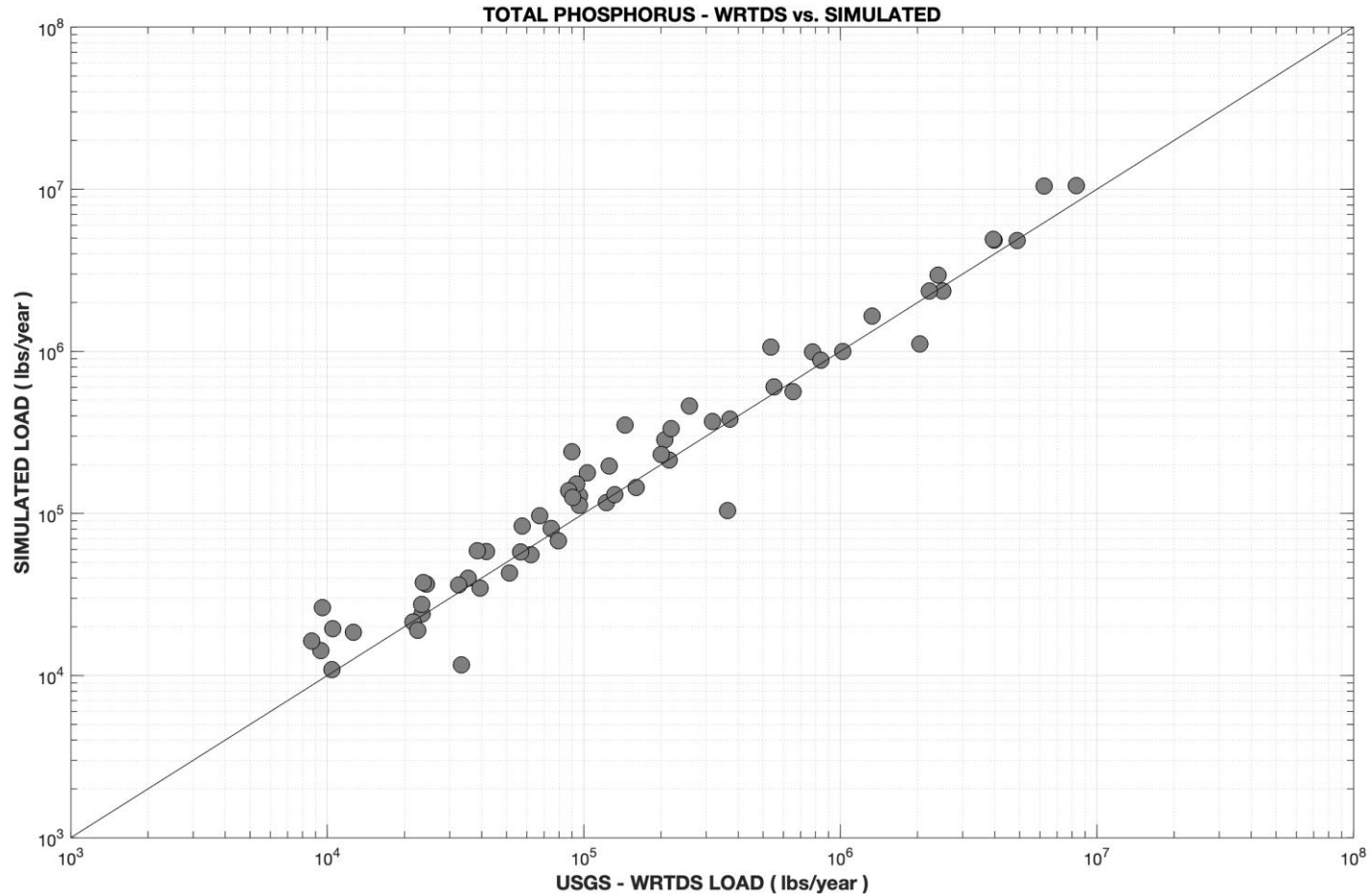
# Other stations – Simulated vs. WRTDS average loads

## Total Nitrogen



# Other stations – Simulated vs. WRTDS average loads

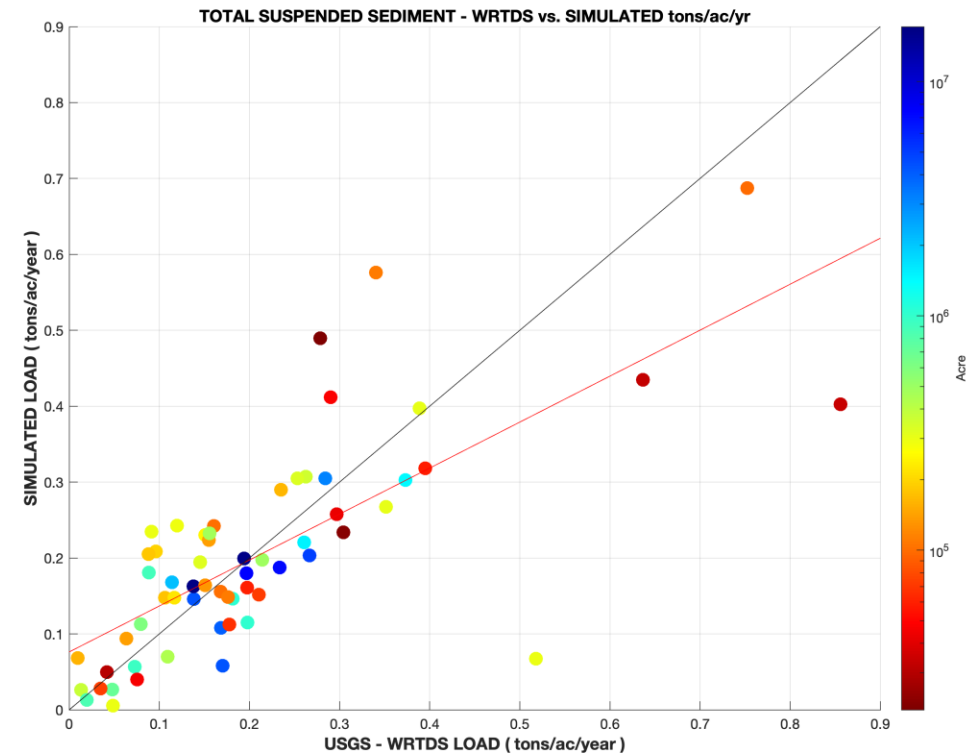
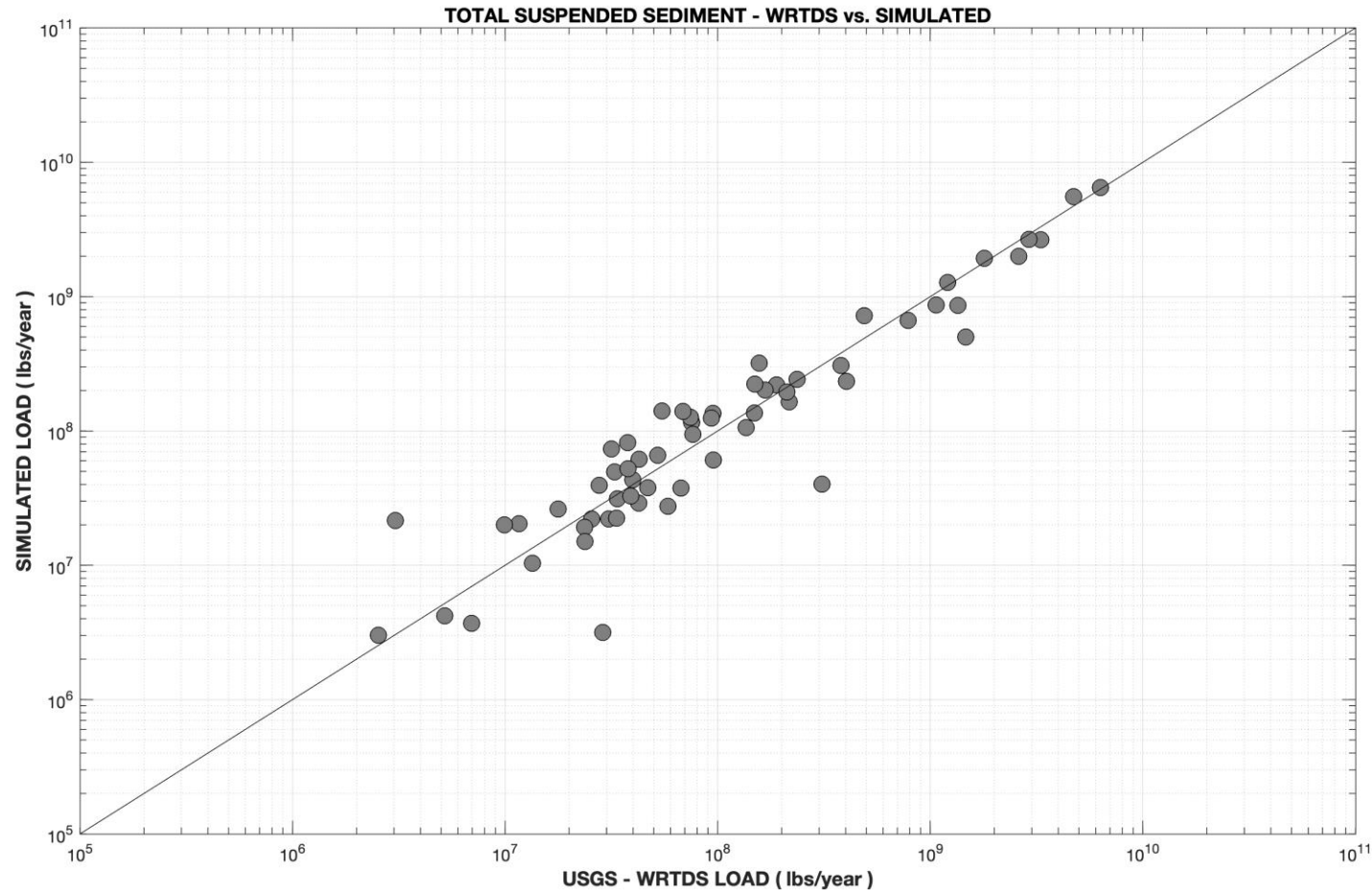
## Total Phosphorus





# Other stations – Simulated vs. WRTDS average loads

## Suspended Sediment



# Summary

**1. Our model calibration of flow, nutrients, and sediment maybe reasonable for linking watershed model flows and loads with the estuarine model given the stage of our models and inputs.**

- we expect to perform a few additional fine tunings
- and collaborate with the MBM team on model linkages

## **>> Next Steps for the Phase 7 Dynamic Watershed Model (DWM)**

**2. We need to incrementally improve the model on multiple fronts: (a) incorporation of new inputs where appropriate; (b) model parameters; (c) calibration methods and processes.**

## >> Next Steps for the Phase 7 Dynamic Watershed Model (DWM)

### 1. Inputs:

- Direct loads – change **point sources**, diversions/withdrawals, and septic from P6 river segment scale to NHD (missing tidal direct loads); add flow with septic (load sensitivity to future climate); treatment of withdrawals in small stream modules and tidal areas with direct discharge to the Bay; Effect of best management practices;
- Replace use of 12 landcover classes fixed in time (inputs do change over time);
- Water quality monitoring data and WRTDS (WRTDS-K);

### 2. Model parameters:

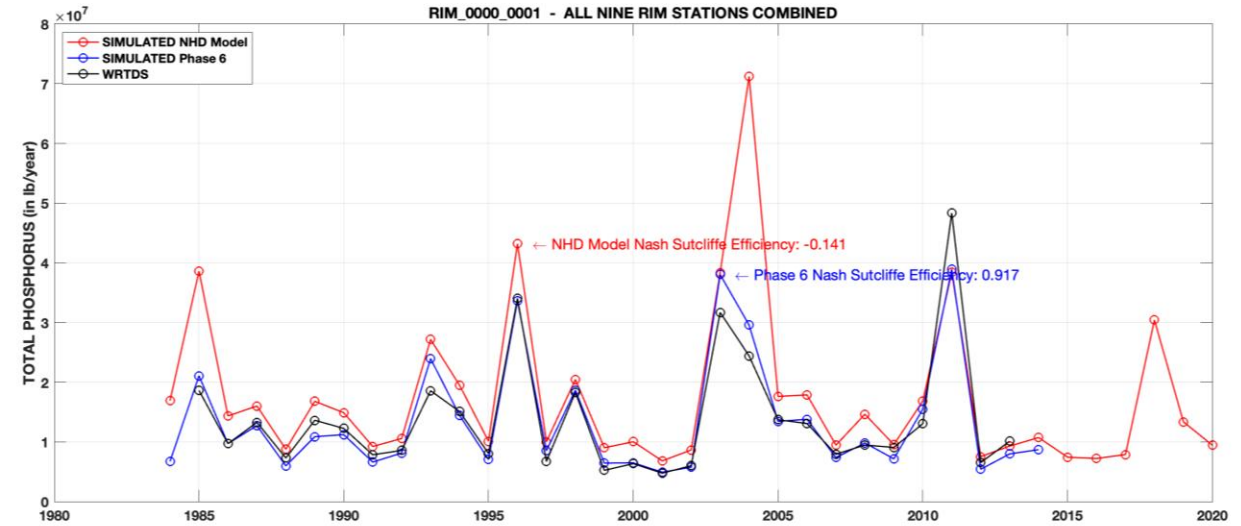
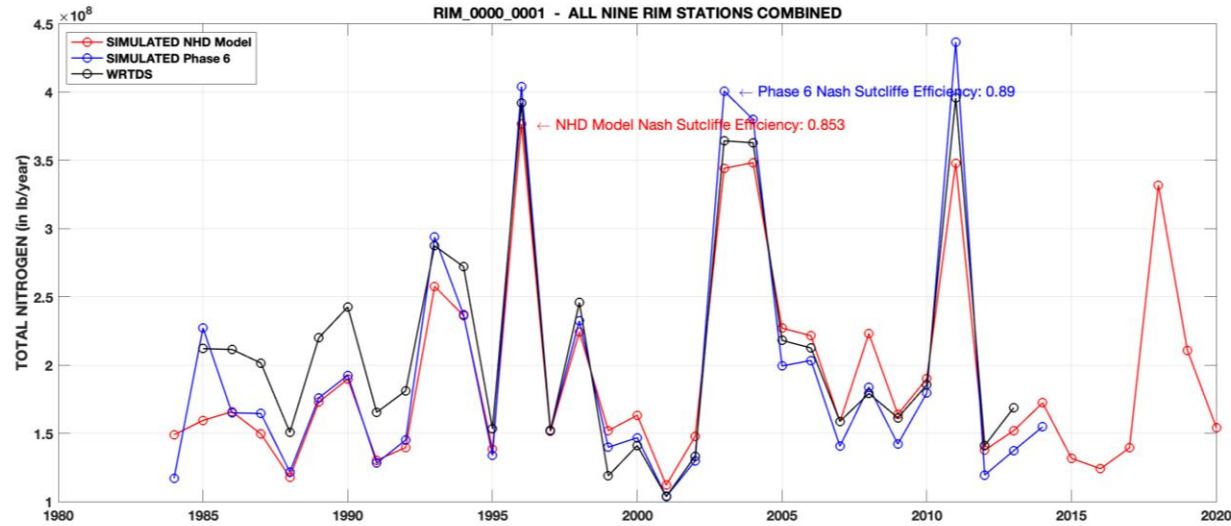
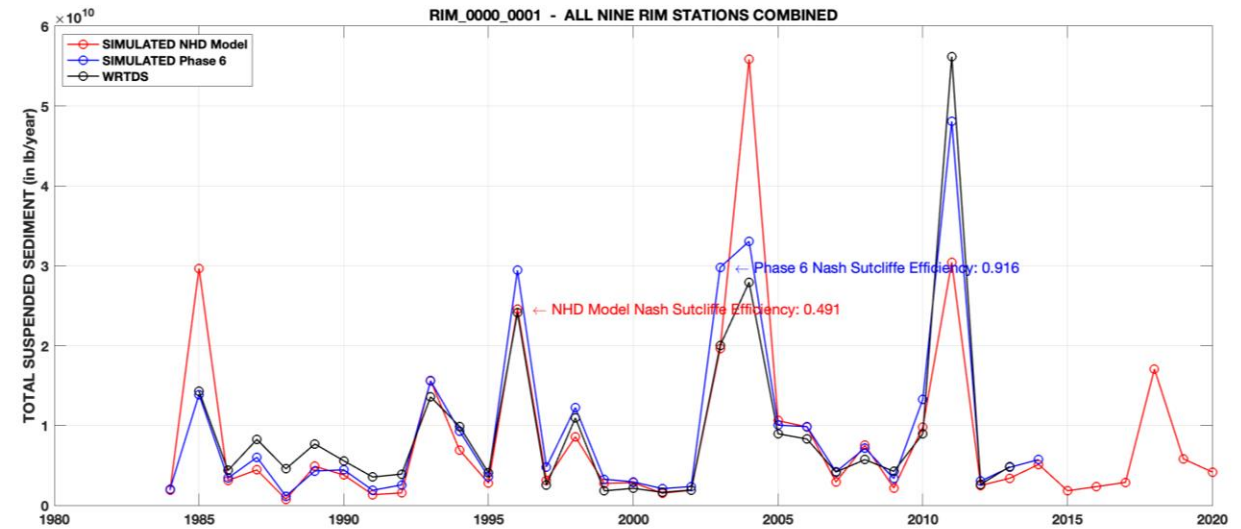
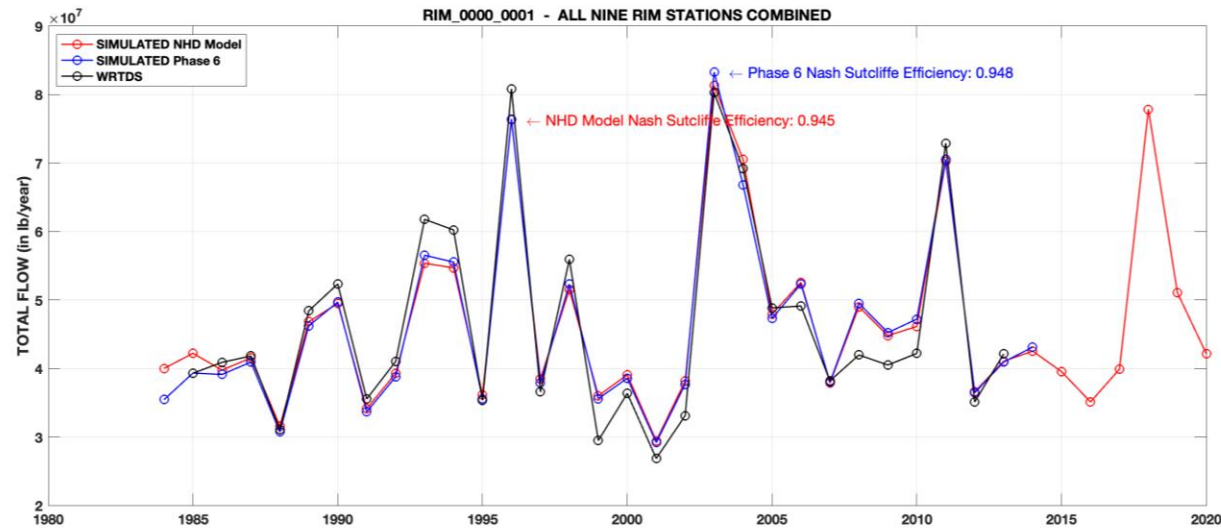
- Beta parameters for flow and seasonal variability; transfer of loading trends from land to stream routing modules; **CalCAST parameters**;

### 3. Calibration:

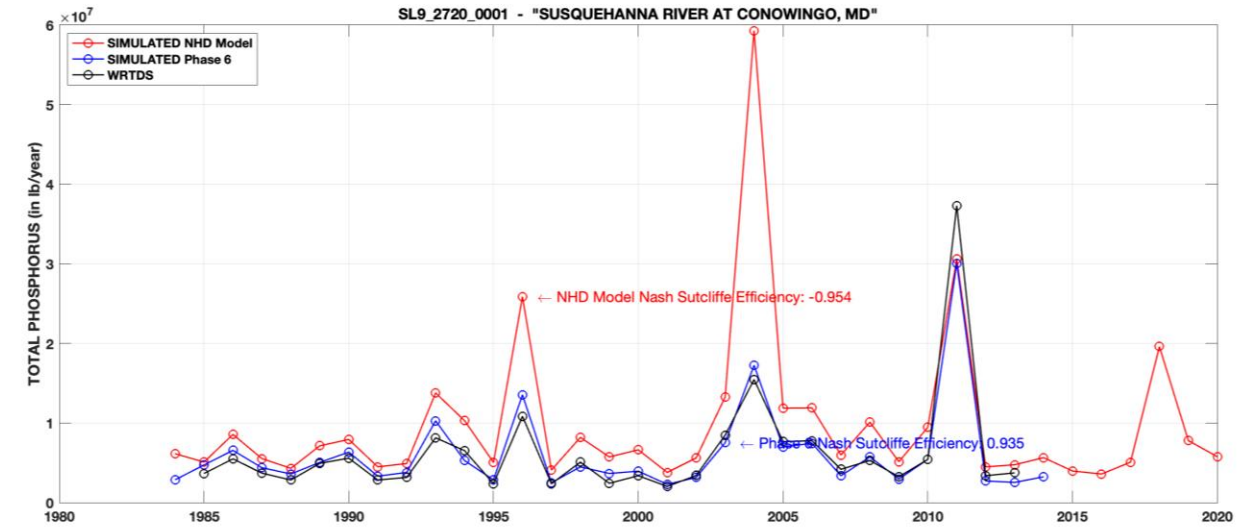
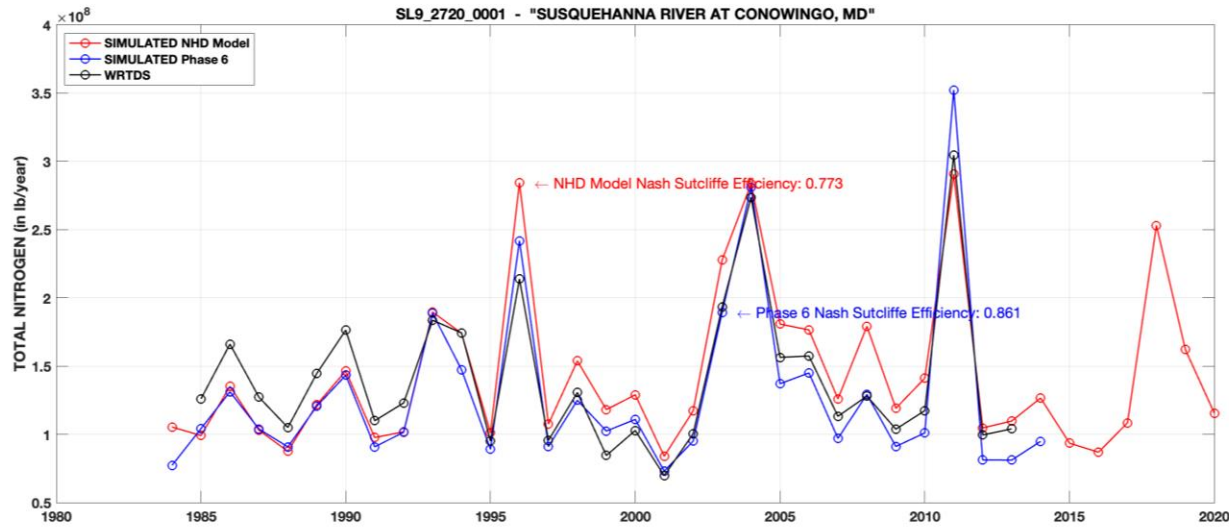
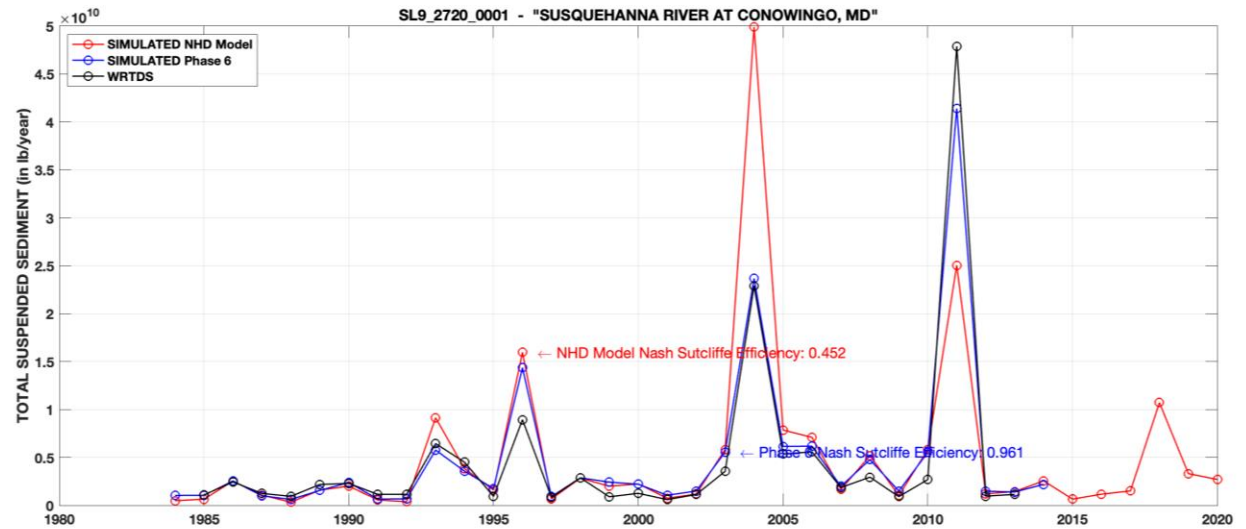
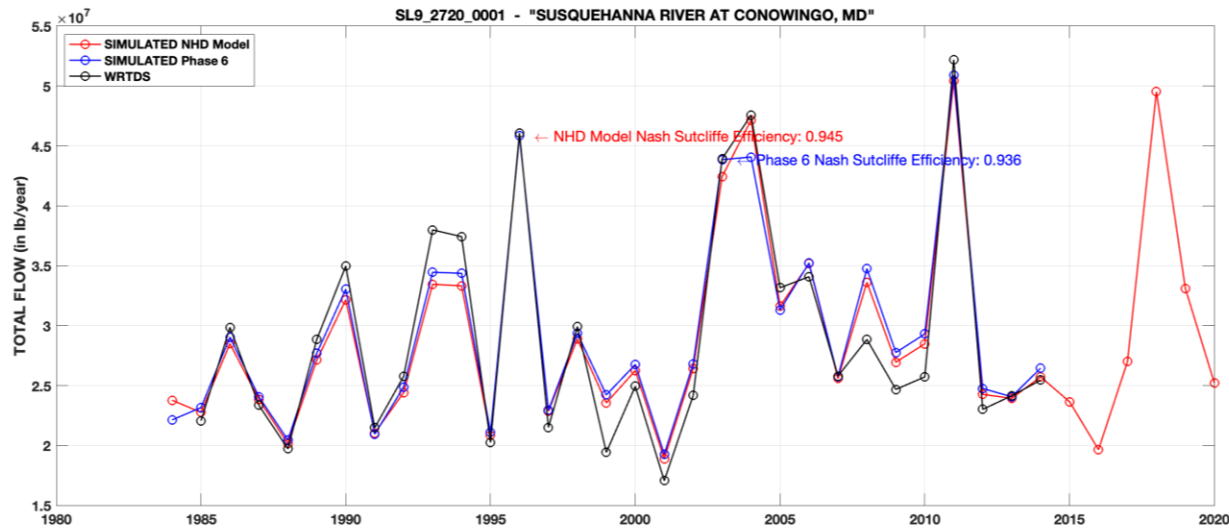
- Calibration methods and watershed processes (e.g., **hydrologic simulation anomalies**; Conowingo infill; module for source of organic nutrients);

# Appendices

# All 9 RIM Stations Combined

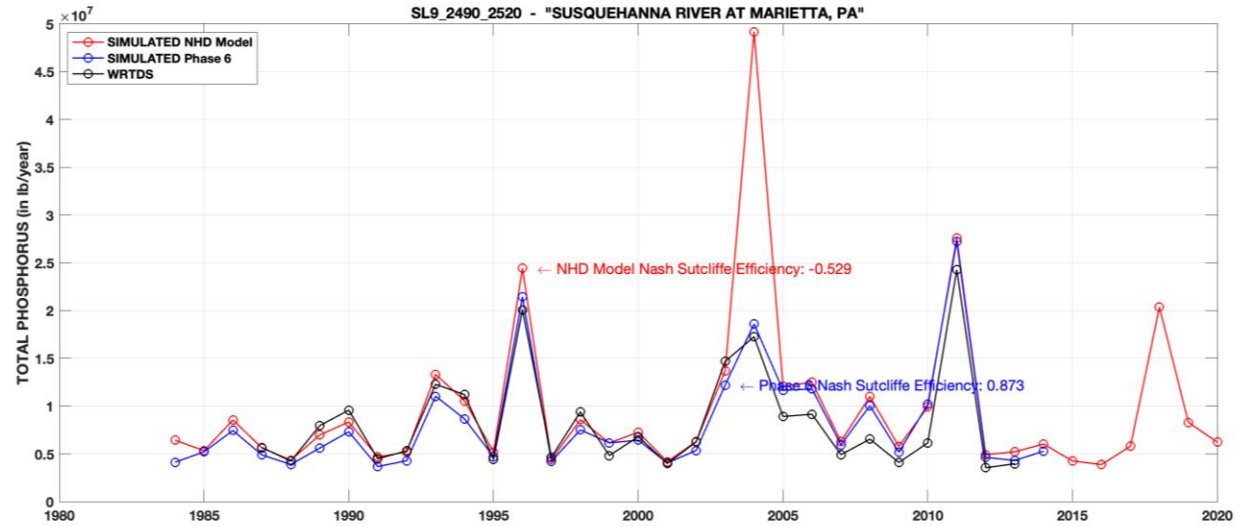
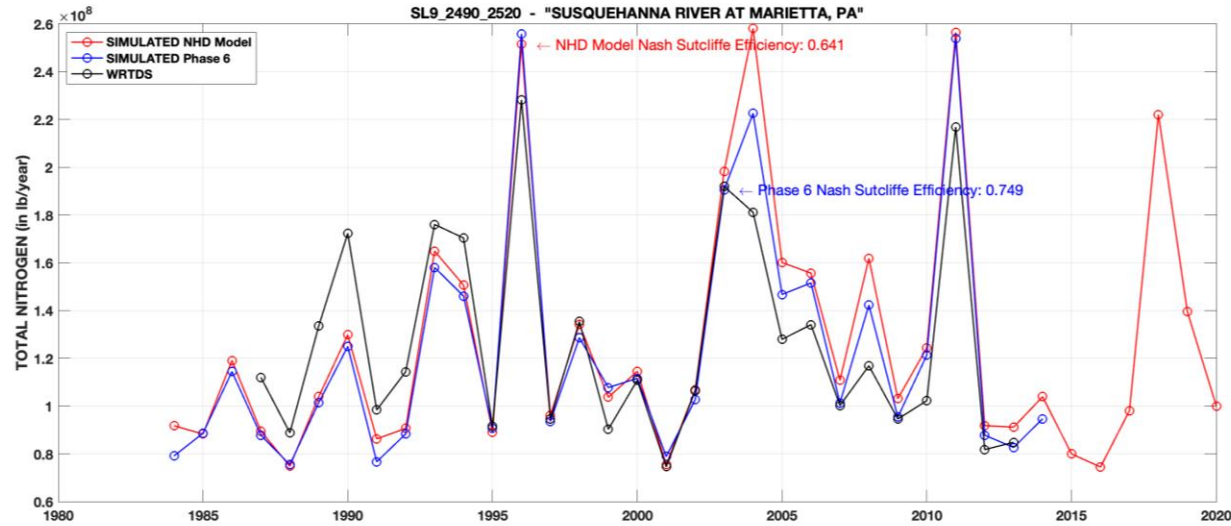
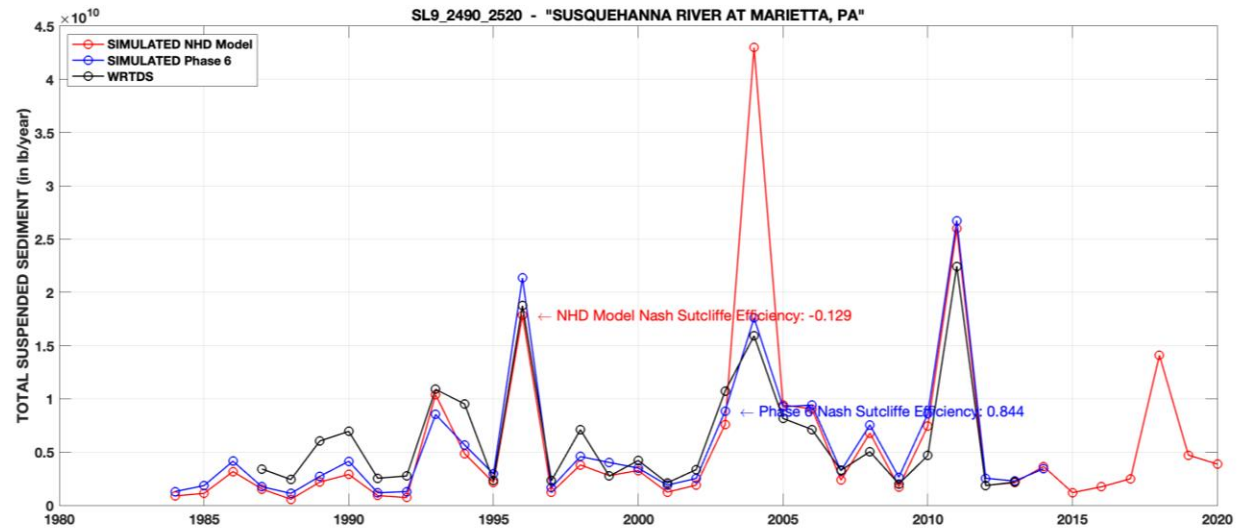
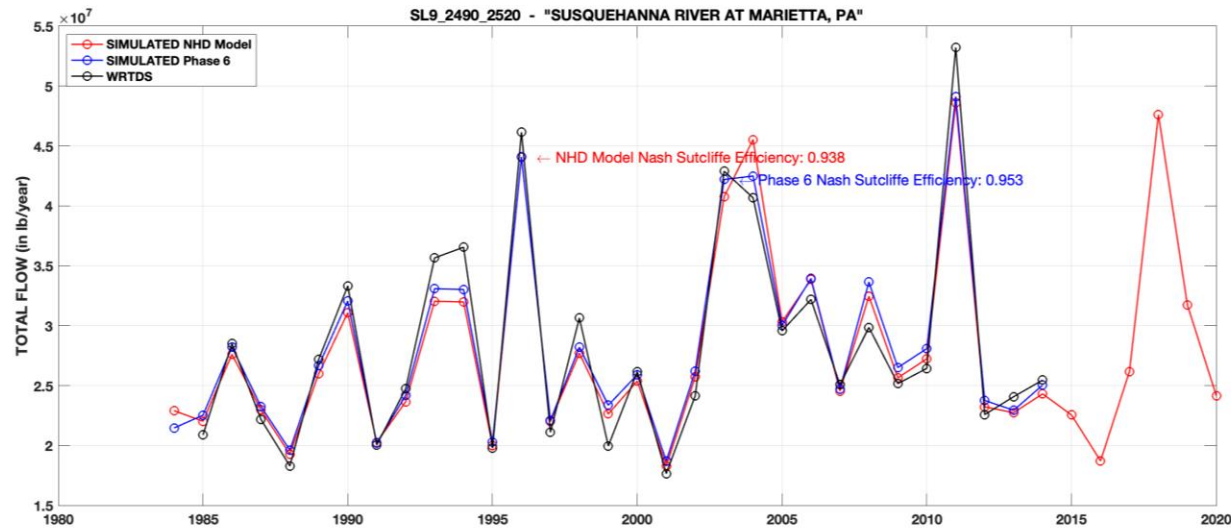


# Susquehanna River at Conowingo, MD

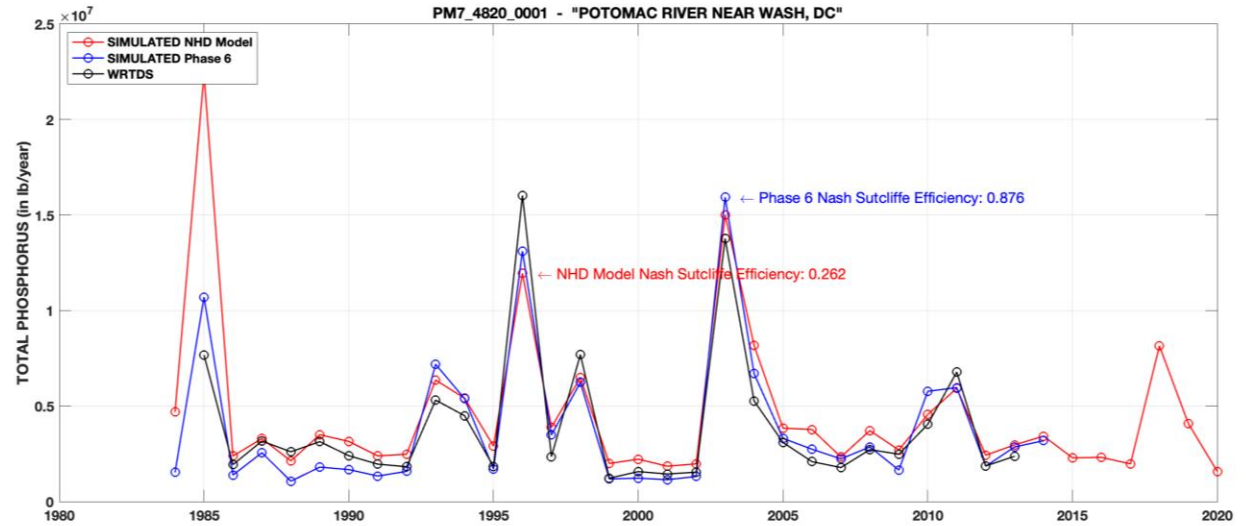
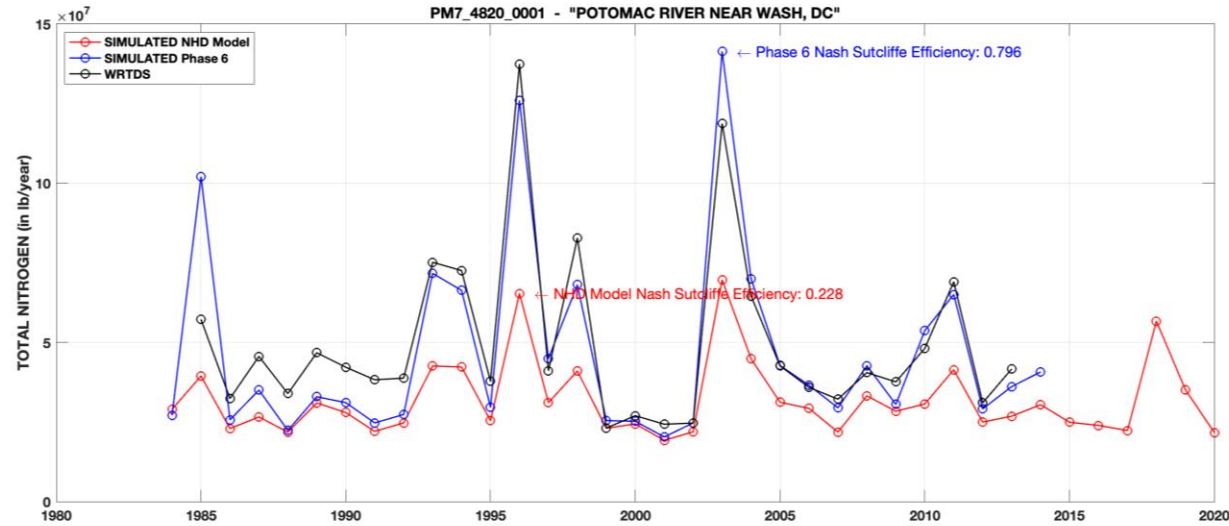
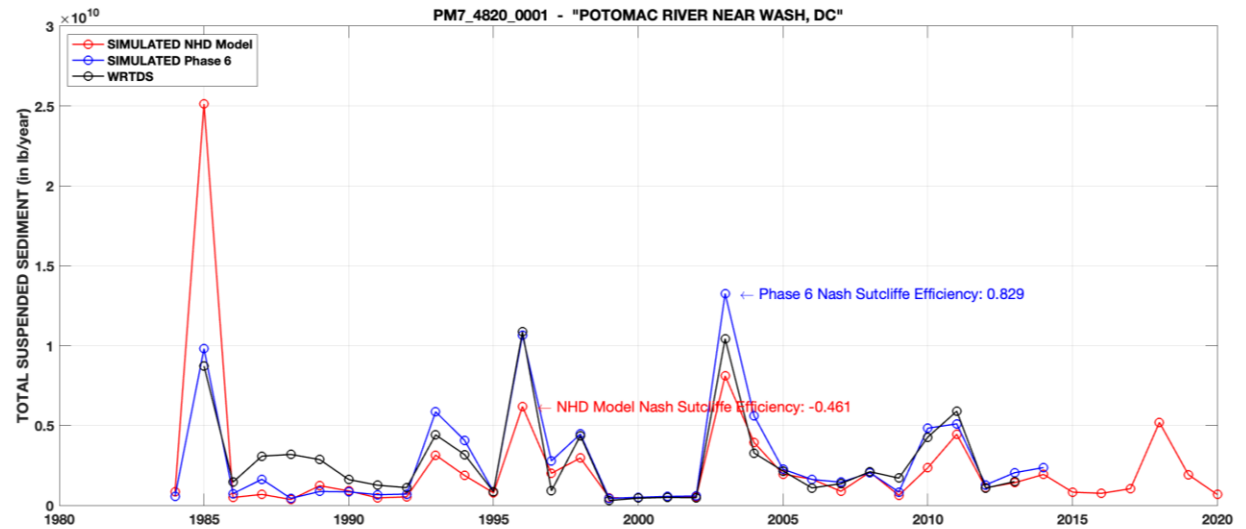
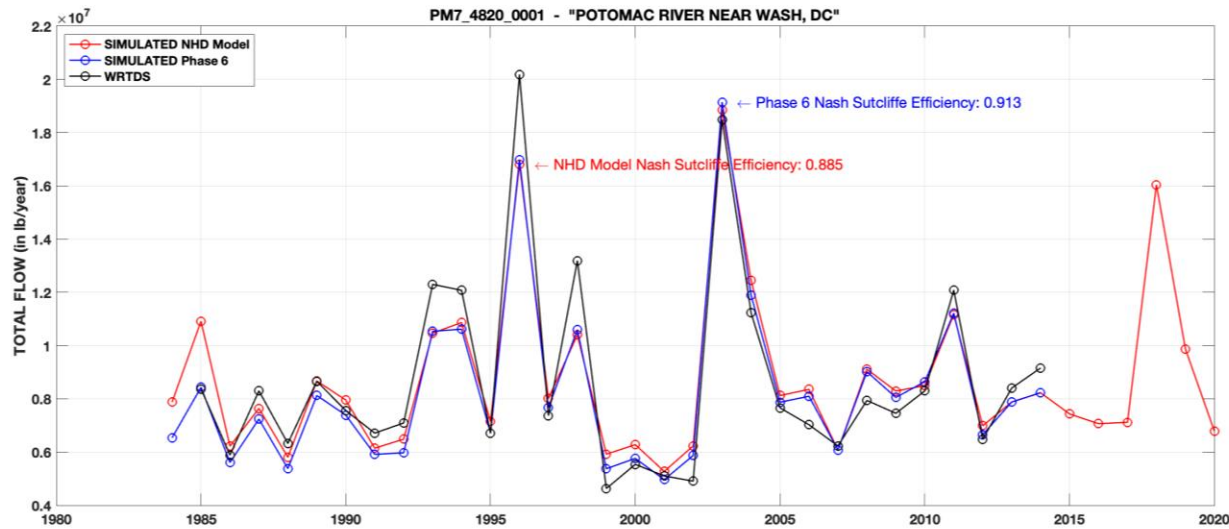




# Susquehanna River at Marietta, PA

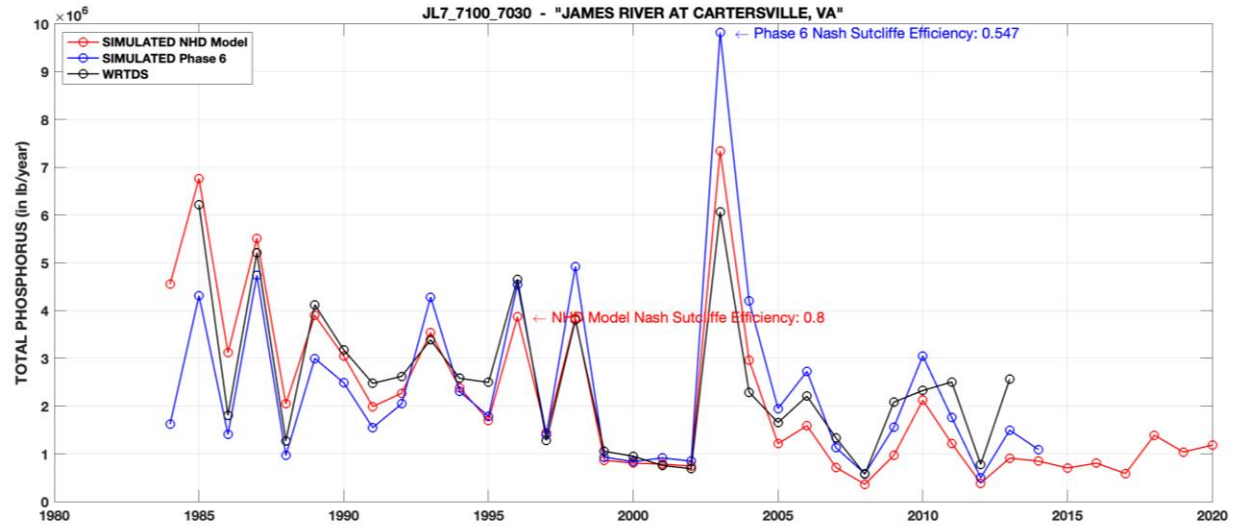
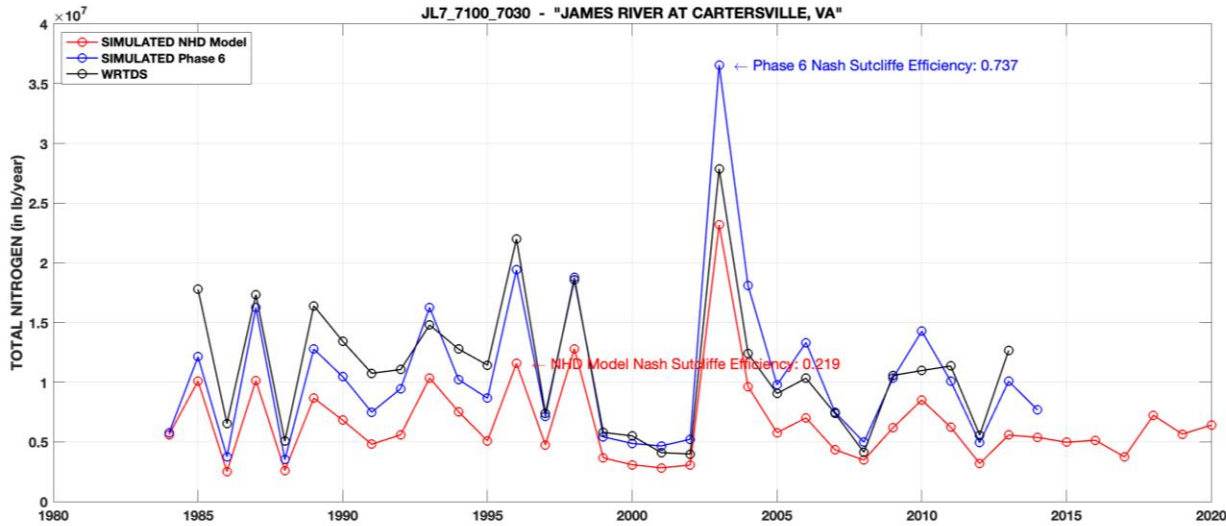
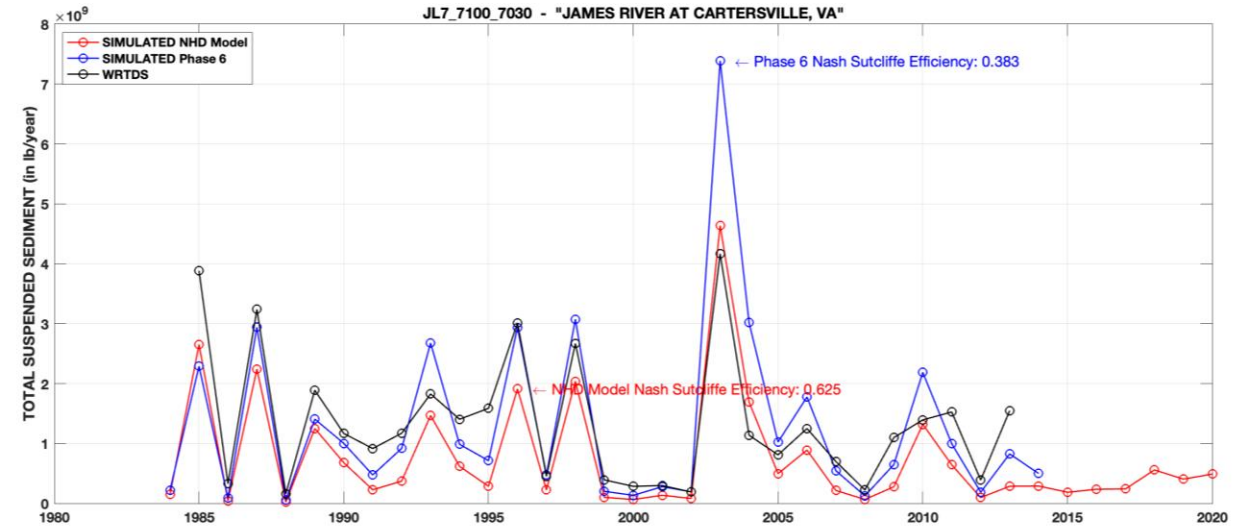
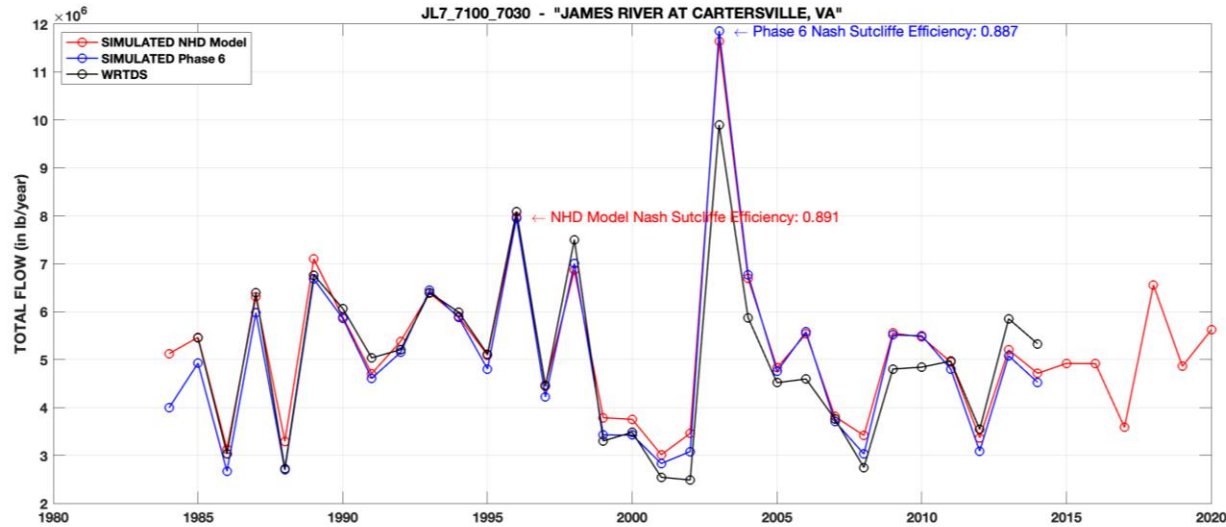


# Potomac River at Washington, DC

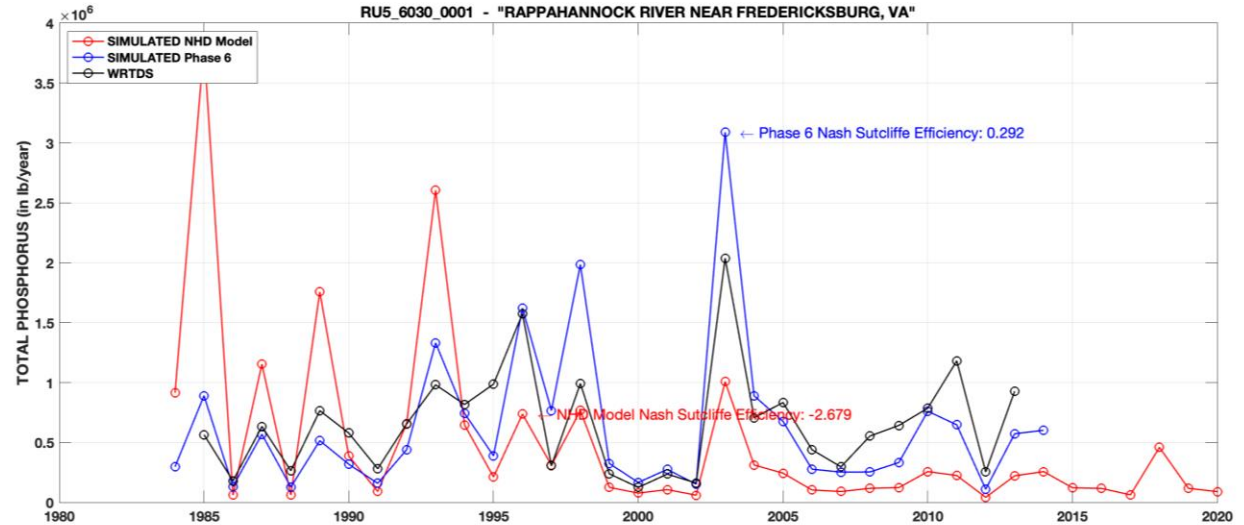
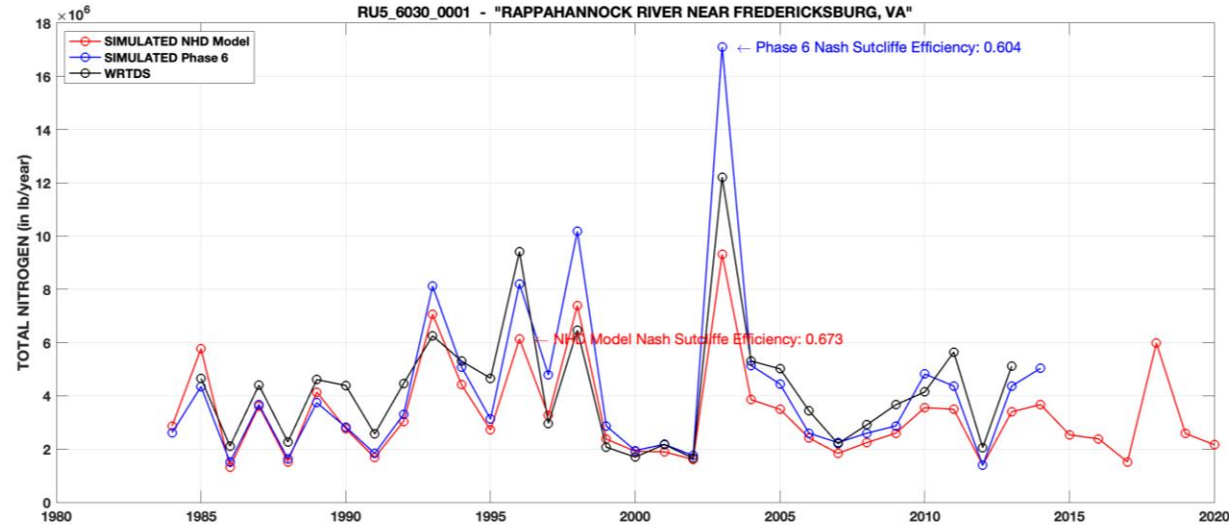
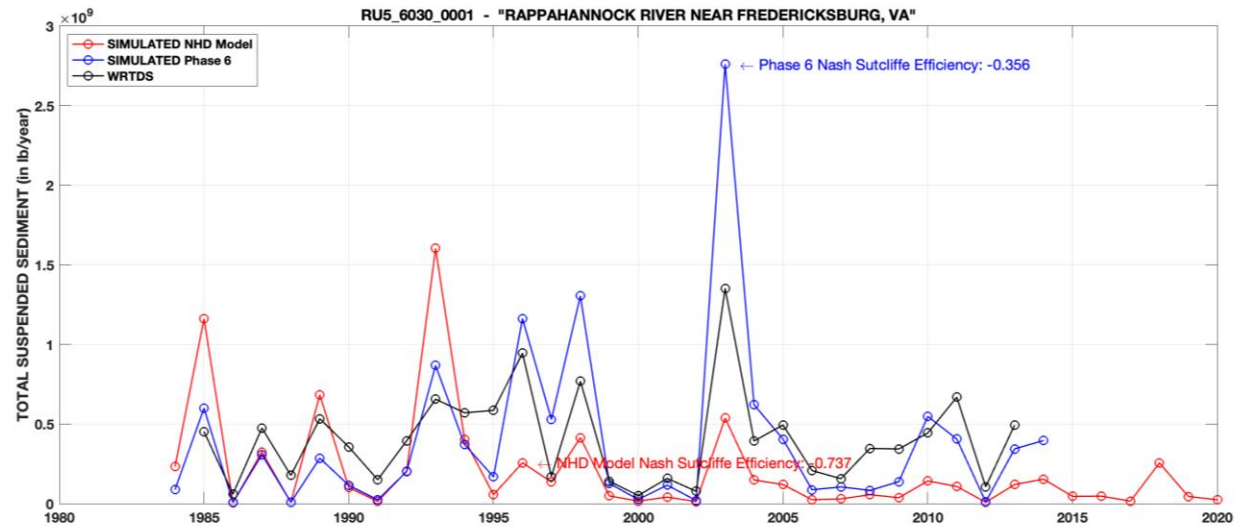
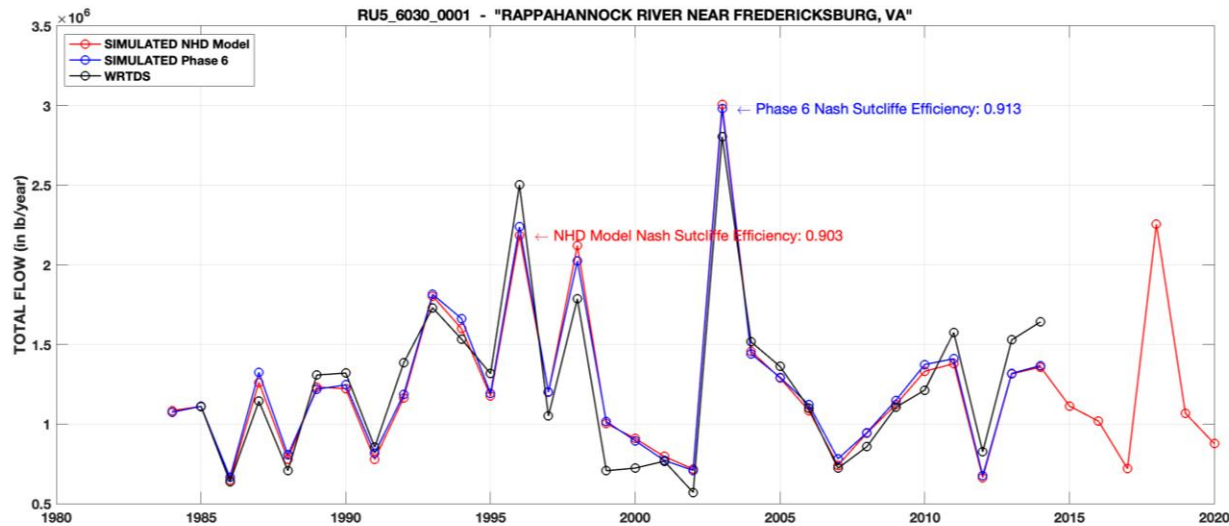




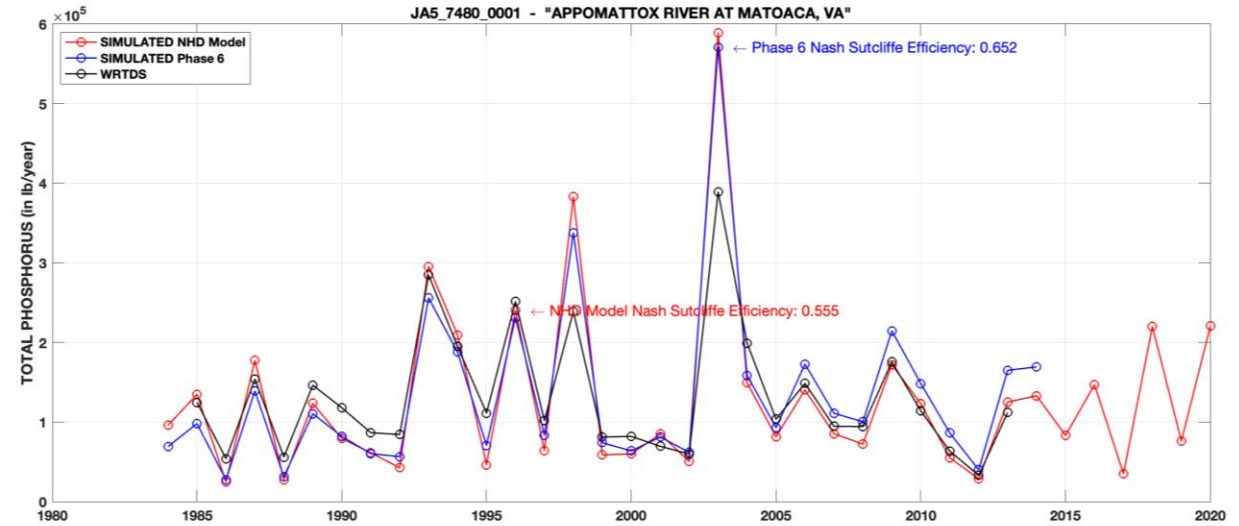
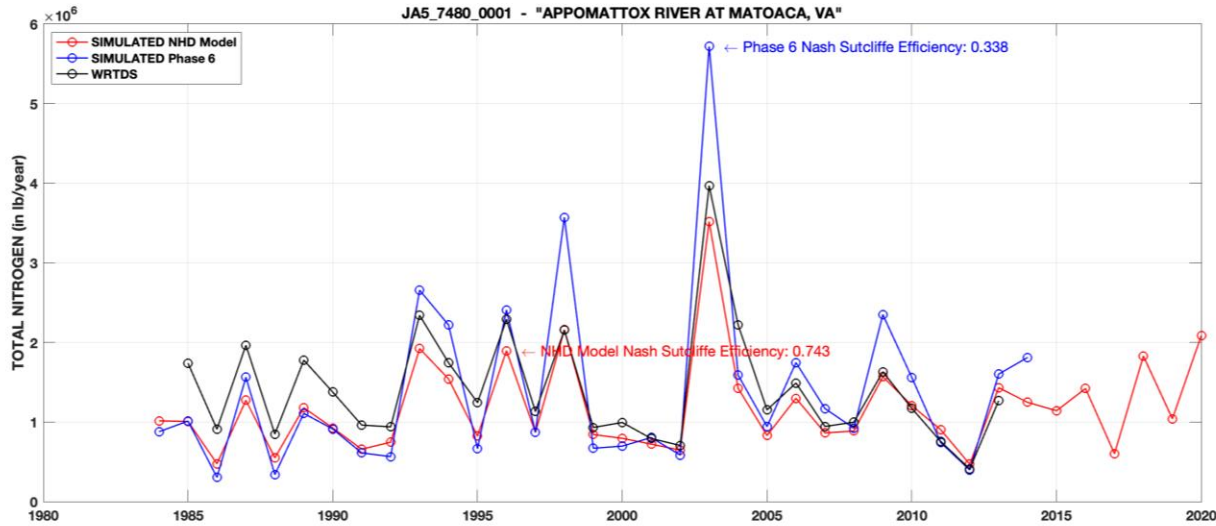
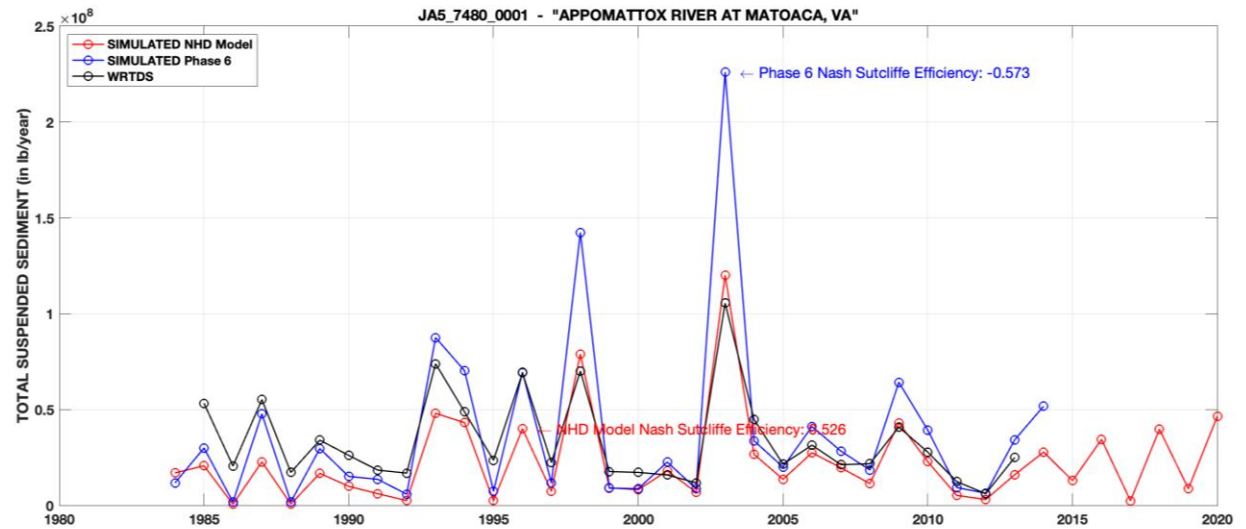
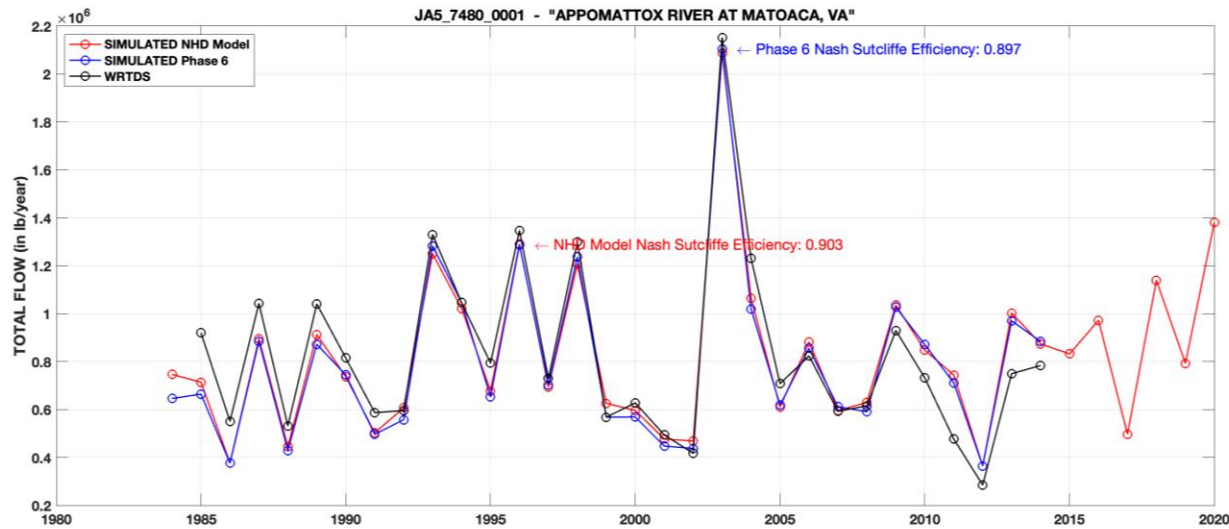
# James River at Cartersville, VA



# Rappahannock River near Fredericksburg, VA

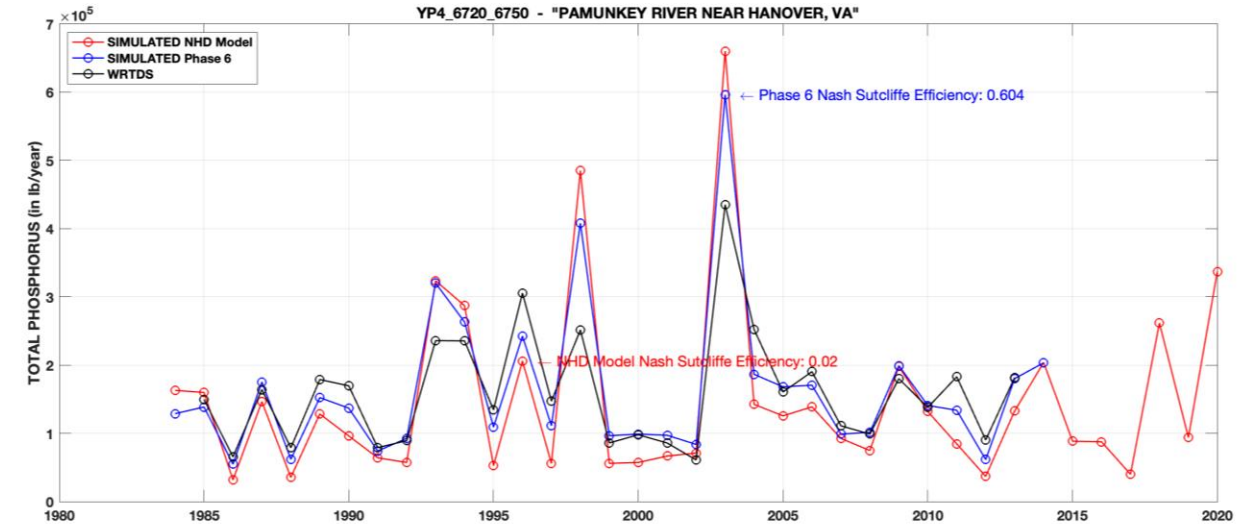
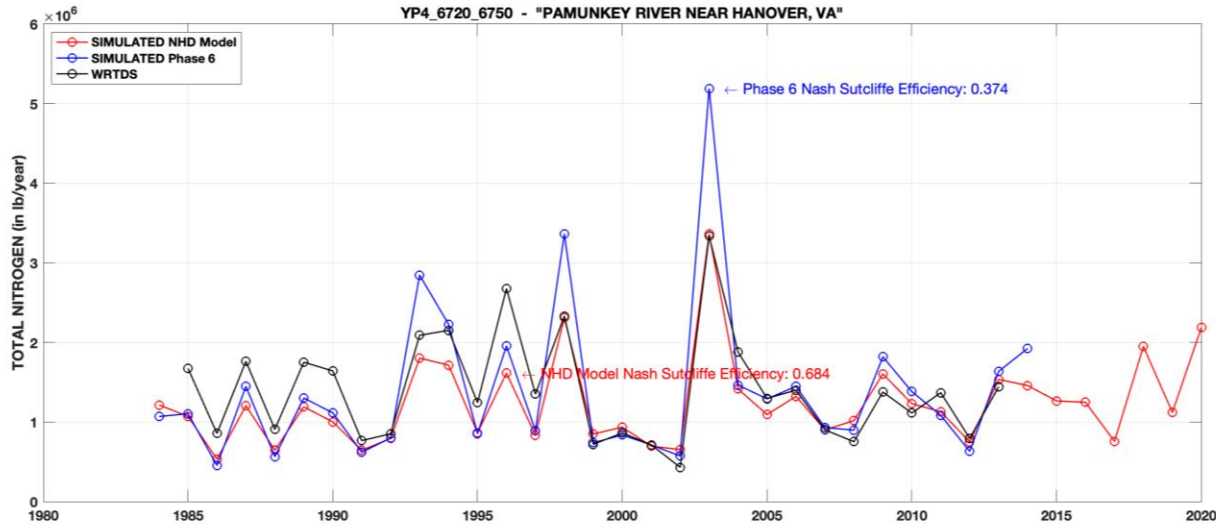
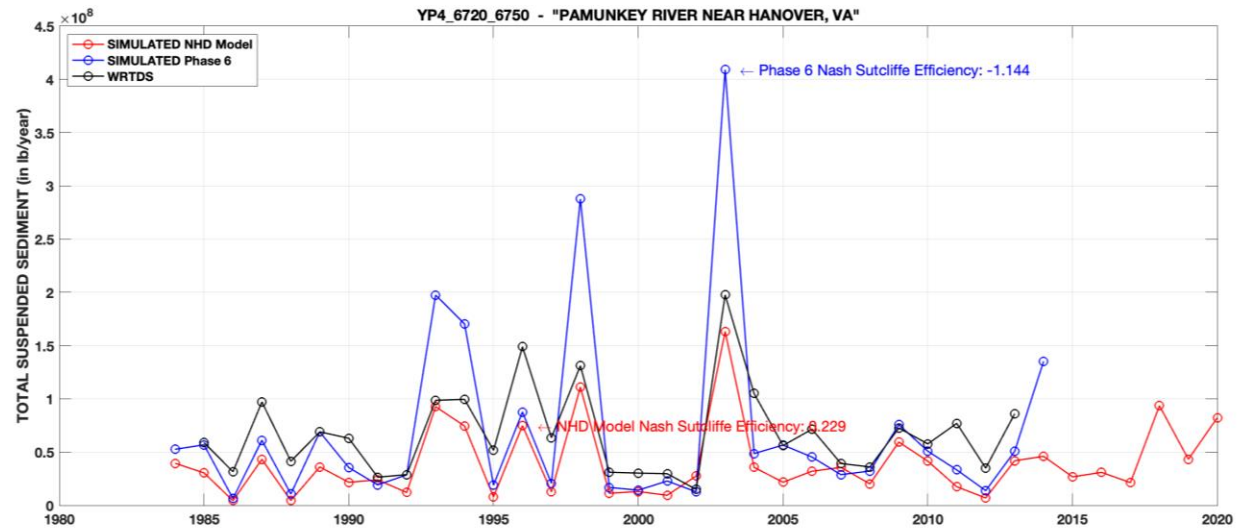
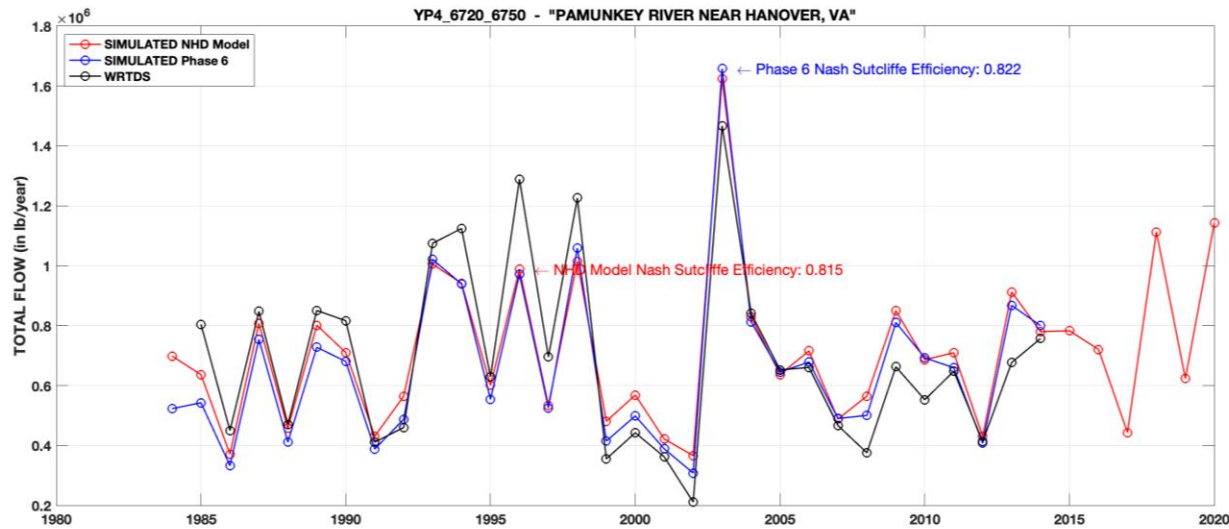


# Appomattox River at Matoaca, VA

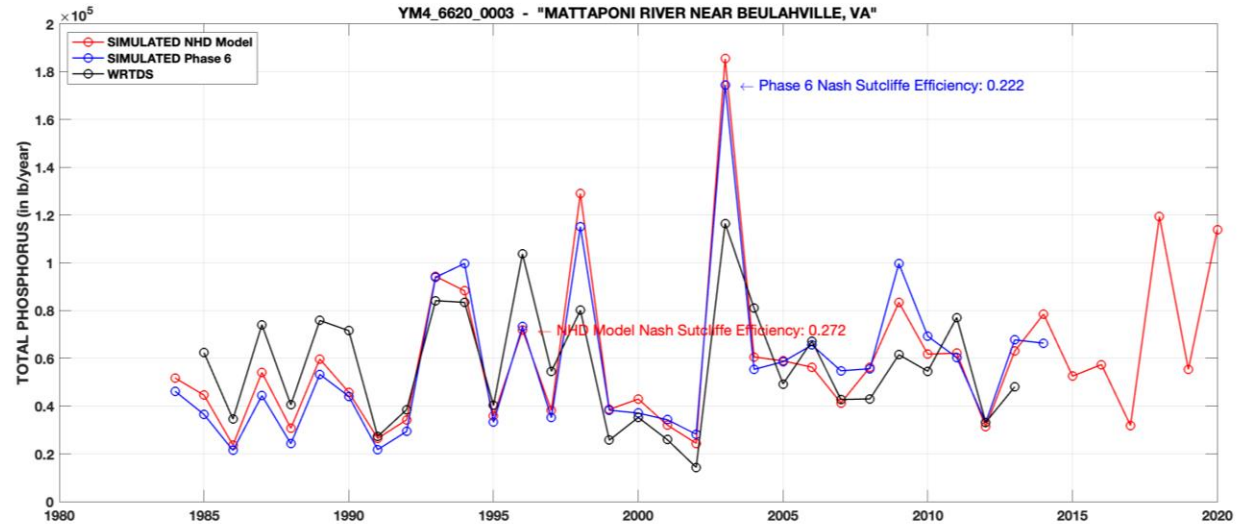
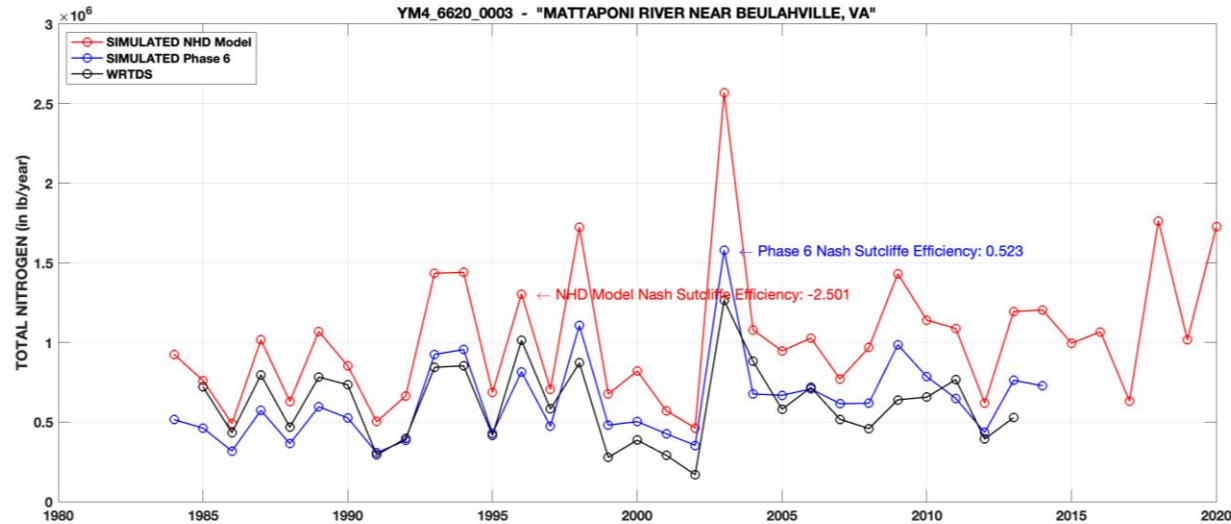
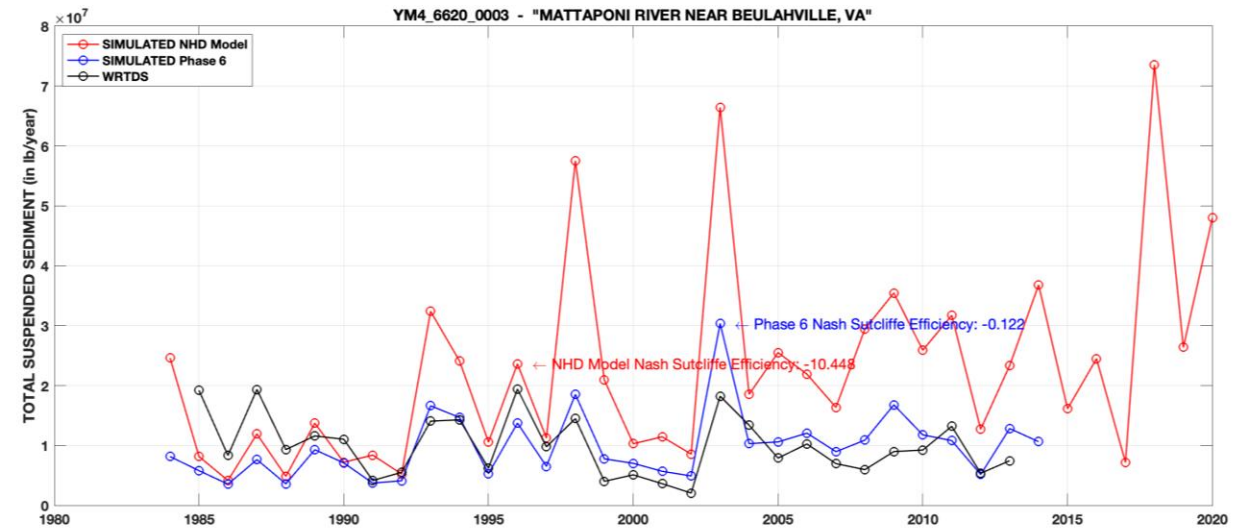
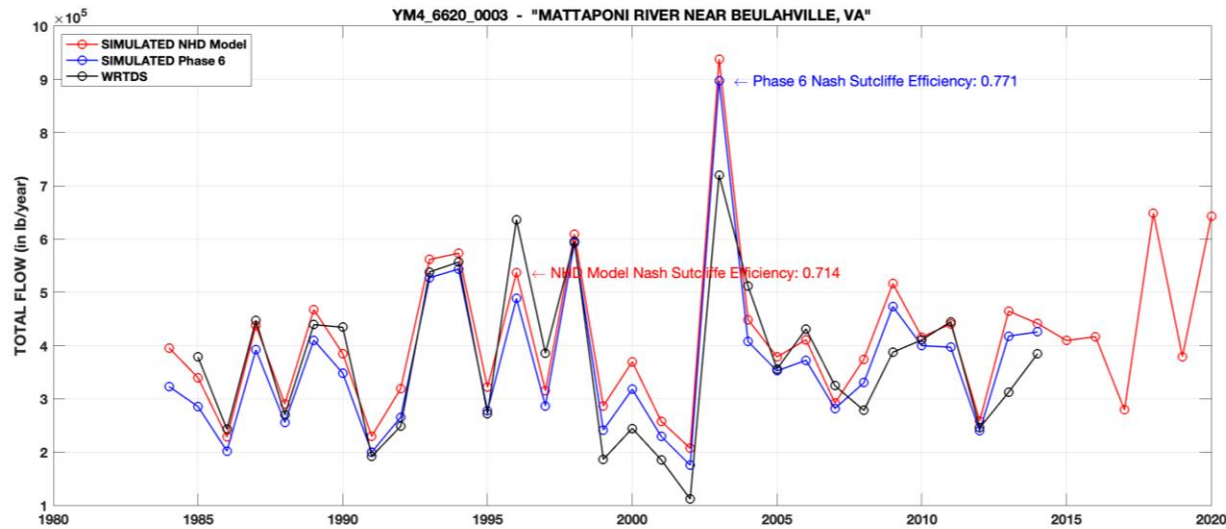




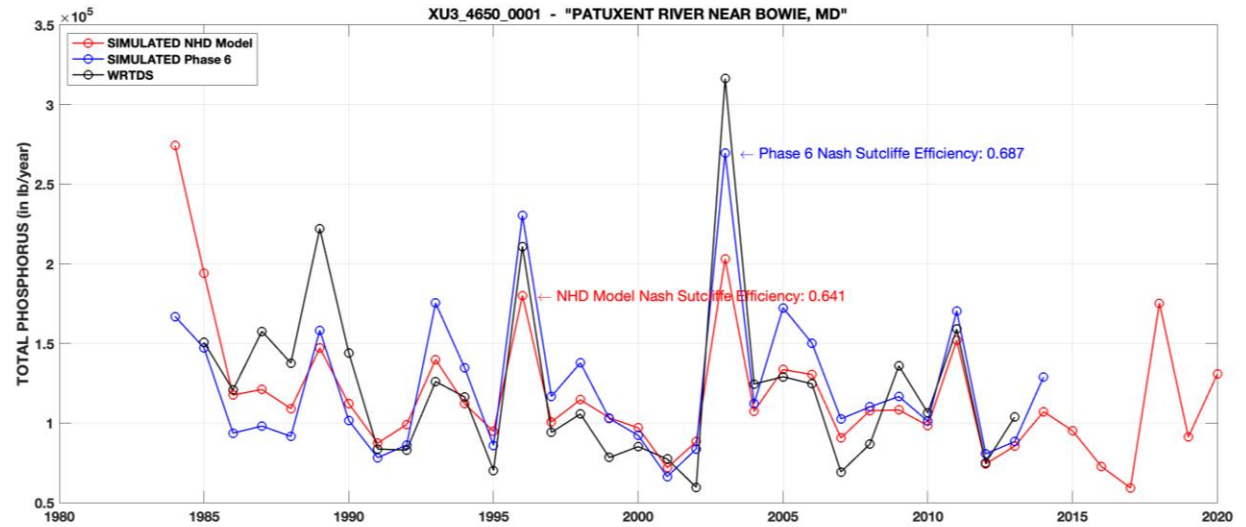
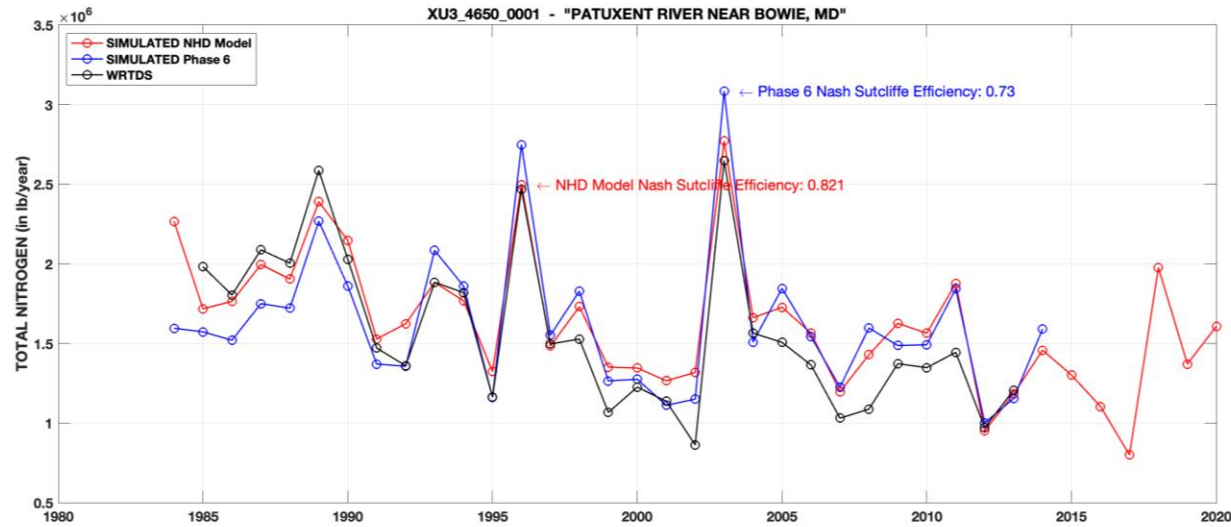
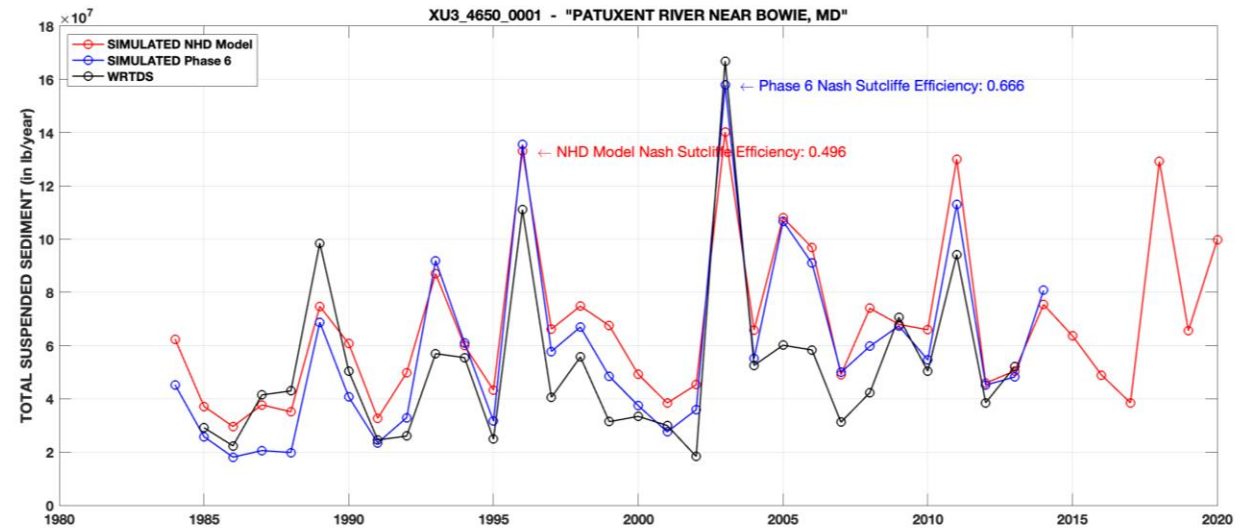
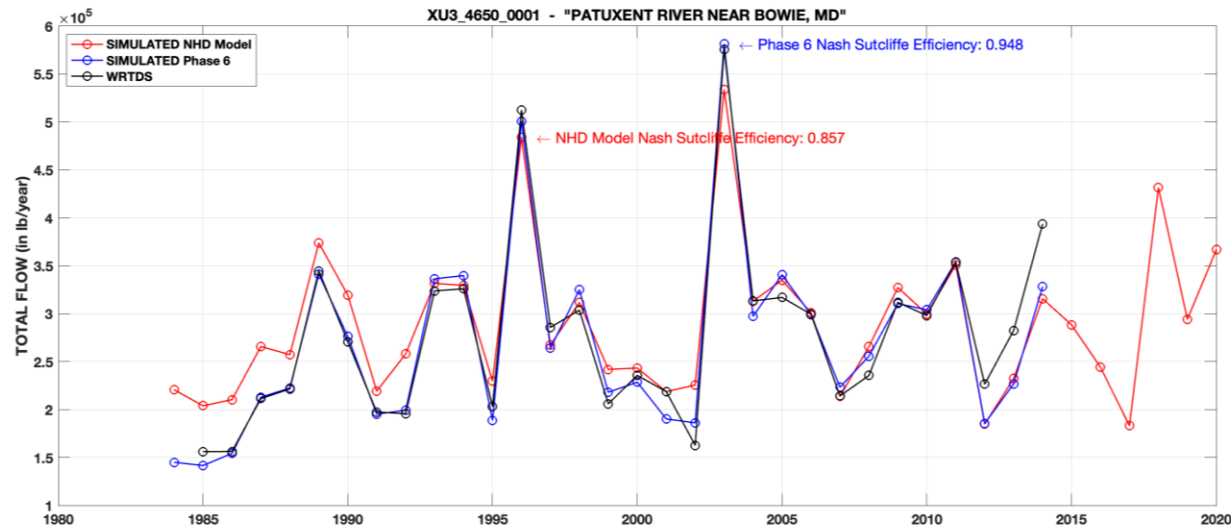
# Pamunkey River near Hanover, VA



# Mattaponi River near Beulahville, VA

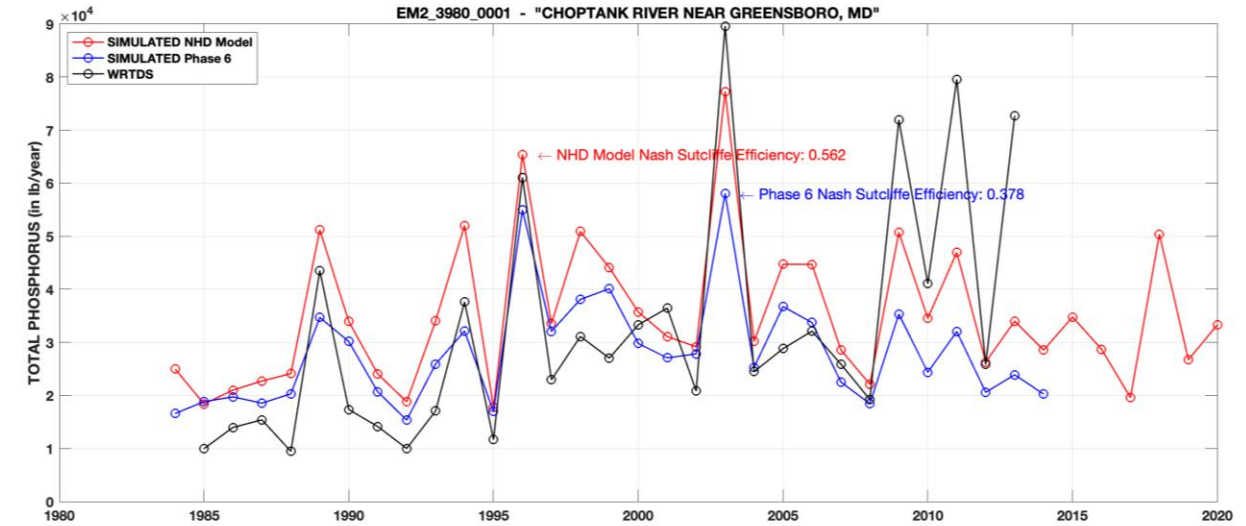
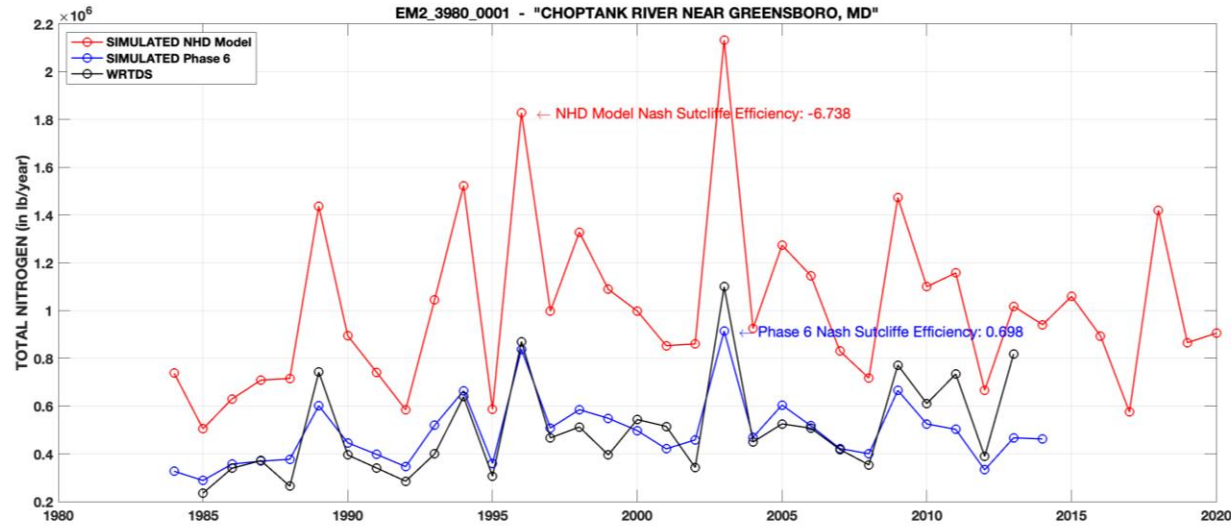
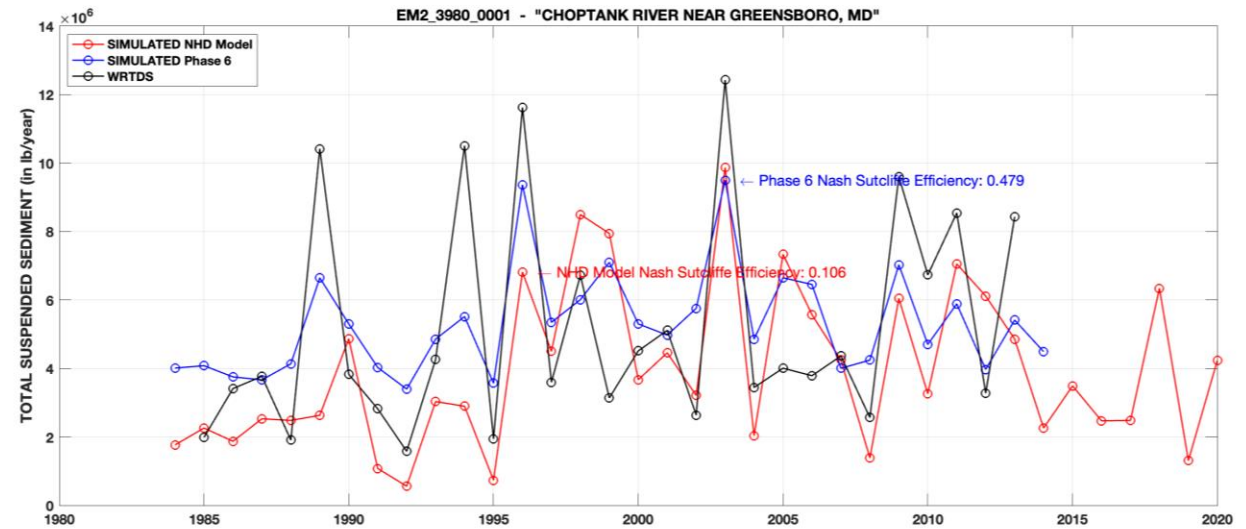
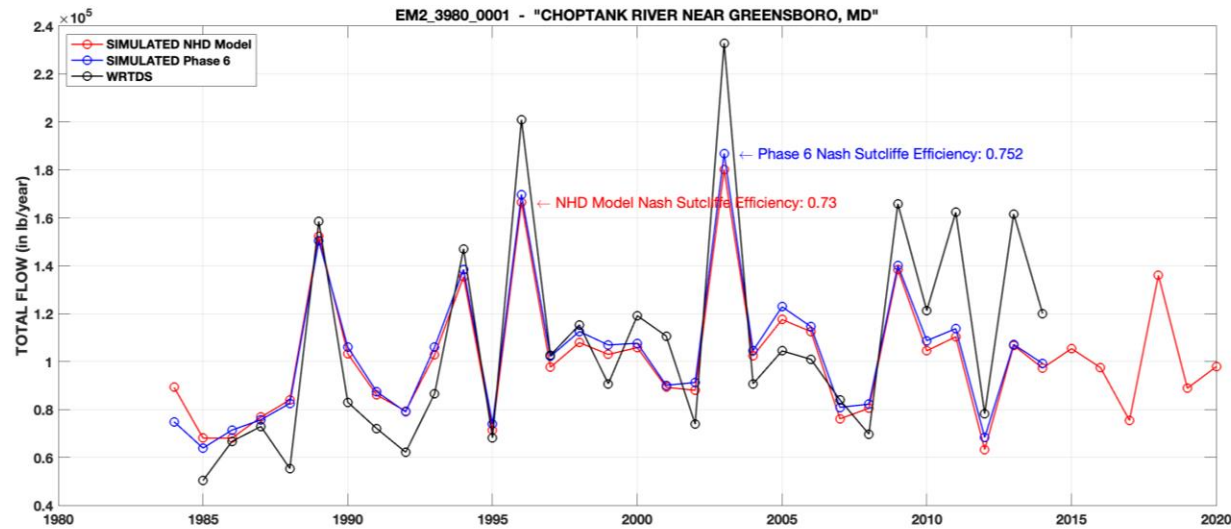


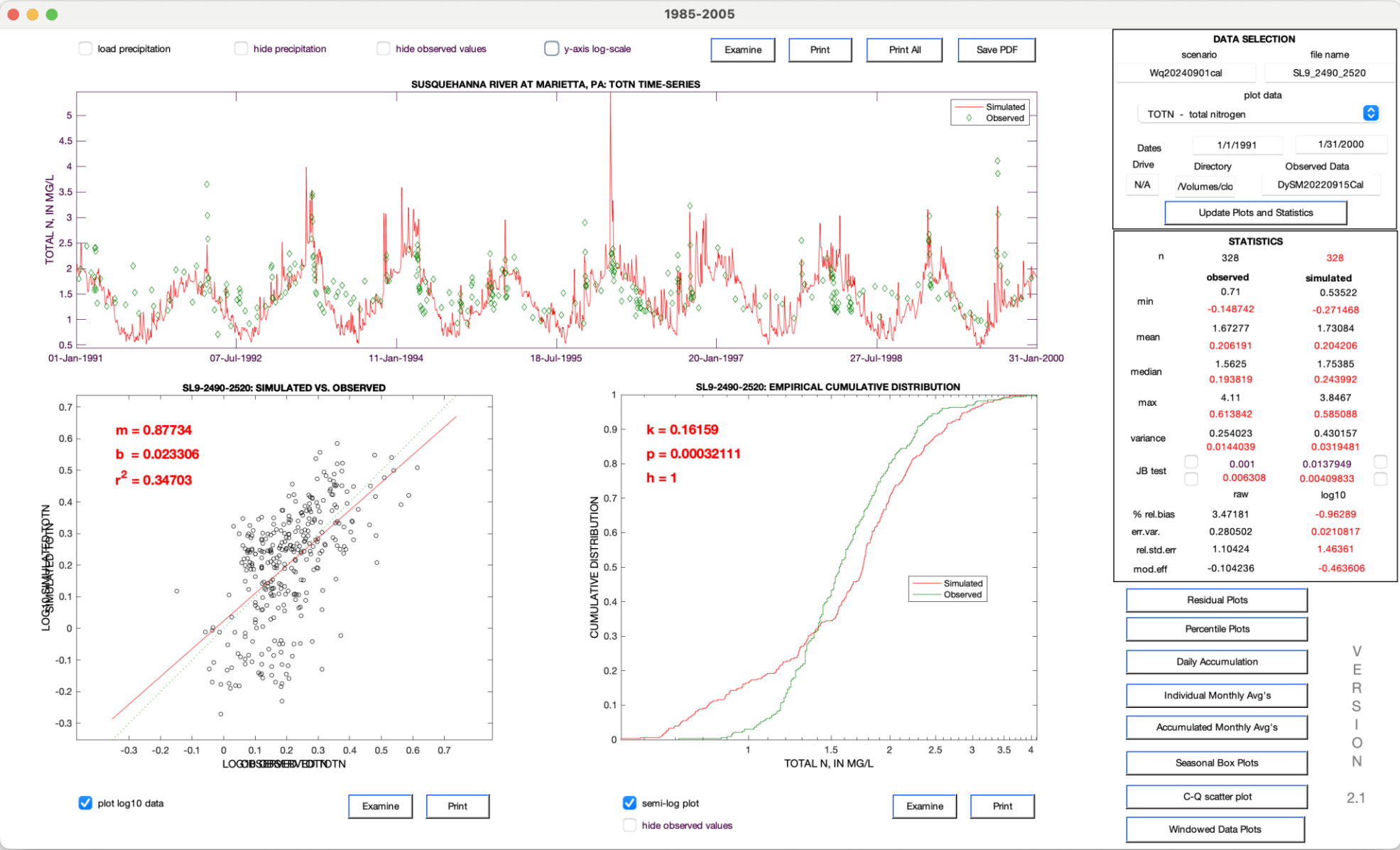
# Patuxent River near Bowie, MD



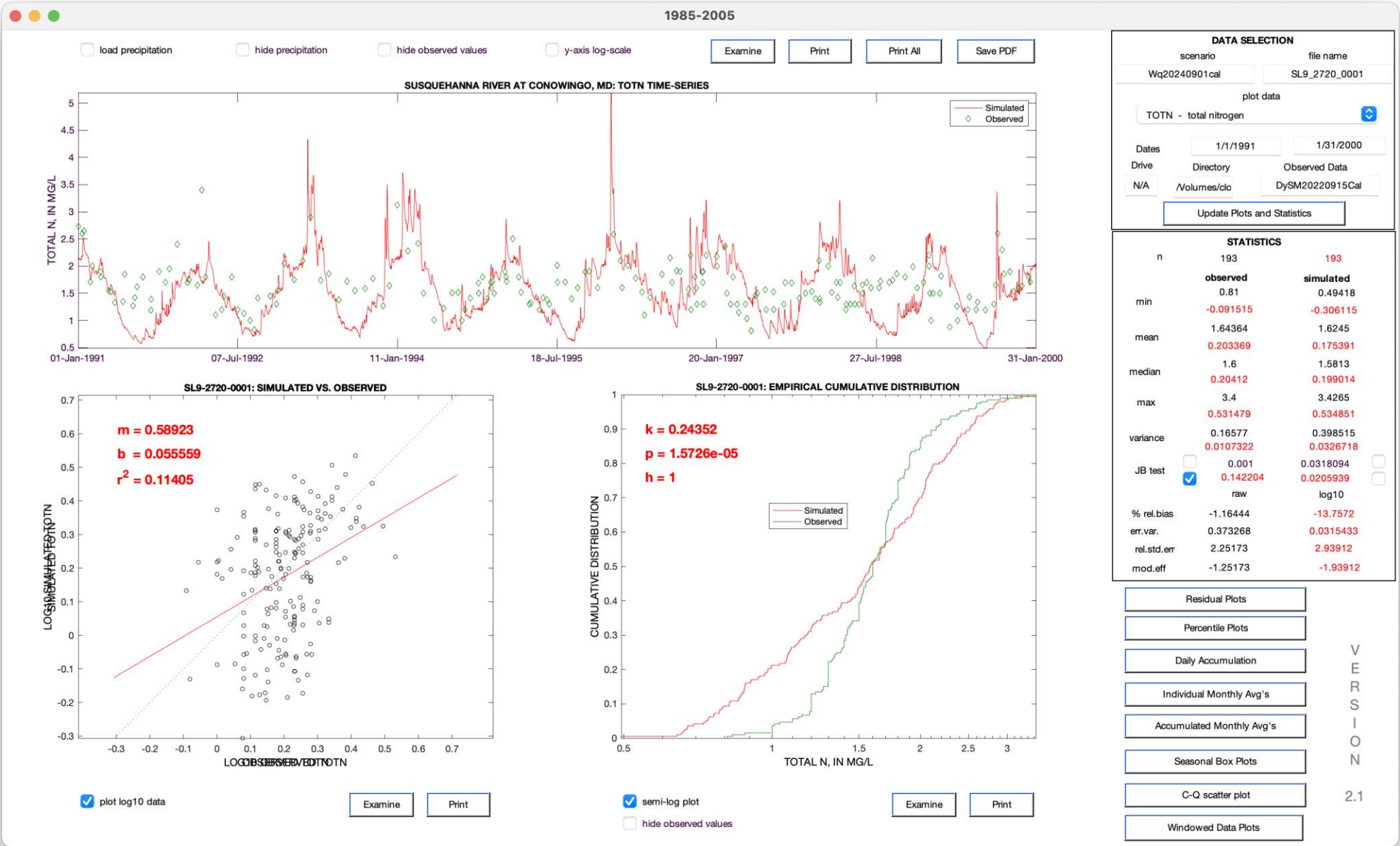


# Choptank River near Greensboro, MD









DATA SELECTION

scenarioWq20240901calfile nameSL9\_2720\_0001

plot dataTOTN - total nitrogen

Dates1/1/19911/31/2000

DriveN/ADirectory/Volumes/cloObserved DataDySM20220915Cal

Update Plots and Statistics

STATISTICS

n	193	193
observed	0.81	0.49418
min	-0.091515	-0.306115
mean	1.64364	1.6245
	0.203369	0.175391
median	1.6	1.5813
	0.20412	0.199014
max	3.4	3.4265
	0.531479	0.534851
variance	0.16577	0.398515
	0.0107322	0.0326718
JB test	0.001	0.0318094
	0.142204	0.0205939
raw		log10
% rel.bias	-1.16444	-13.7572
err.var.	0.373268	0.0315433
rel.std.err	2.25173	2.93912
mod.eff	-1.25173	-1.93912

Residual Plots

Percentile Plots

Daily Accumulation

Individual Monthly Avg's

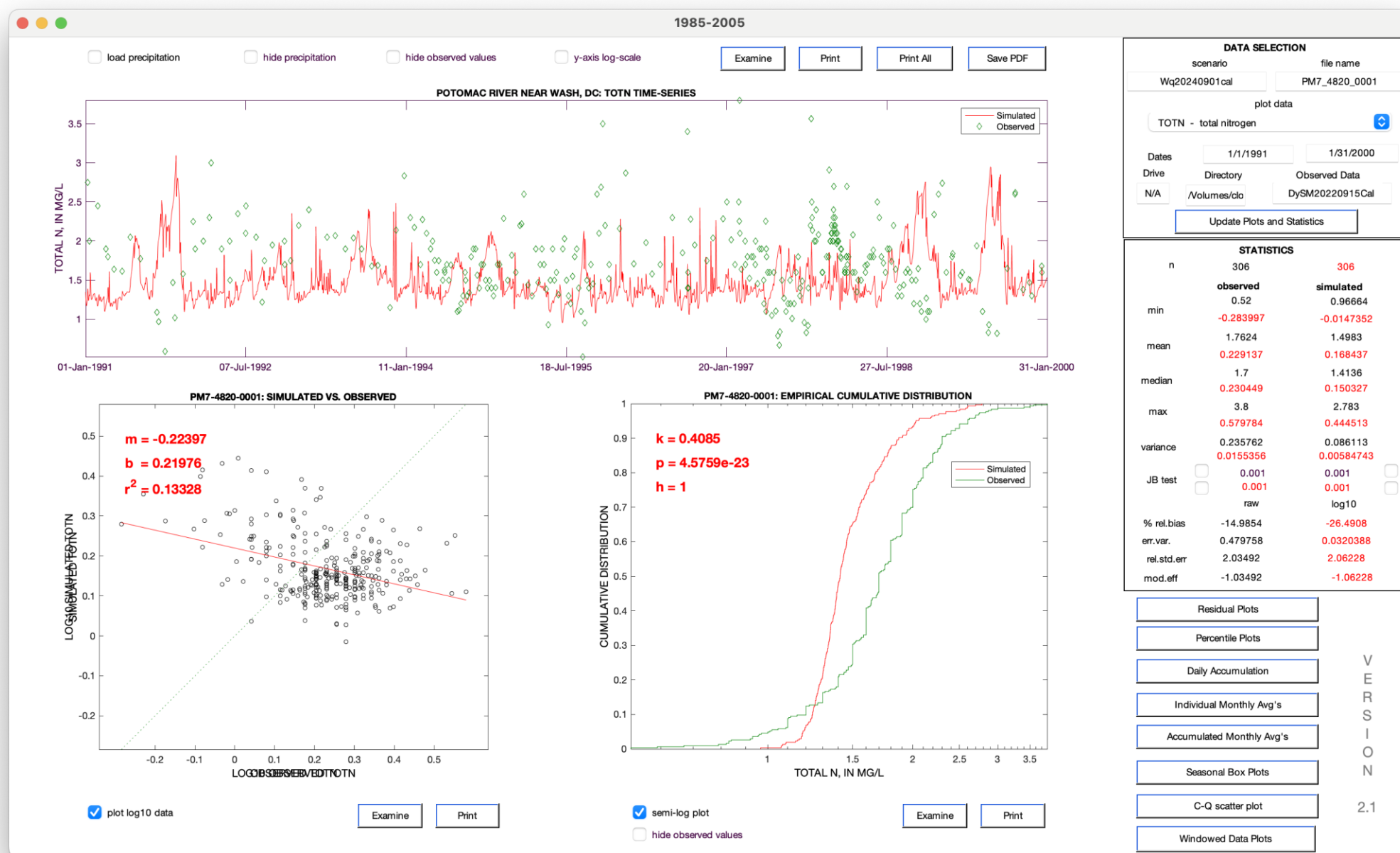
Accumulated Monthly Avg's

Seasonal Box Plots

C-Q scatter plot

Windowed Data Plots

VERSION2.1

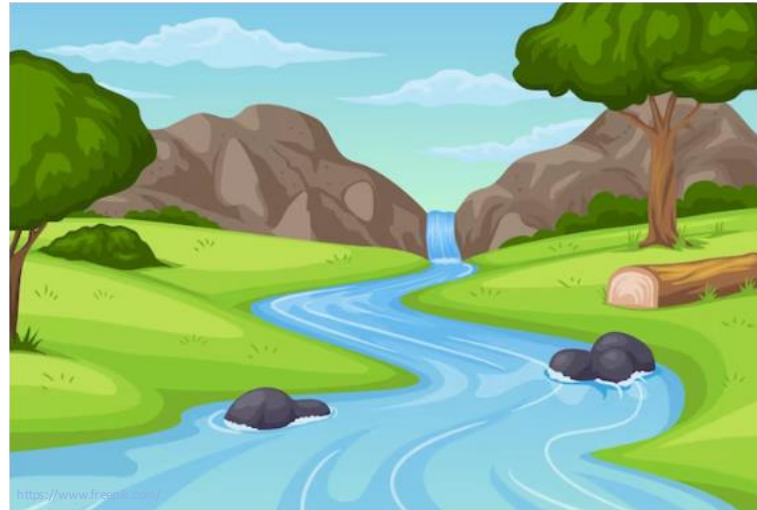


# Small-stream flow and concentration (Q-C) relationship



HSPF: hourly surface and groundwater hydrology of land uses

UNEC: annual surface and groundwater concentrations as a function of input history and estimates of lag-times

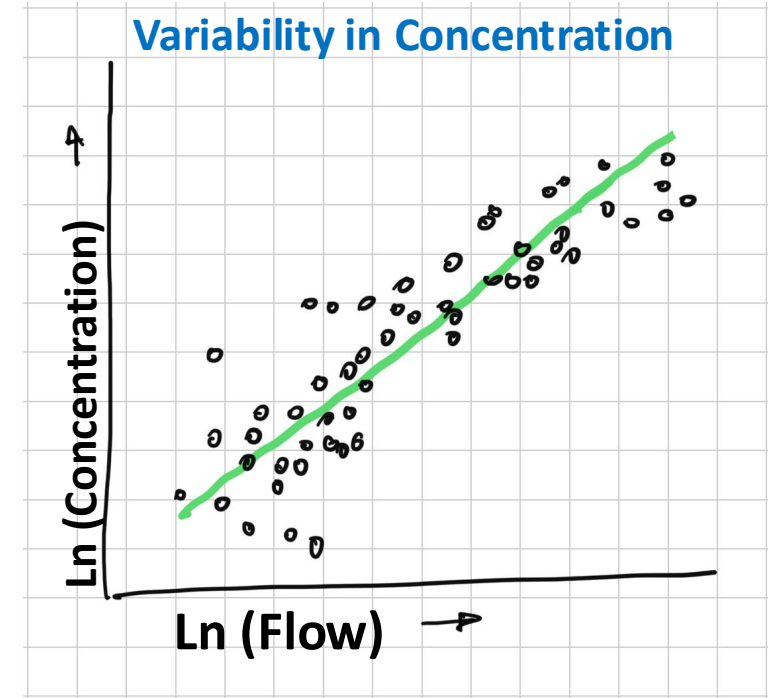


Biogeochemical processing,  
Storage/deposition, Scour  
→ Fate and Transport

Stream Transport Factor (STF)



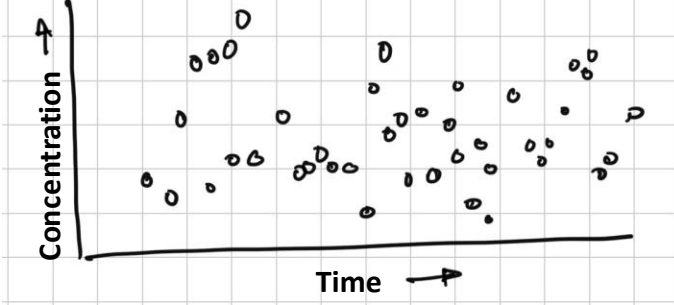
Variability in Concentration



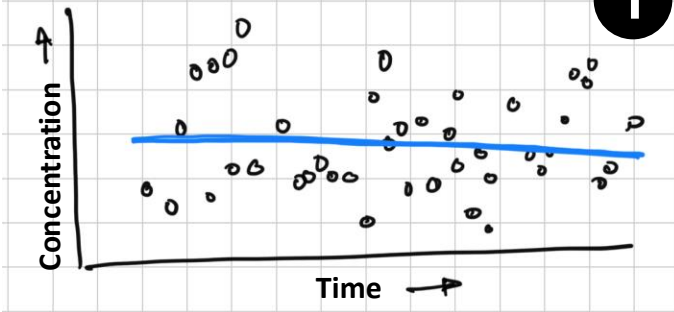
? ... emergent behavior

# Small-stream flow and concentration (Q-C) relationship

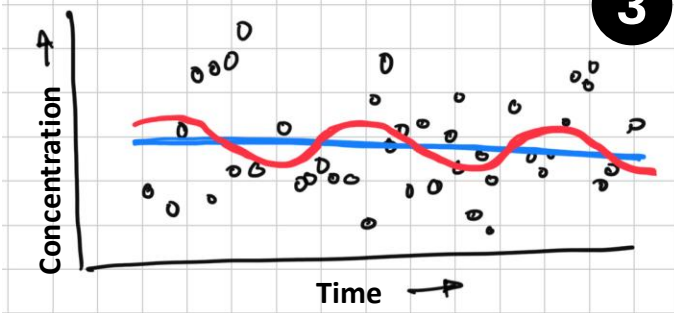
> data at a monitoring station



$$\ln(c_{trend}) = \beta_x + \beta_1 t$$



$$\ln(c_{season}) = \beta_3 \sin(2\pi t) + \beta_4 \cos(2\pi t)$$



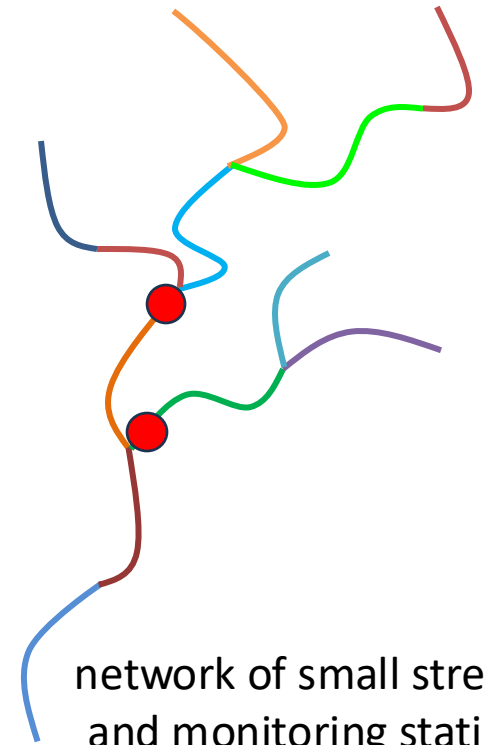
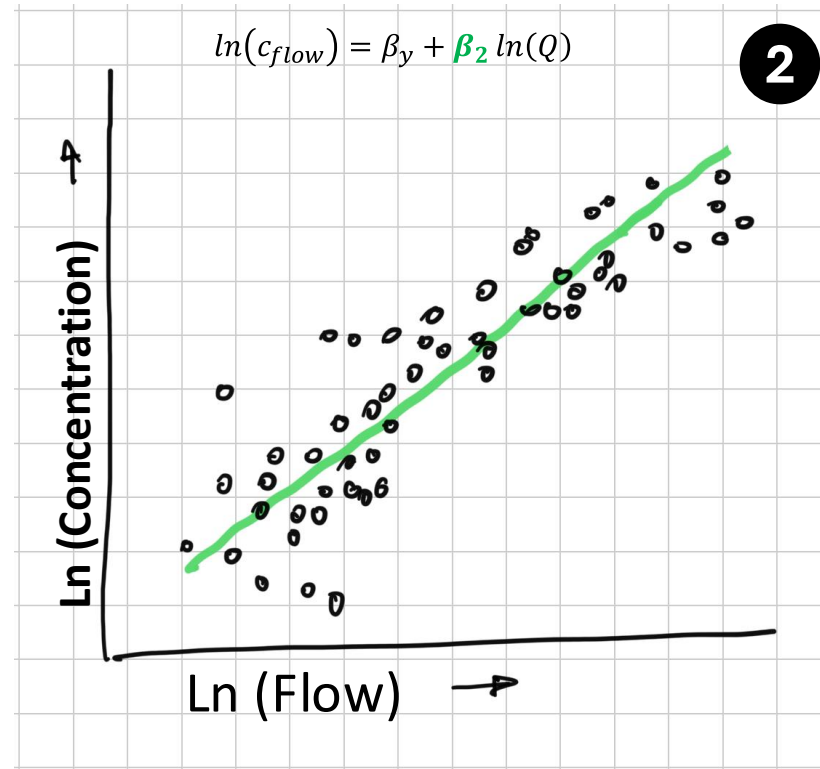
$$\ln(c) = \underbrace{\beta_o}_{1} + \underbrace{\beta_1 t}_{2} + \underbrace{\beta_2 \ln(Q) + \beta_3 \sin(2\pi t) + \beta_4 \cos(2\pi t)}_{3} + \varepsilon \quad [\text{FluxMaster}]$$

1

2

3

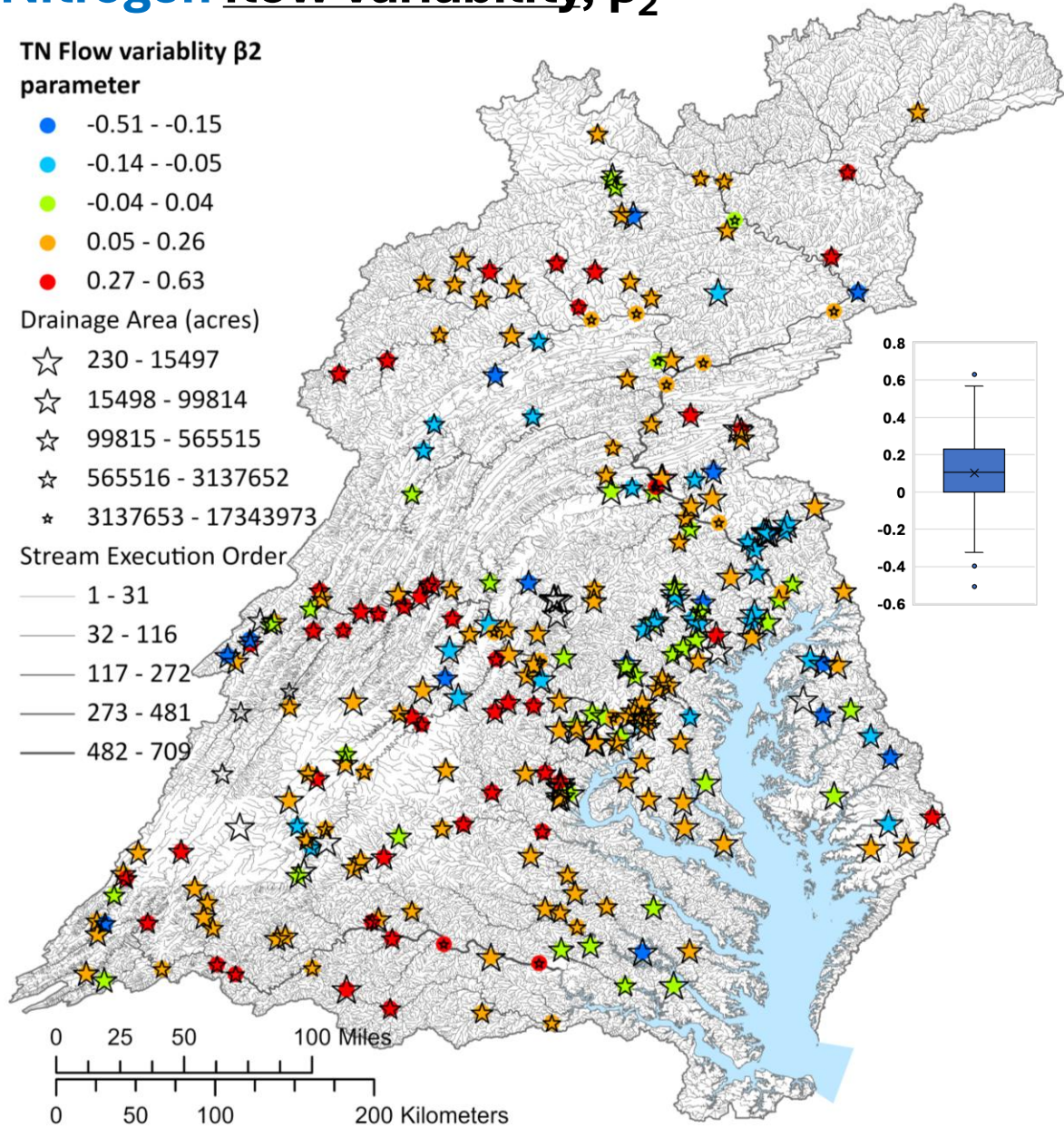
$$\ln(c_{flow}) = \beta_y + \beta_2 \ln(Q)$$



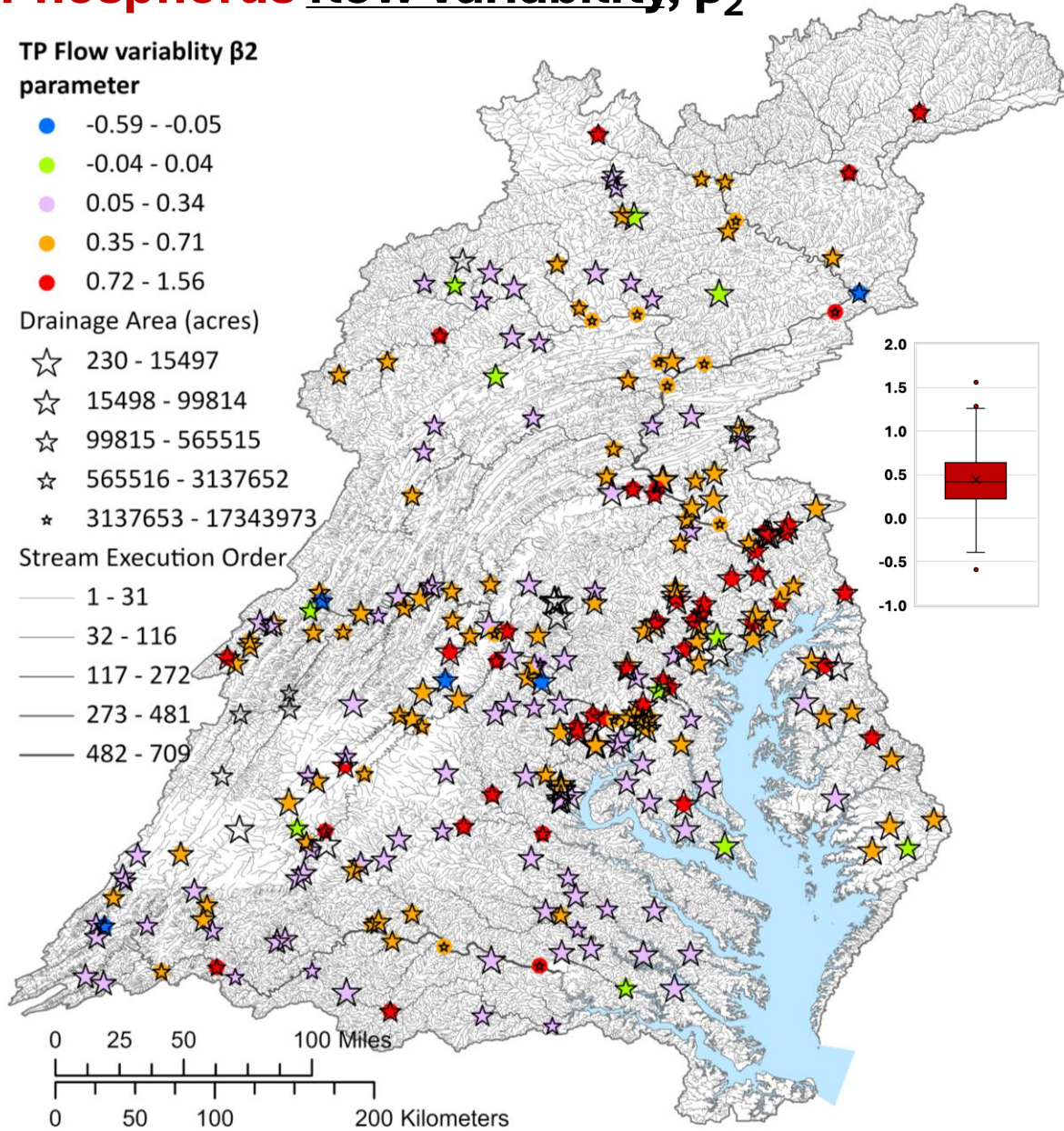
network of small streams  
and monitoring stations  
with water quality and  
streamflow data



# Nitrogen flow variability, $\beta_2$



# Phosphorus flow variability, $\beta_2$

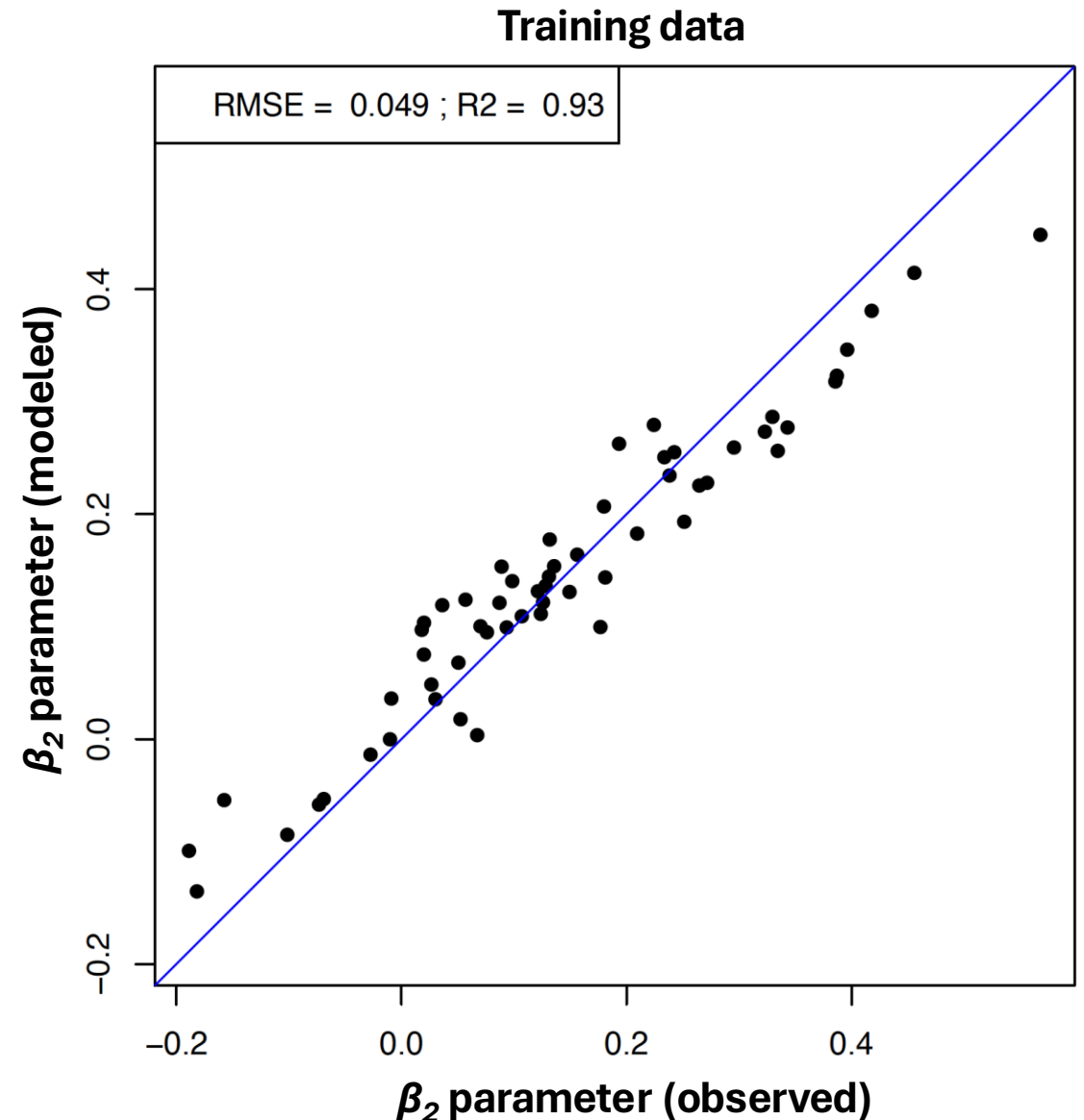


$$\ln(c) = \beta_o + \beta_1 t + \beta_2 \ln(Q) + \beta_3 \sin(2\pi t) + \beta_4 \cos(2\pi t) + \varepsilon$$

# Generalization of $\beta$ parameters – Qian Zhang

An initial *Random Forest* model was developed:

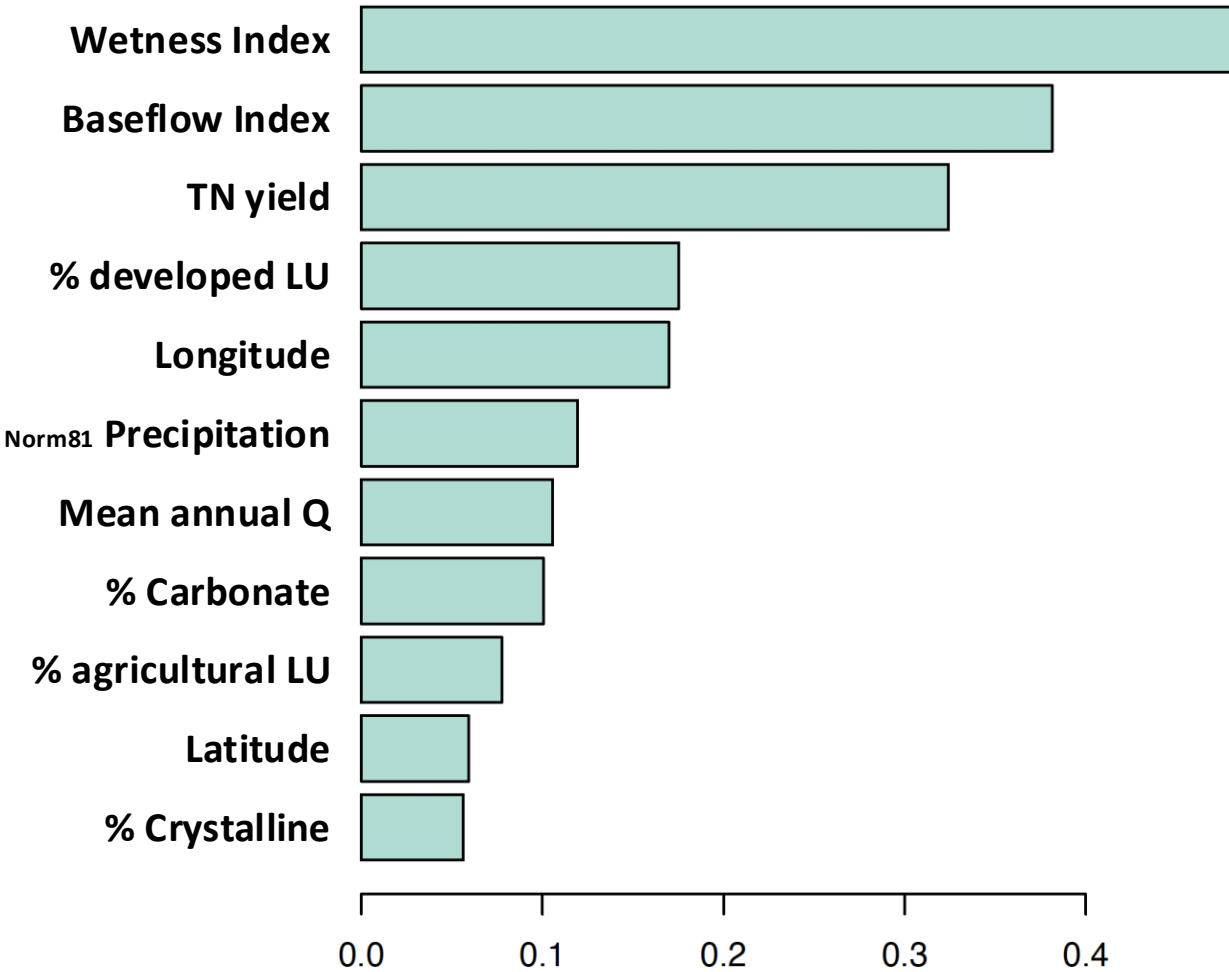
- The model links  $\beta_2$  parameter with watershed attributes
- Performance of the model for training data is shown in the figure
- Currently using data for NTN stations; an expansion would require watershed attributes for additional stations



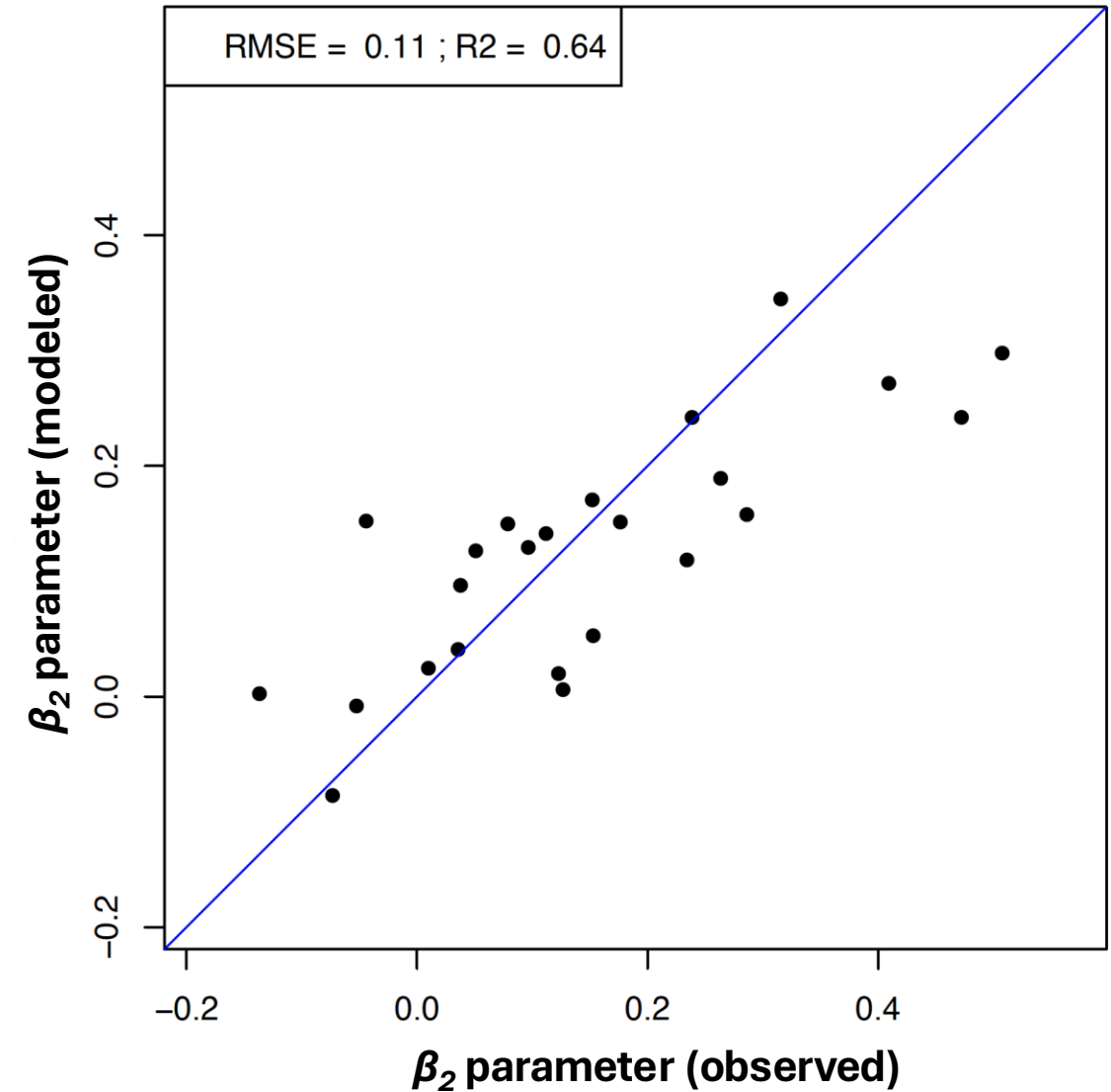


# Generalization of $\beta$ parameters – Qian Zhang

Importance of watershed attributes



Validation data



# Scale and Simulation of Small Streams

**nested model  
segmentation of streams  
and river mainstems →**

100K NHD  
STREAMS

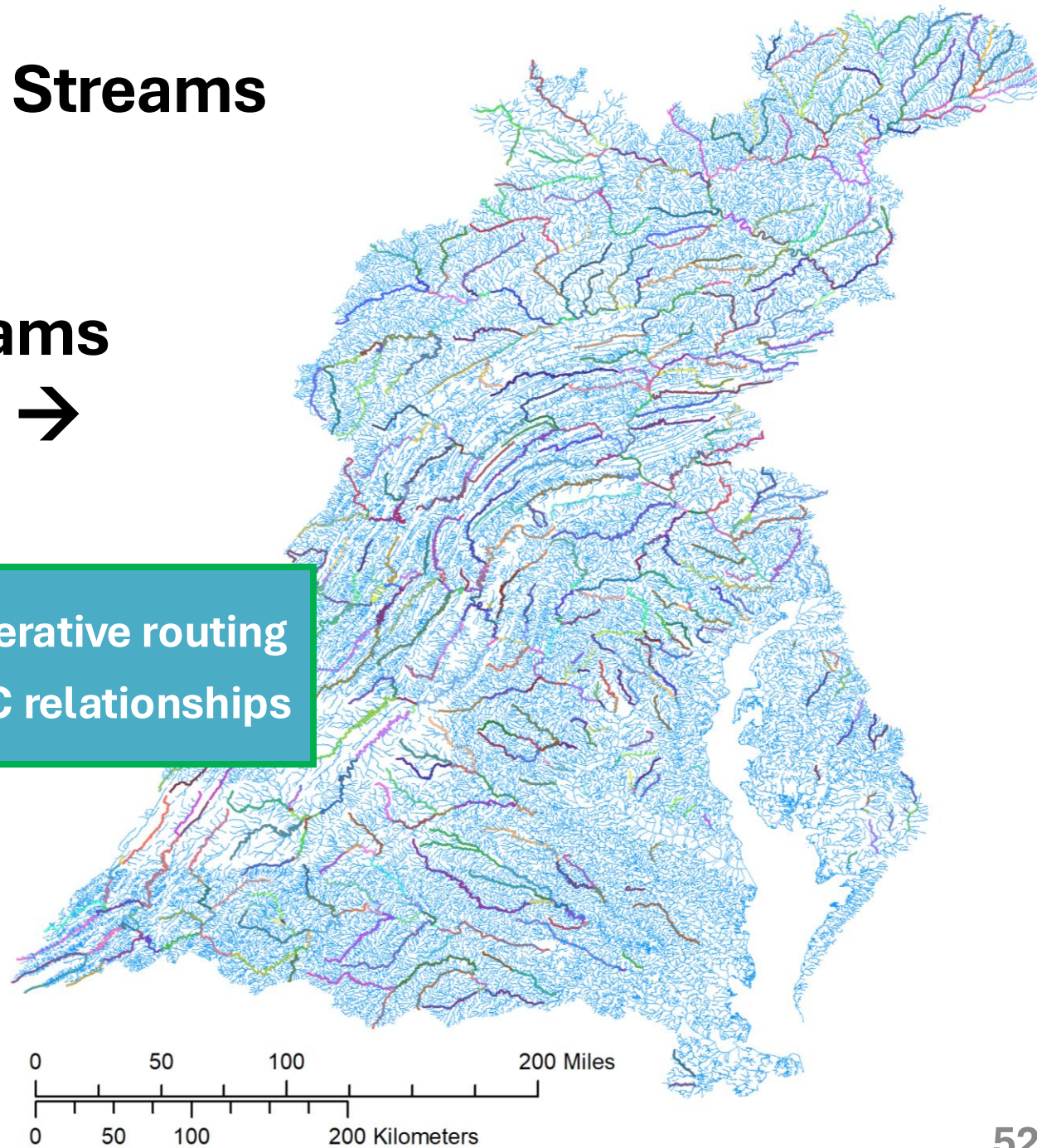


Hydrology: Non-iterative routing  
Water Quality: Q-C relationships

RIVER  
MAINSTEM

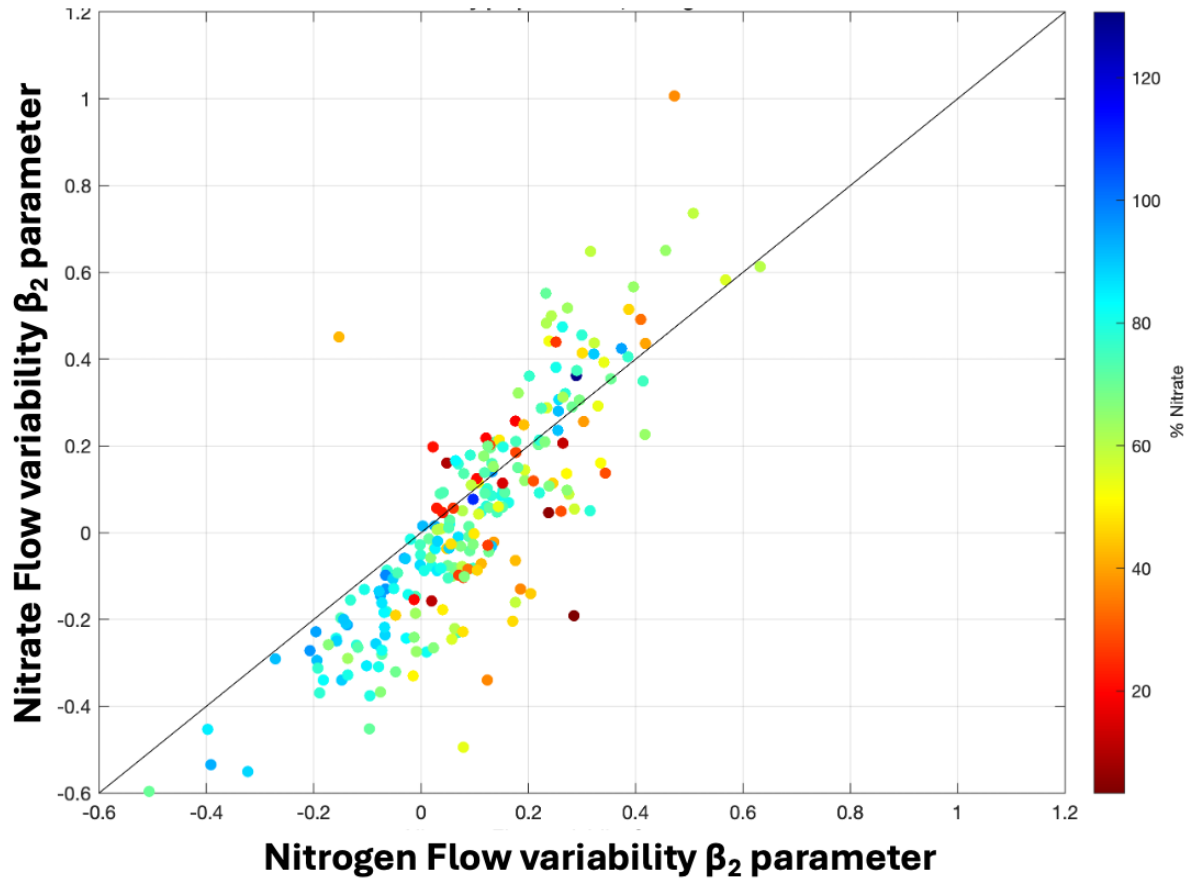


HSPF

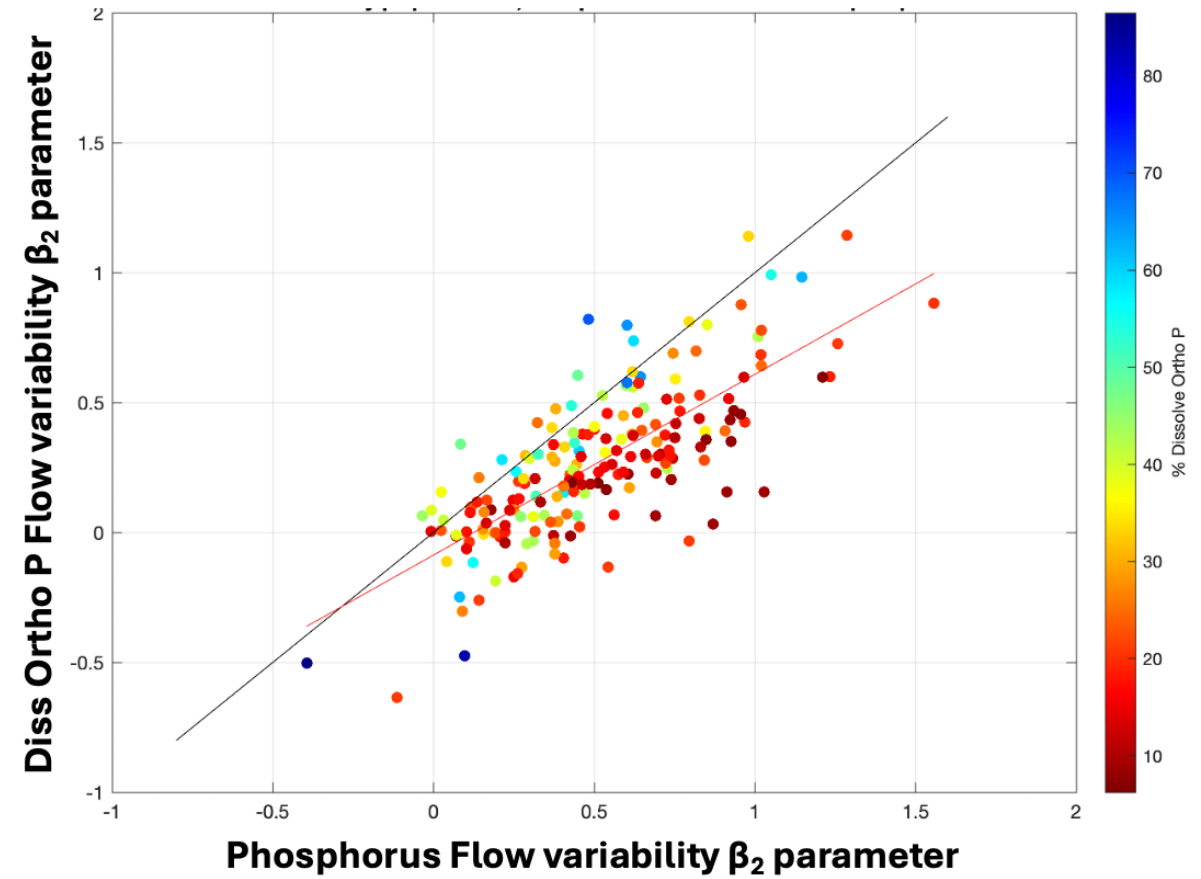


# Flow variability, $\beta_2$ parameter

## Nitrogen vs. Nitrate

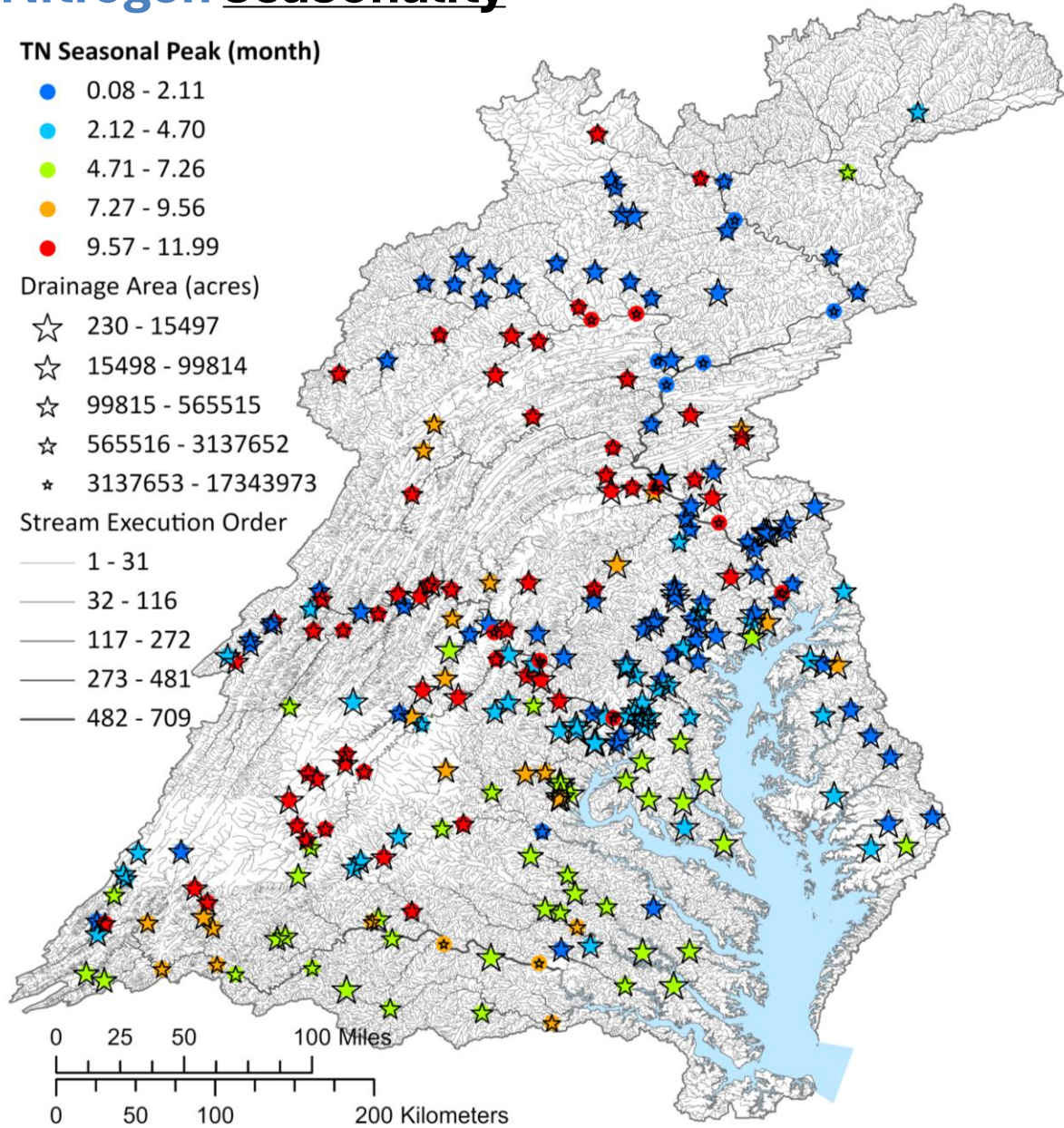


## Phosphorus vs. Dissolved Orthophosphate

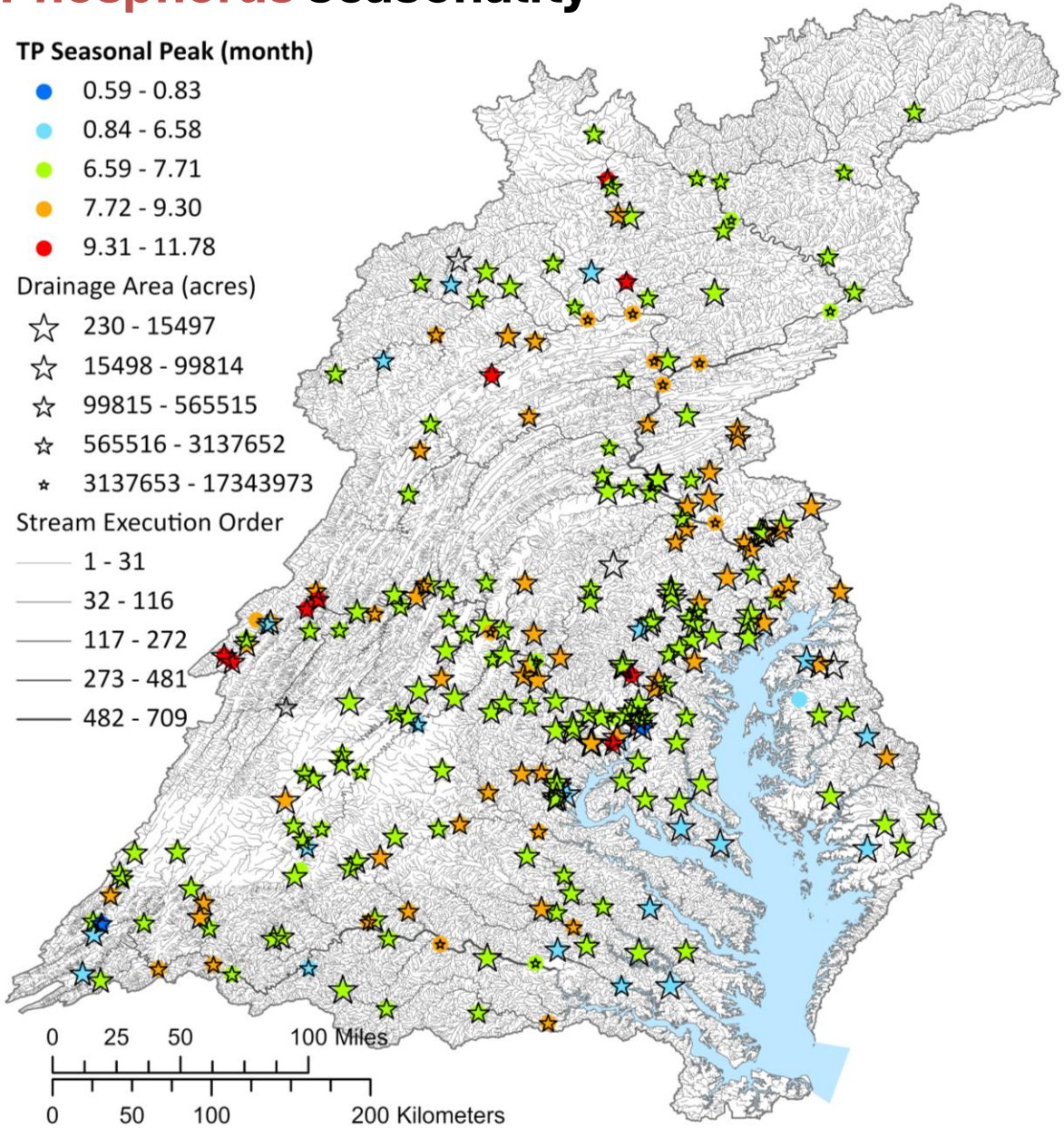




# Nitrogen seasonality

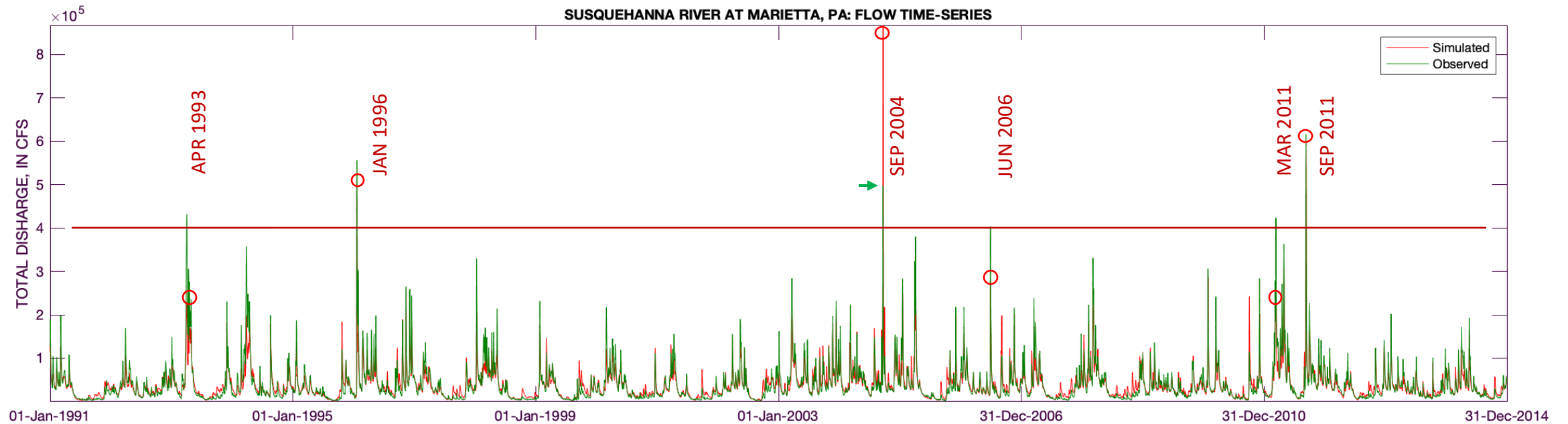


# Phosphorus seasonality

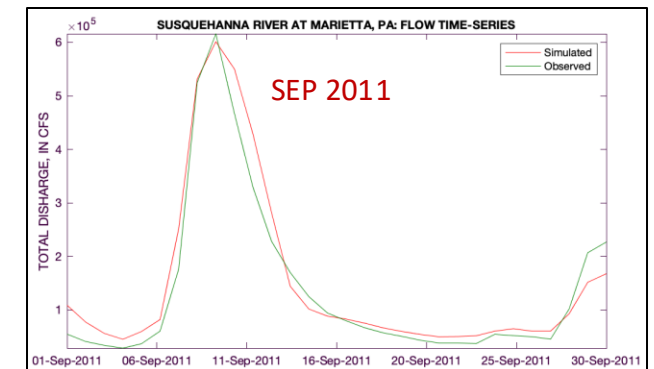
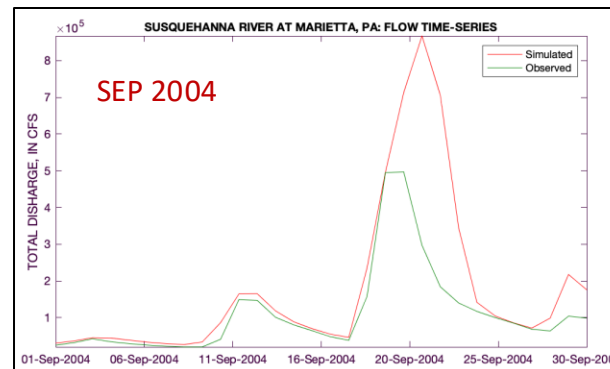
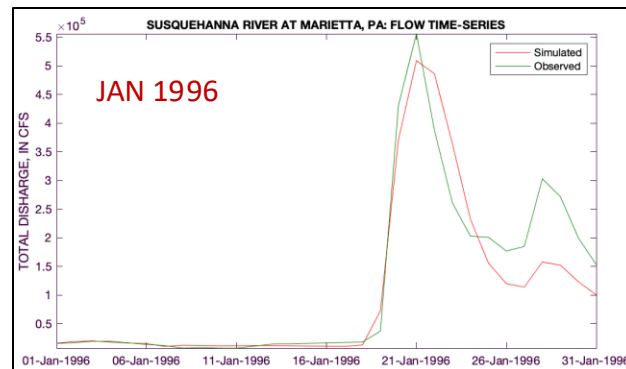


$$\ln(c) = \beta_o + \beta_1 t + \beta_2 \ln(Q) + \beta_3 \sin(2\pi t) + \beta_4 \cos(2\pi t) + \varepsilon$$

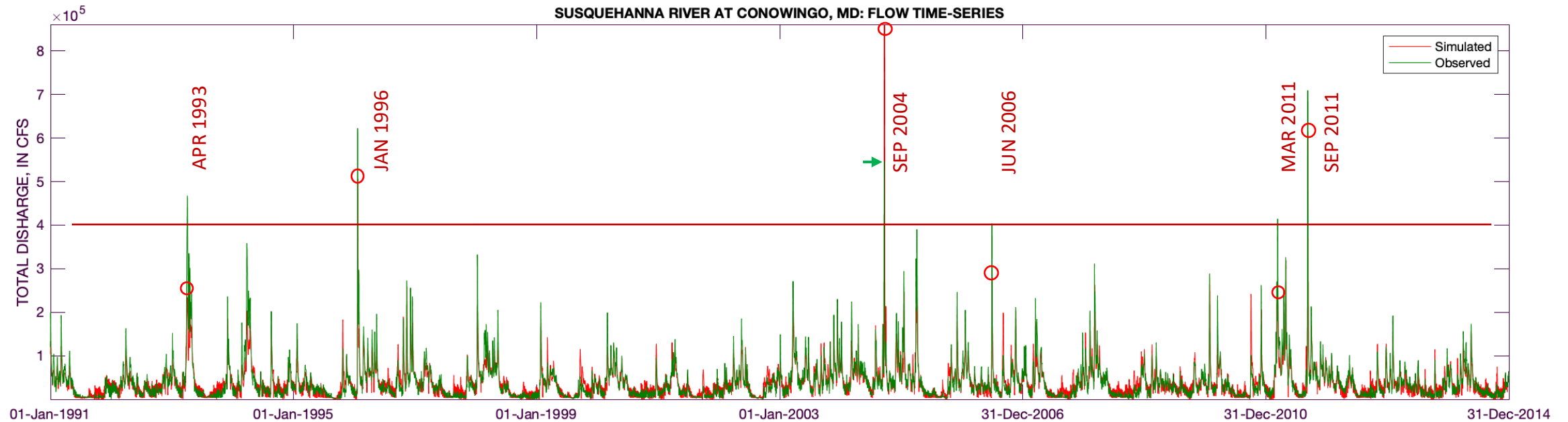
# Susquehanna River at Marietta, PA



*There were 6 events when flow exceeded 400,000 cfs and most of them were under simulated, except for 2004*



# Susquehanna River at Conowingo, MD



*There were 6 events when flow exceeded 400,000 cfs and most of them were under simulated, except for 2004*

