Outline

- Water Quality Modeling 101
- How to Use Models Correctly?
- Are Your Model Results Right?
- Post Audit
- Case Studies
- Data Never Sufficient
- Take-Home Messages
- Discussions

Why Water Quality Model?

- Establish a quantitative cause-effect relationships between **sources** and **receiving water responses**

Input → **System** → **Output**

Sources

Receiving Water

Response

Model Types

Empirical models

(經驗模式)

- Mathematical relationship(數學關係)
- Based on observed data (基於觀察)
- Not theoretical

Deterministic models

(定率模式)

- Mathematical models (數學模式)
- Designed to produce system responses or outputs

Water Quality Model Representation

Water **transport** through the system (水體於系統內之傳輸)

- Physical conditions and transport properties of the water system

Reactions within the system (系統內的反應)

- Physical, Biological, Chemical, and Biochemical

Inputs or withdrawals from the system due to anthropogenic activities or natural phenomena (因人類活動或自然現象對系統之貢獻)

Driving Forces for Mass Transport

Freshwater stream/river with unidirectional flow (河流/單一方向之河流)

- Gravitational force (proportional to gradient)
- Tributary inflows
- Direct runoff into water body during runoff events
- Wind

Lake/reservoir

(湖泊/水庫)

- Wind
- Tributary inflows
- Discharge from dam
- Direct runoff into water body during runoff events

Stream/river with oscillatory flow

(流量不固定之河流)

- Gravitational force (proportional to gradient)
- Astronomical tides(潮汐)
- Tributary inflows
- Spatial (horizontal and vertical) salinity gradients
- Direct runoff into water body during runoff events
- Wind

Estuary/bay/coastal seas

(河口/海灣/海岸)

- Astronomical tides(潮汐)
- Freshwater discharge
- Wind
- Coriolis force (科氏力)
- Atmospheric pressure gradients
- Direct runoff into water body during runoff events

Basic Principle – Mass Conservation

behind a Water Quality Model

$$V\frac{dC}{dt} = J + \sum R + \sum T + \sum W$$

V = volume

C = concentration of constituent

t = time

J = mass transport through the system

R = reaction within the system

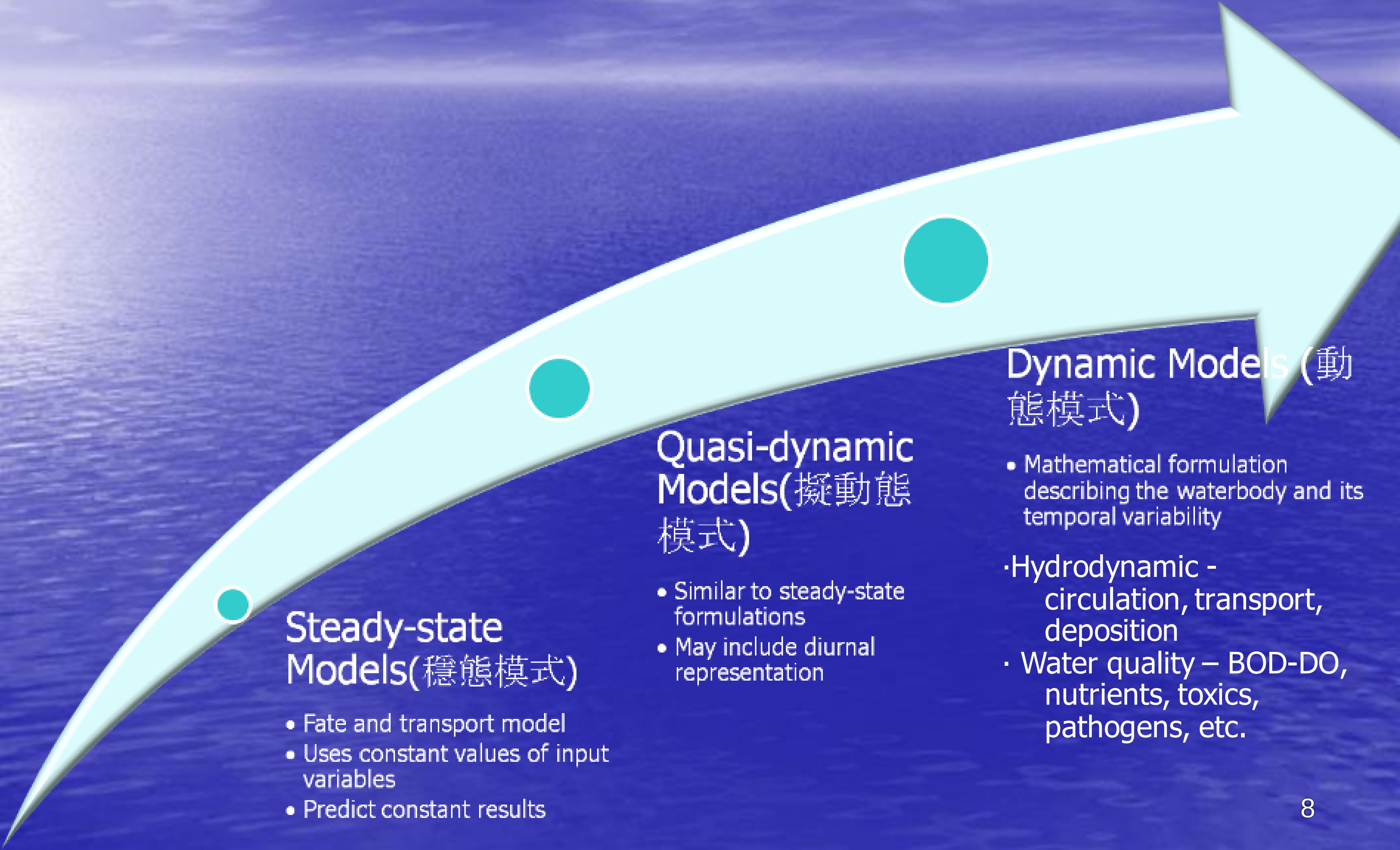
T = transfer from one phase to another

W = input

Water Quality Model Applications

- Simple, steady state models typically used to assess response under a specific flow condition. e.g., low flow (簡單、穩態的模式用於建立特定流量情況下的模擬，例如低流量)
  - Best suited to point sources/steady state inputs (最適用於點源/穩態流量)
- Dynamic models consider time varying conditions (動態模式考慮隨時間變化的環境)
  - Typically more processes simulated allowing evaluation of interactions among constituents(原則上，模式評估並考慮不同機制間的互動)
  - Consider distributed nonpoint inputs(考慮非點源污染)
  - Often provide multidimensional simulations(多維度模擬)
  - Usually used for lakes, estuaries, and streams exhibiting complex interactions (通常用於湖泊、河口及河流之較複雜的機制)

Temporal Complexity



Steady-state Models(穩態模式)

- Fate and transport model
- Uses constant values of input variables
- Predict constant results

Quasi-dynamic Models(擬動態模式)

- Similar to steady-state formulations
- May include diurnal representation

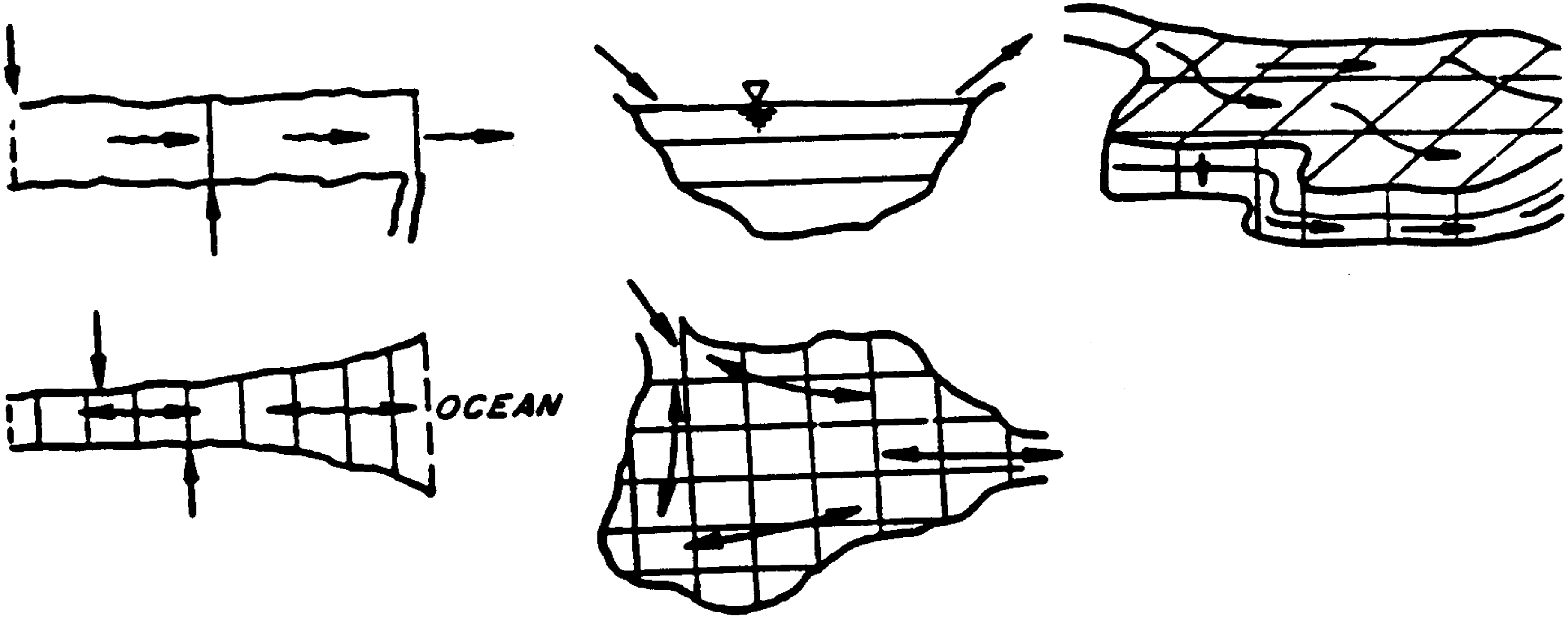
Dynamic Models (動態模式)

- Mathematical formulation describing the waterbody and its temporal variability

·Hydrodynamic - circulation, transport, deposition

· Water quality – BOD-DO, nutrients, toxics, pathogens, etc.

Spatial Discretization of Water Systems



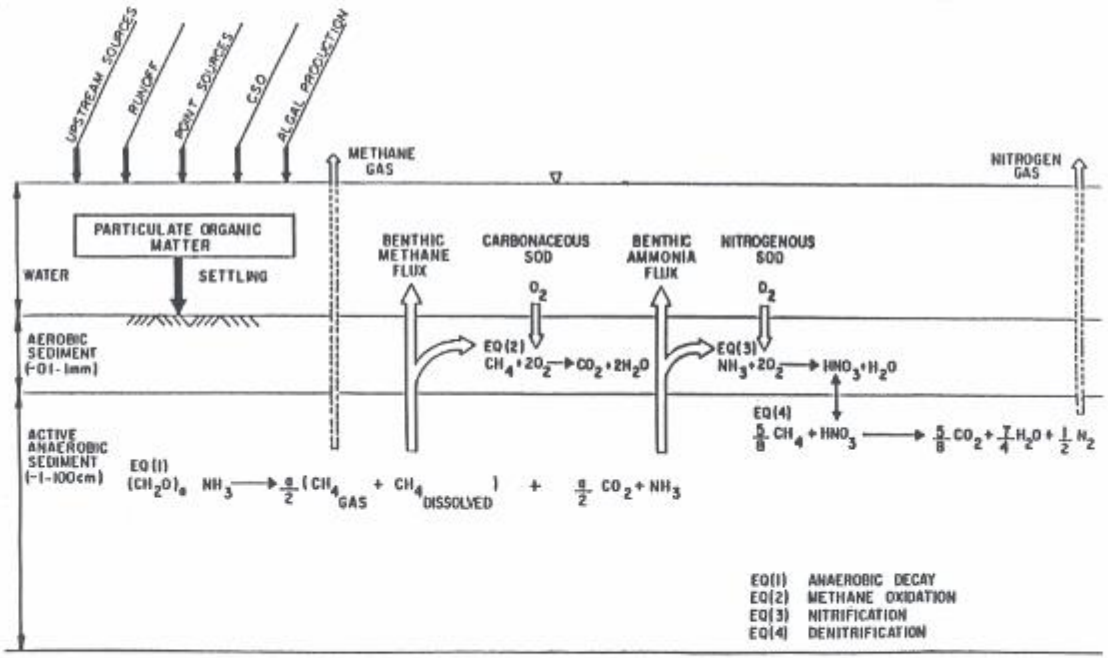
1-D longitudinal
(rivers)

2-D in the vertical
(narrow and deep lakes and reservoirs)
2-D in the horizontal
(shallow and large lakes and reservoirs,
shallow coastal areas, wide rivers)

Full 3-D
(estuaries, large & deep
lakes
and reservoirs)

BOD-Related DO Problems

- Dissolved Oxygen (溶氧) as End Point
- Biochemical Oxygen Demand (生化需氧量)
  - **C**arbonaceous **B**iochemical **O**xygen **D**emand(碳生化需氧量)
  - **N**itrogenous **B**iochemical **O**xygen **D**emand(氮生化需氧量)
  - **S**ediment **O**xygen **D**emand(底泥需氧量)

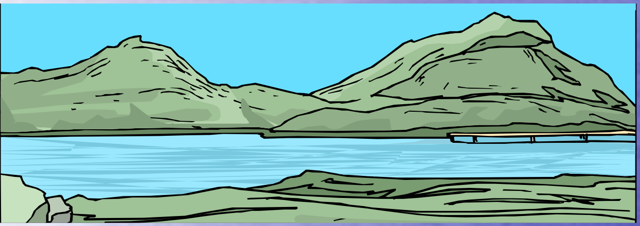


Source: HydroQual, 1992.

How Does a Stream BOD/DOModel Look Like?

A Simple Analytical Solution from Streeter & Phelps

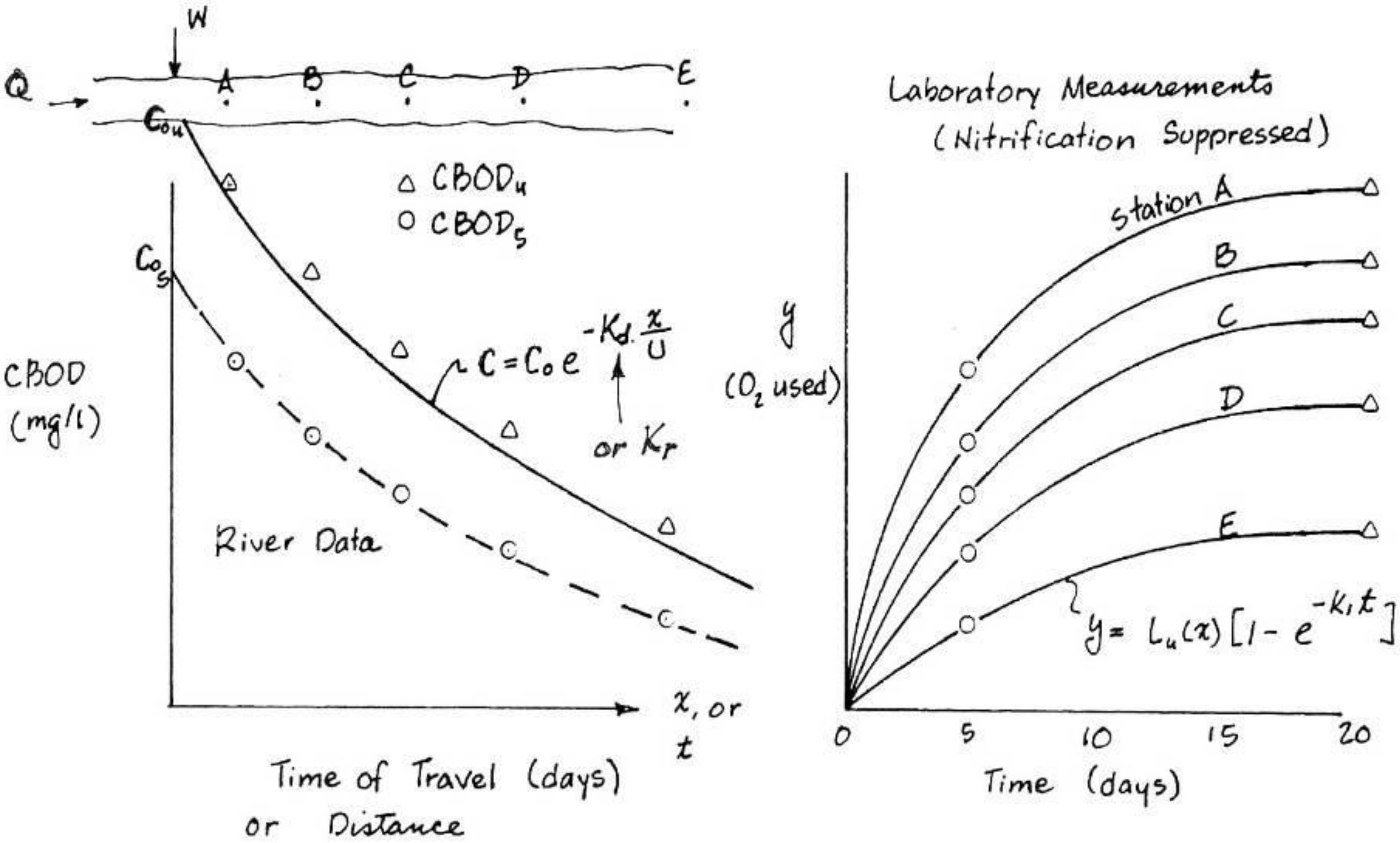
Prototype Process



$$
\begin{aligned}
D = {} & \frac{K_d L_0}{K_a - K_r}\left(e^{-K_r \frac{x}{U}} - e^{-K_a \frac{x}{U}}\right) && \text{CBOD}_u \\
& + \frac{K_n N_0}{K_a - K_n}\left(e^{-K_n \frac{x}{U}} - e^{-K_a \frac{x}{U}}\right) && \text{NBOD} \\
& + D_0 e^{-K_a \frac{x}{U}} && \text{Initial Deficit} \\
& - \frac{P}{K_a}\left(1 - e^{-K_a \frac{x}{U}}\right) && \text{Algal Photosysthesis} \\
& + \frac{R}{K_a}\left(1 - e^{-K_a \frac{x}{U}}\right) && \text{Algal Respiration} \\
& + \frac{SOD}{H\,K_a}\left(1 - e^{-K_a \frac{x}{U}}\right) && \text{Sediment Oxygen Demand}
\end{aligned}
$$

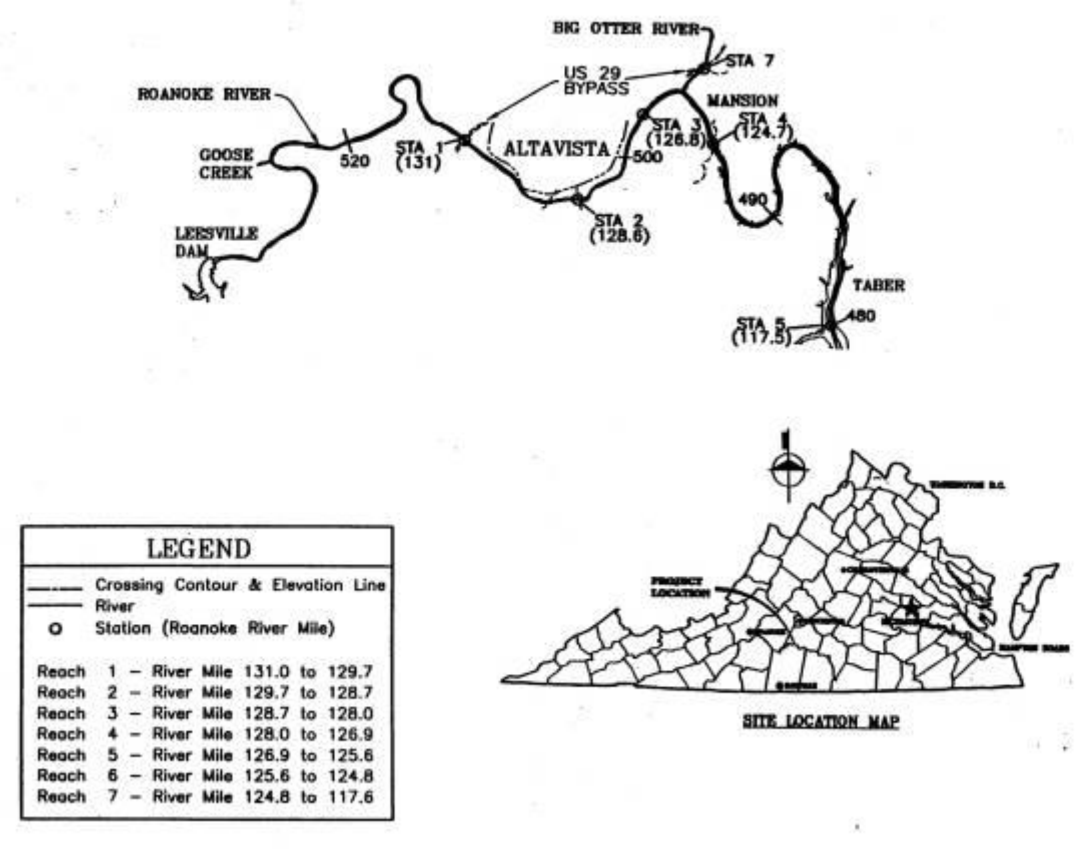
- A theoretical representation of prototype processes
- Incorporating some prior observations drawn from field and laboratory data
- Relating external inputs or forcing functions to system variable responses

Understanding CBOD Removal and Deoxygenation Rates in Streams



BOD/DO Modeling of the Roanoke River

$$\gamma = 10138 \frac{(DO_{mix})^{1.094} Q^{0.864} S^{0.06}}{T^{1.423} (DO_{sag})^{1.474}}$$

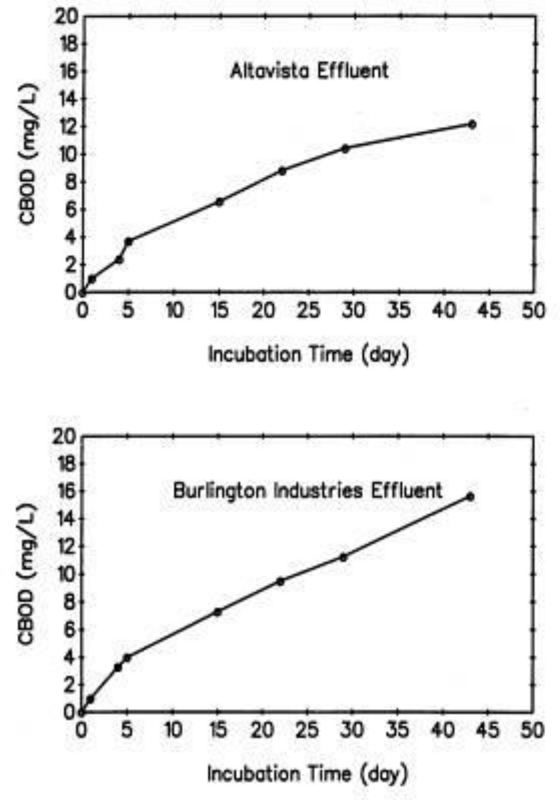


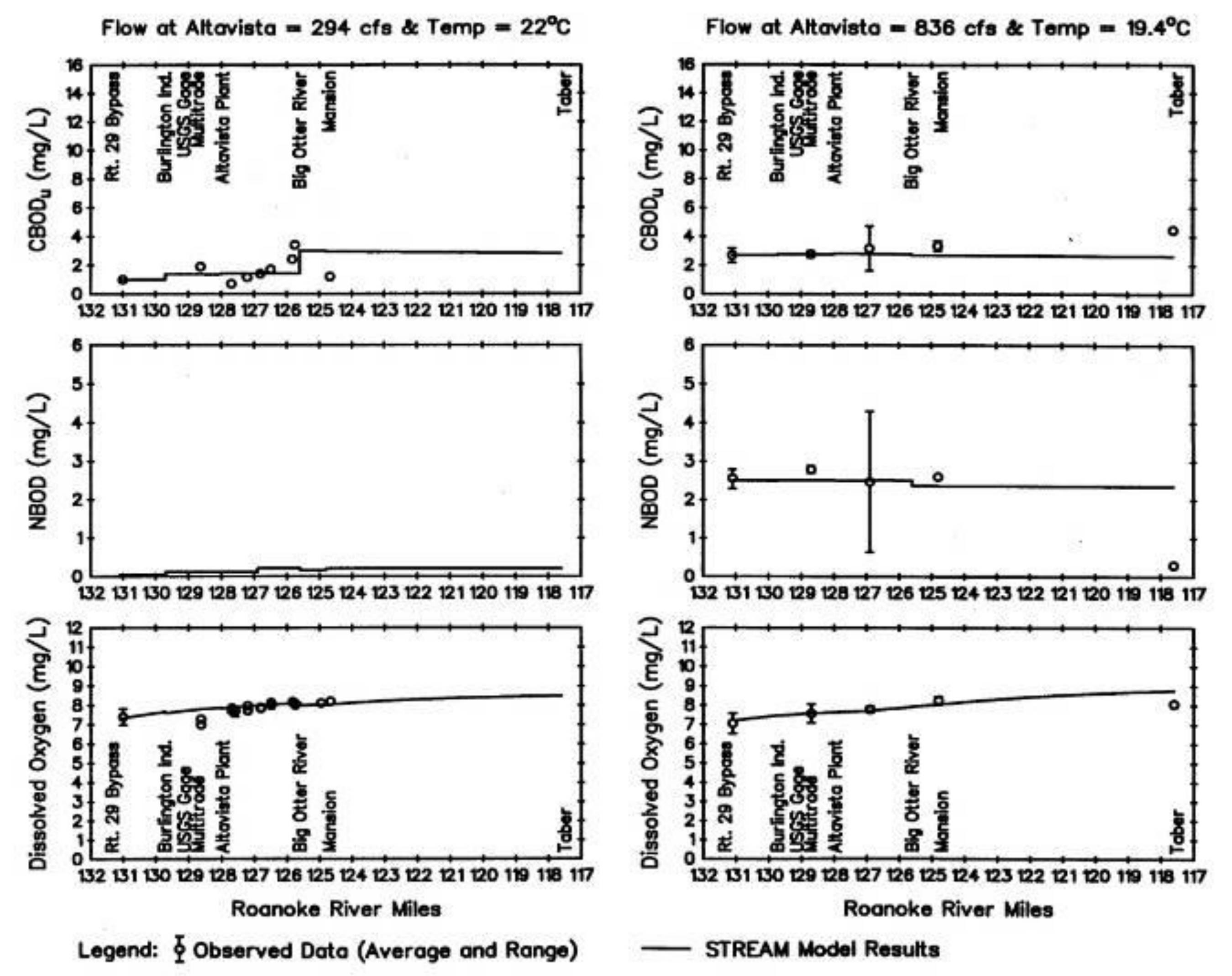
LEGEND

- Crossing Contour & Elevation Line
- River
- ○ Station (Roanoke River Mile)

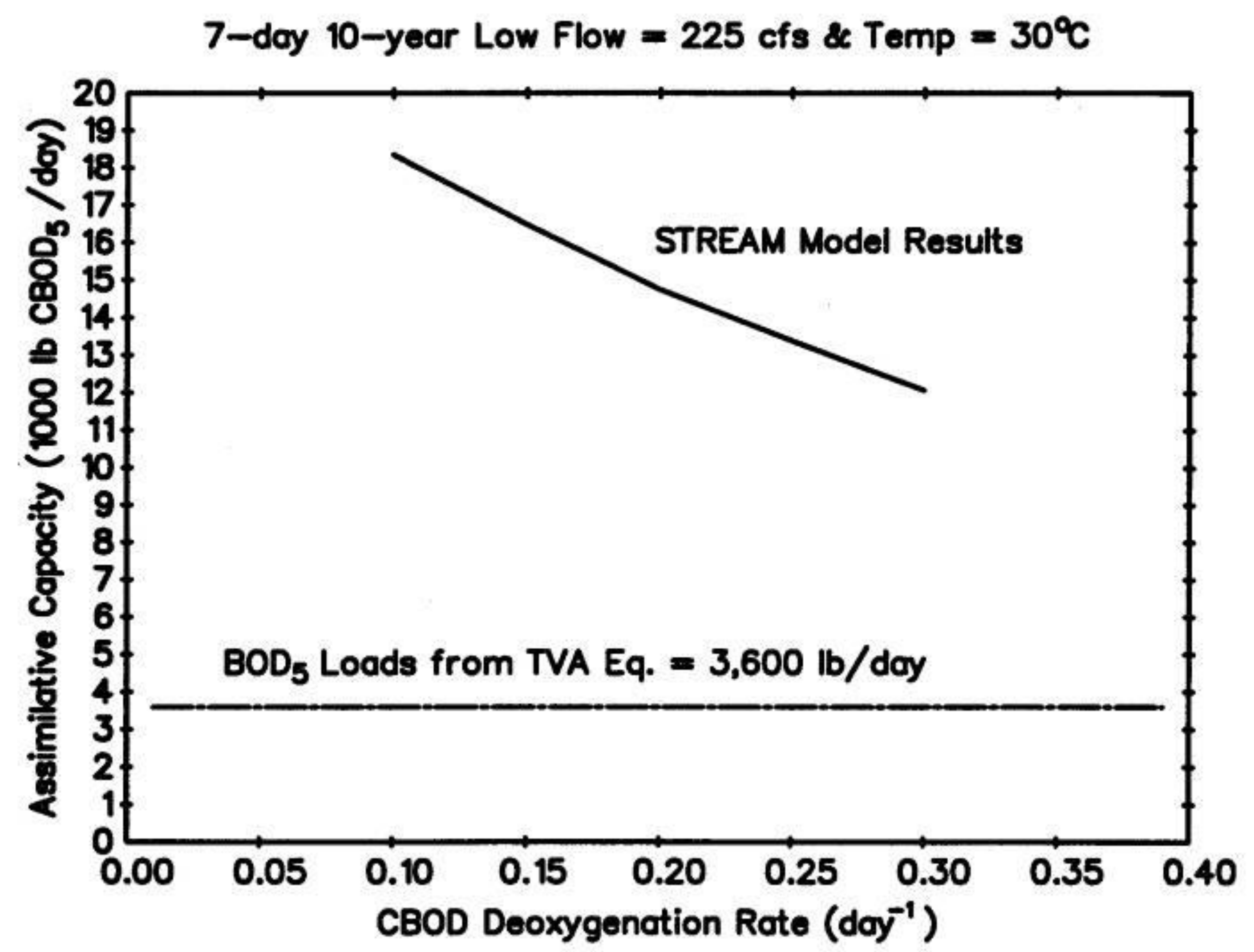
Reach 1 – River Mile 131.0 to 129.7
Reach 2 – River Mile 129.7 to 128.7
Reach 3 – River Mile 128.7 to 128.0
Reach 4 – River Mile 128.0 to 126.9
Reach 5 – River Mile 126.9 to 125.6
Reach 6 – River Mile 125.6 to 124.8
Reach 7 – River Mile 124.8 to 117.6

New Data to Support Modeling for Water Quality Management





Assimilative Capacity vs. CBOD Deoxygenation Rate



Comparing Reaeration Coefficients for Shirtee Creek, Alabama

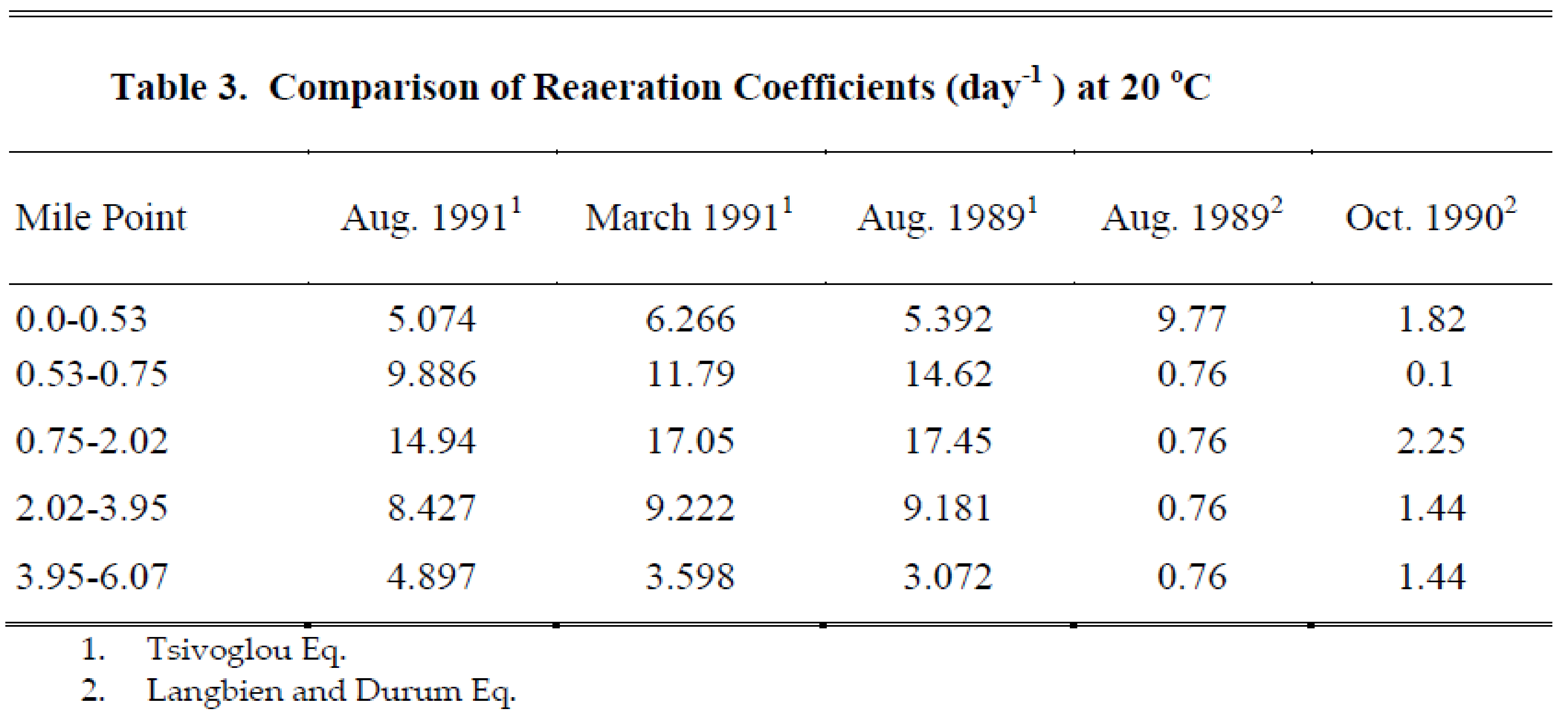


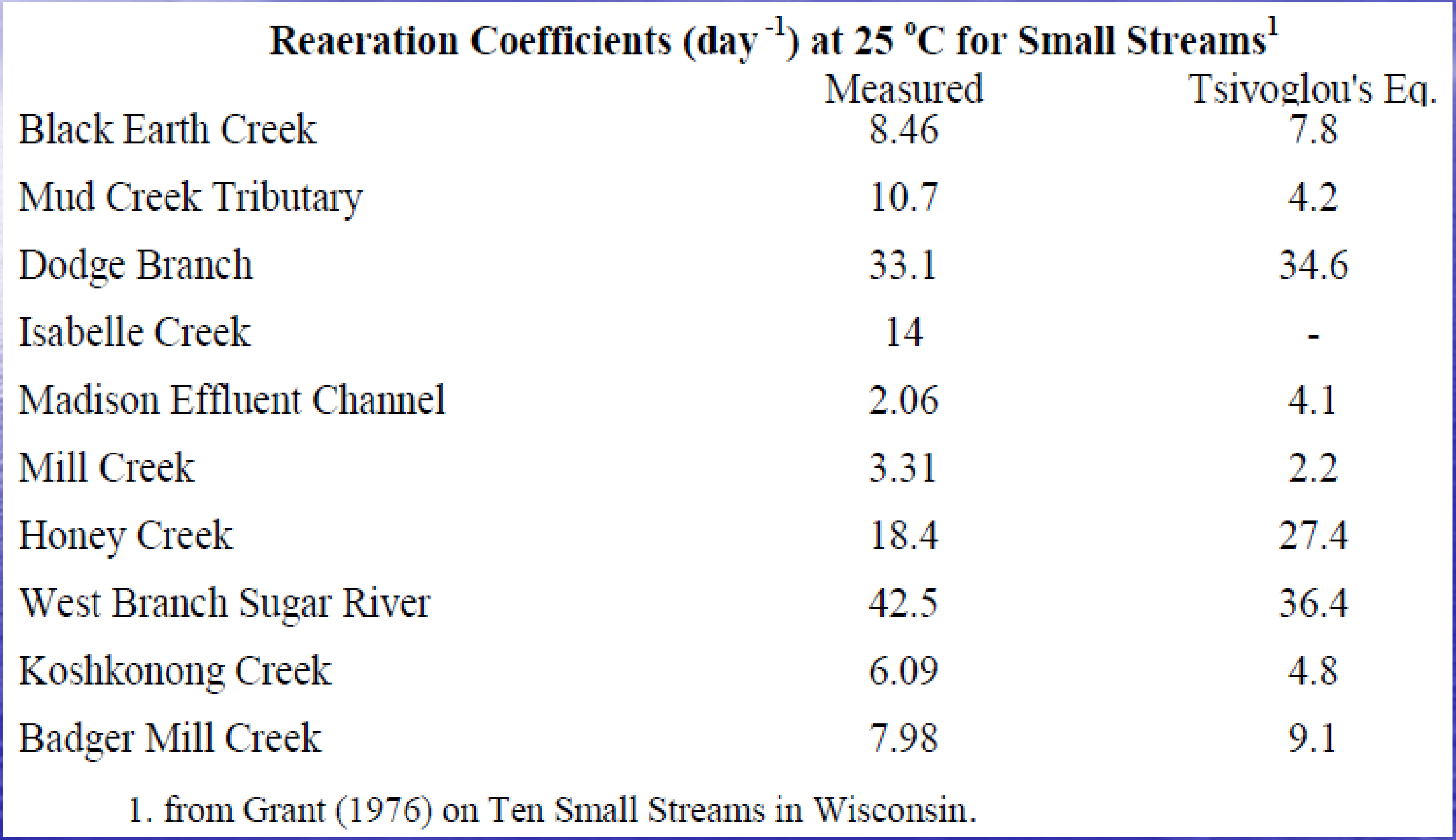
Table 3. Comparison of Reaeration Coefficients (day^{-1}) at 20 °C

Mile Point	Aug. 1991[1]	March 1991[1]	Aug. 1989[1]	Aug. 1989[2]	Oct. 1990[2]
0.0-0.53	5.074	6.266	5.392	9.77	1.82
0.53-0.75	9.886	11.79	14.62	0.76	0.1
0.75-2.02	14.94	17.05	17.45	0.76	2.25
2.02-3.95	8.427	9.222	9.181	0.76	1.44
3.95-6.07	4.897	3.598	3.072	0.76	1.44

1. Tsivoglou Eq.
2. Langbien and Durum Eq.

Alabama Department of Environmental Management (ADEM) Used L&D Eq. in their Wasteload Allocation Model, Resulting in Very Stringent Effluent Limits for the Point Source. The L&D Eq. Proved to be Inappropriate for This Shallow Water. The Tsivoglou Eq. Should Have Been Used Instead!!

Testing the Tsivoglou Equation

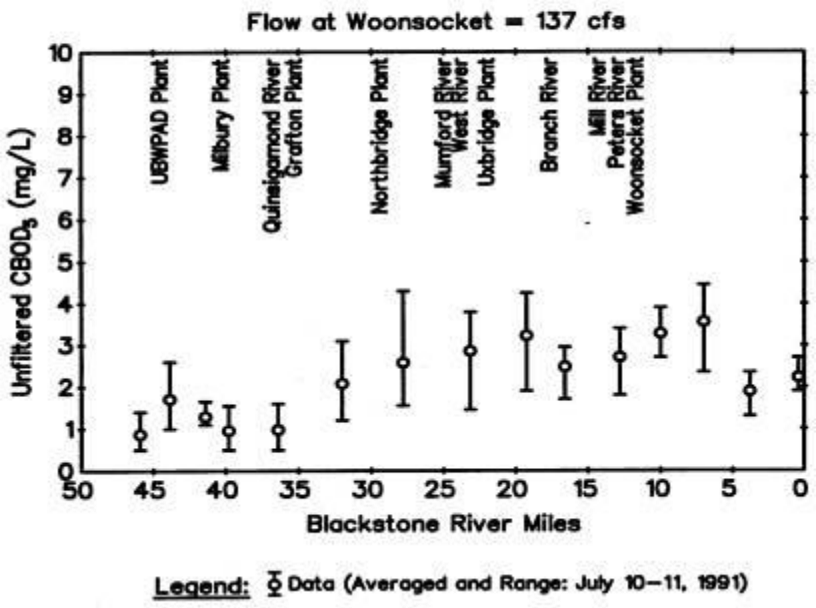


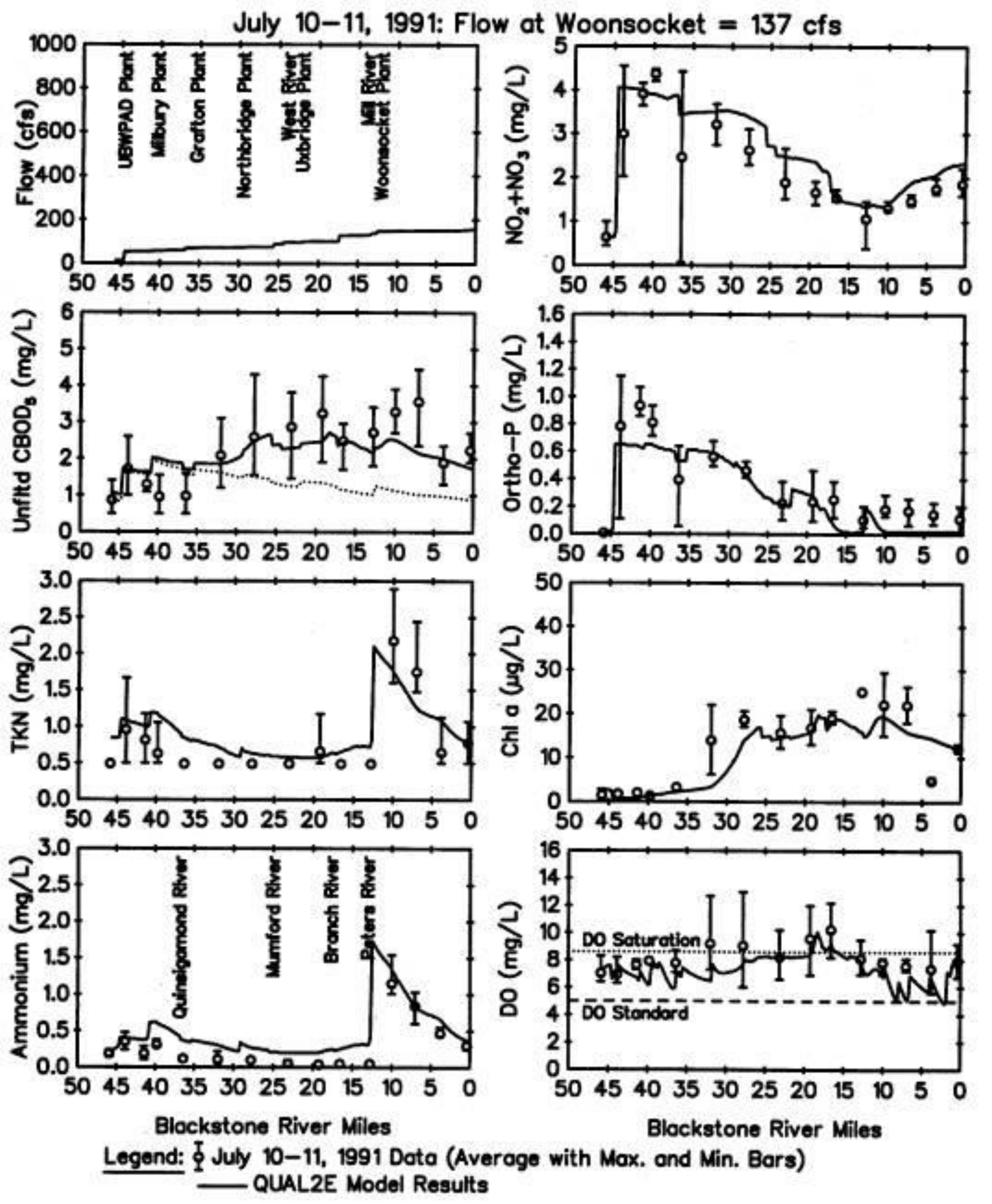
Reaeration Coefficients (day^{-1}) at 25 °C for Small Streams[1]

	Measured	Tsivoglou's Eq.
Black Earth Creek	8.46	7.8
Mud Creek Tributary	10.7	4.2
Dodge Branch	33.1	34.6
Isabelle Creek	14	-
Madison Effluent Channel	2.06	4.1
Mill Creek	3.31	2.2
Honey Creek	18.4	27.4
West Branch Sugar River	42.5	36.4
Koshkonong Creek	6.09	4.8
Badger Mill Creek	7.98	9.1

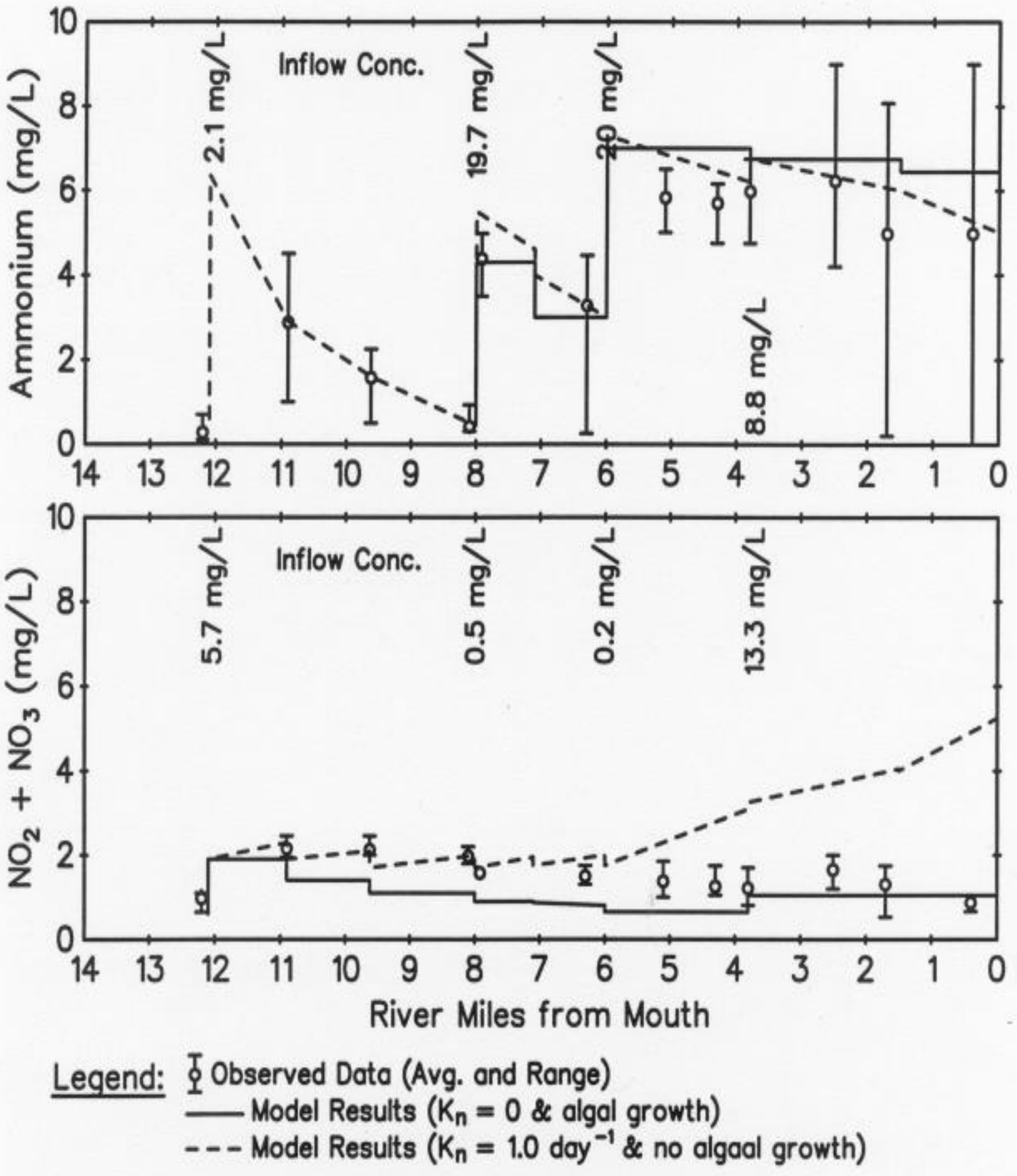
1. from Grant (1976) on Ten Small Streams in Wisconsin.

BOD/DO Modeling of the Blackstone River

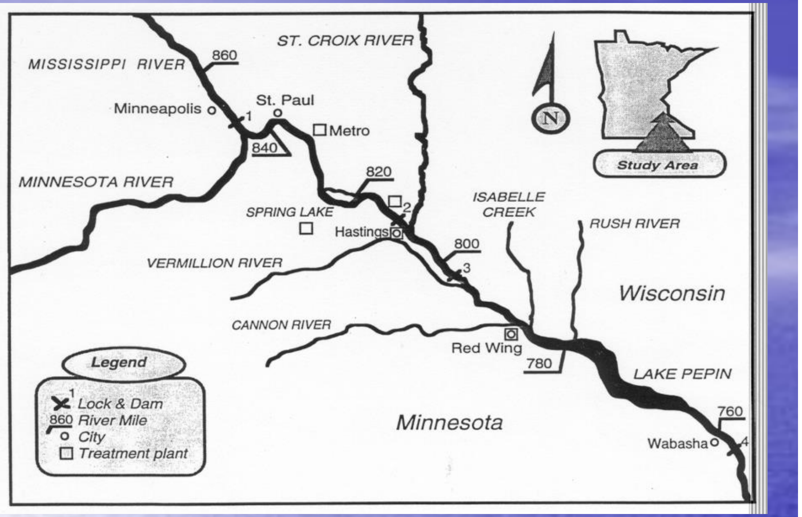




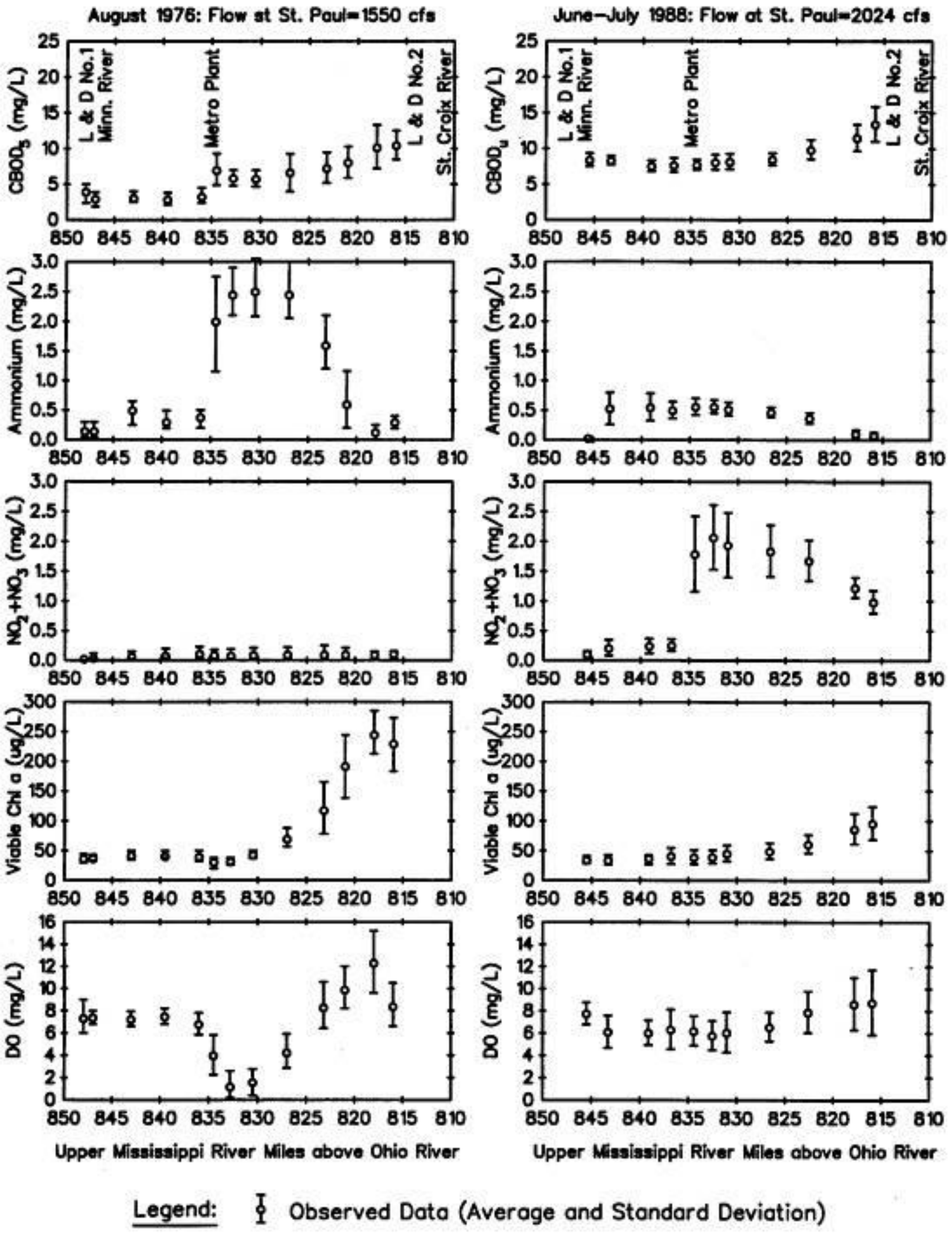
Trying to Justify Nitrification Process with Model Results



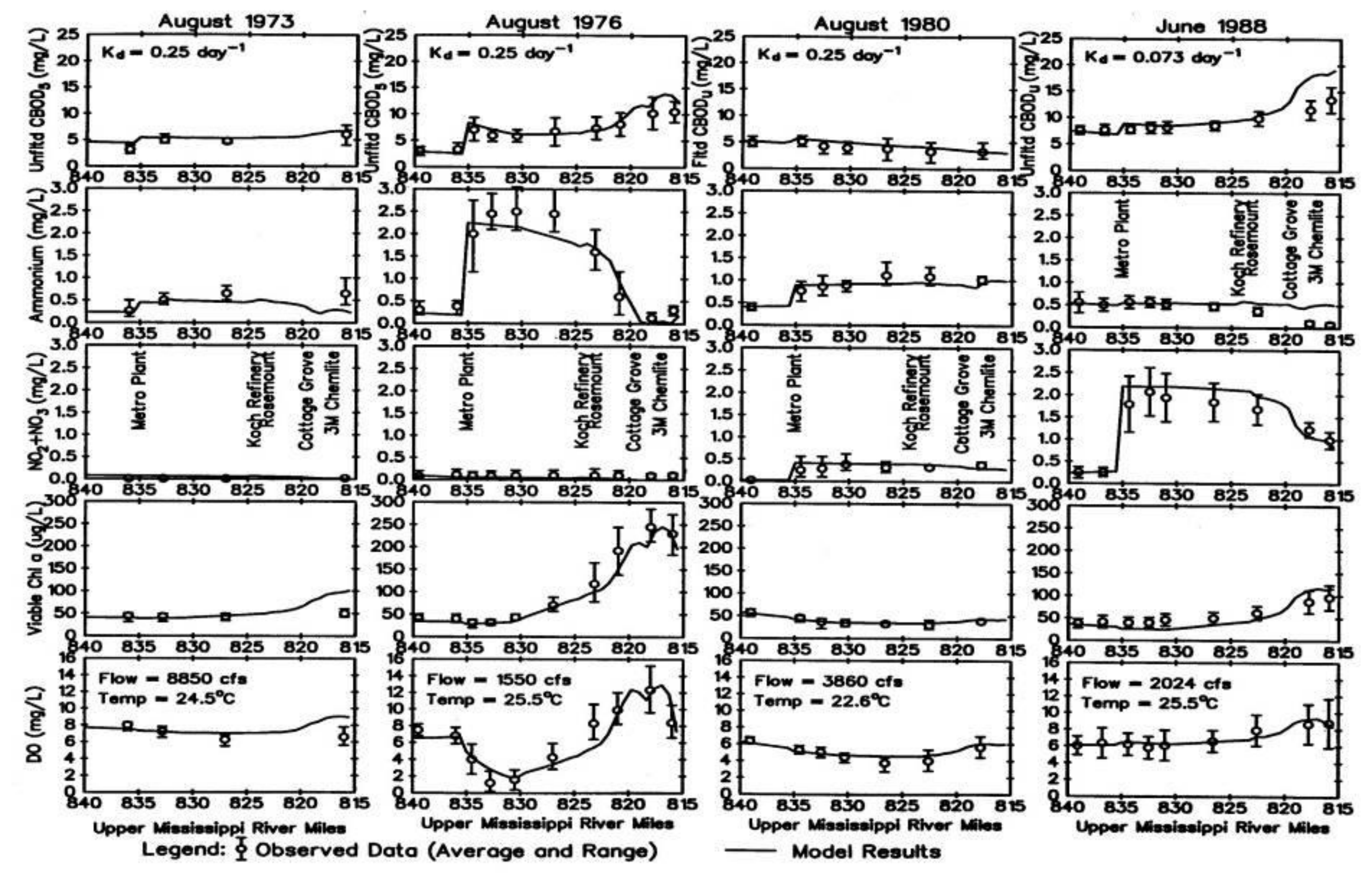
The Upper Mississippi River



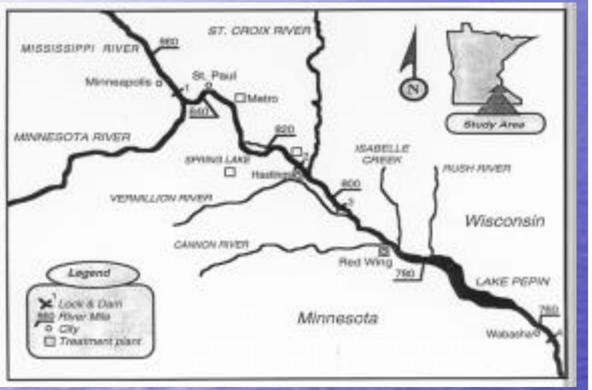
A BOD/DO Model Was Developed, Calibrated, and Verified to Design the Nitrification Process at the Metro Plant. The Regulatory Agency Required that a Model Post-Audit be Performed under Low Flow Conditions. Finally, the Summer 1988 Presented a Ideal Low Flow for the Model Post-Audit Analysis.



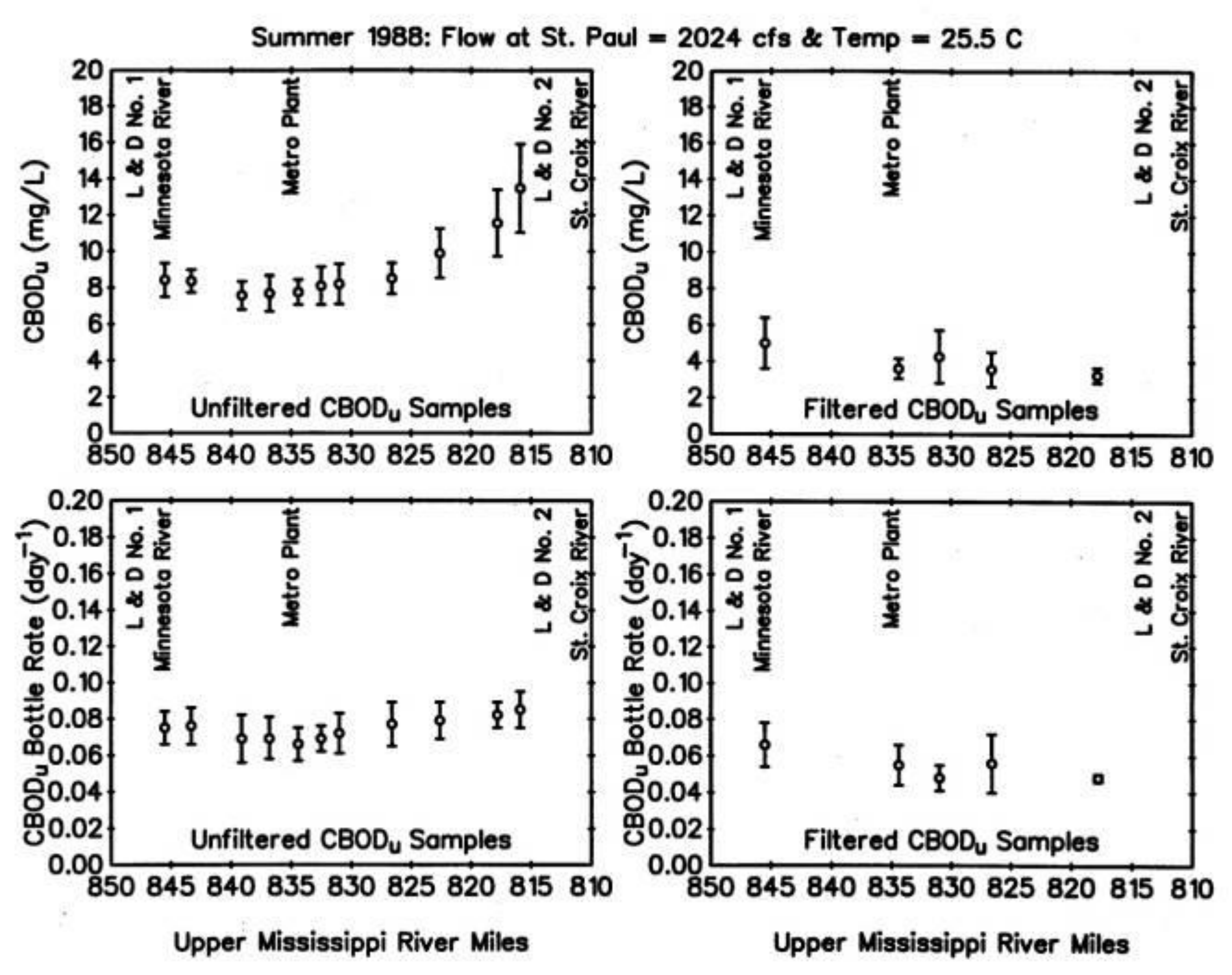
Post-Audit of the Upper Mississippi River BOD/DO Model



CBOD (Filtered and Unfiltered) Conc. And CBOD Bottle Rate

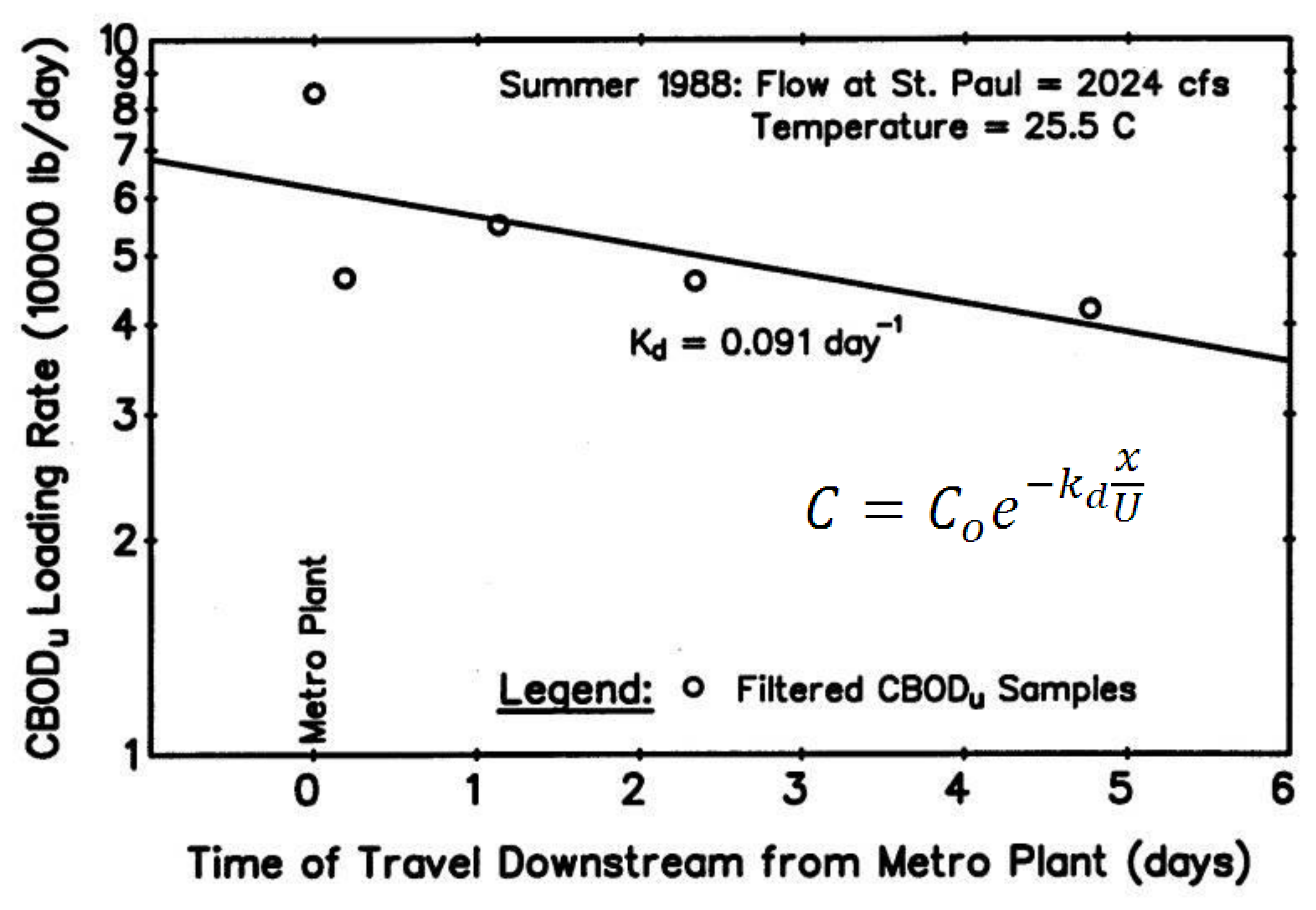


Unfiltered CBOD Levels Increase and Filtered CBOD Levels Decrease in the Downstream Direction


Summer 1988: Flow at St. Paul = 2024 cfs & Temp = 25.5 C

Deriving CBOD Deoxygenation Rate

TO ACCOUNT FOR TRIBUTARY INFLOWS, USE CBOD LOADS!!



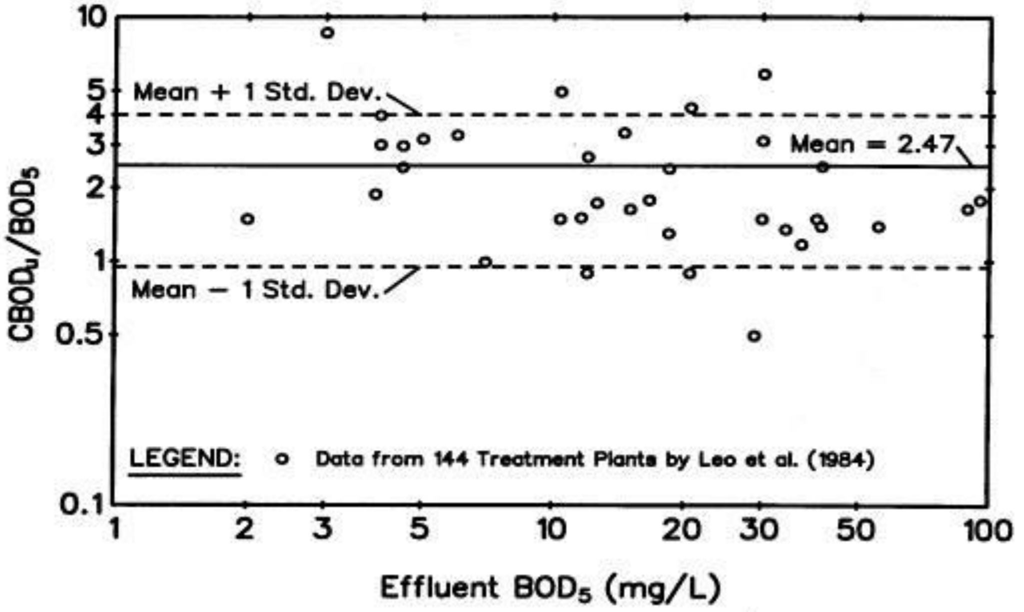
$$C = C_o e^{-k_d \frac{x}{U}}$$

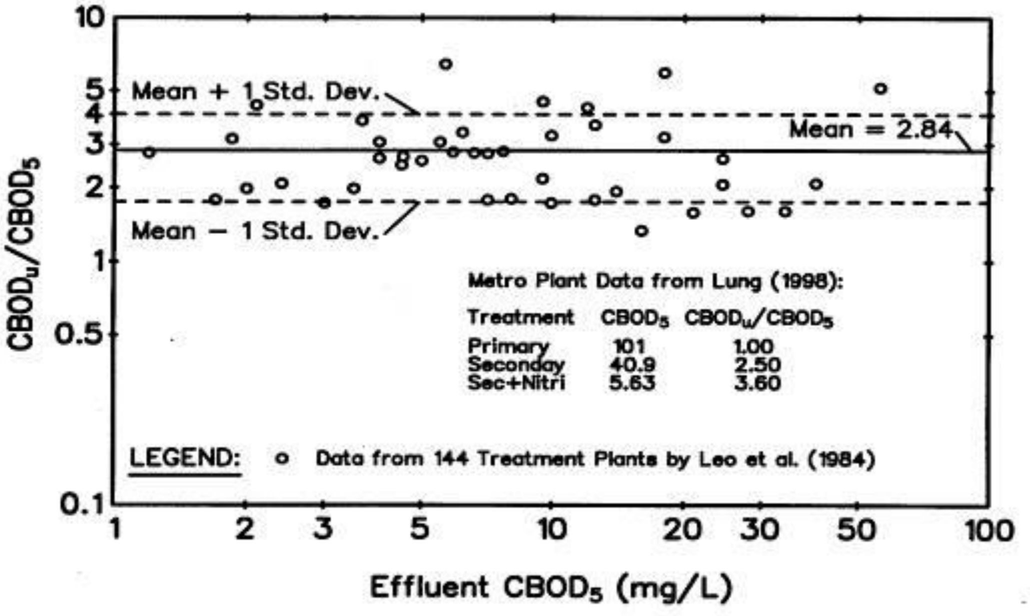
CBOD$_u$ to CBOD$_5$ Ratio in Wastewater

$$y = L_u(1 - e^{-kt})$$

$$\frac{CBOD_u}{CBOD_5} = \frac{1}{1 - e^{-(k_1)(5)}}$$

Note the Increase of CBOD$_u$ to CBOD$_5$ Ratio with Treatment Upgrade at the Metro Plant (Lung, 1988).
K Rates Also Decrease with Treatment Upgrade!!!!

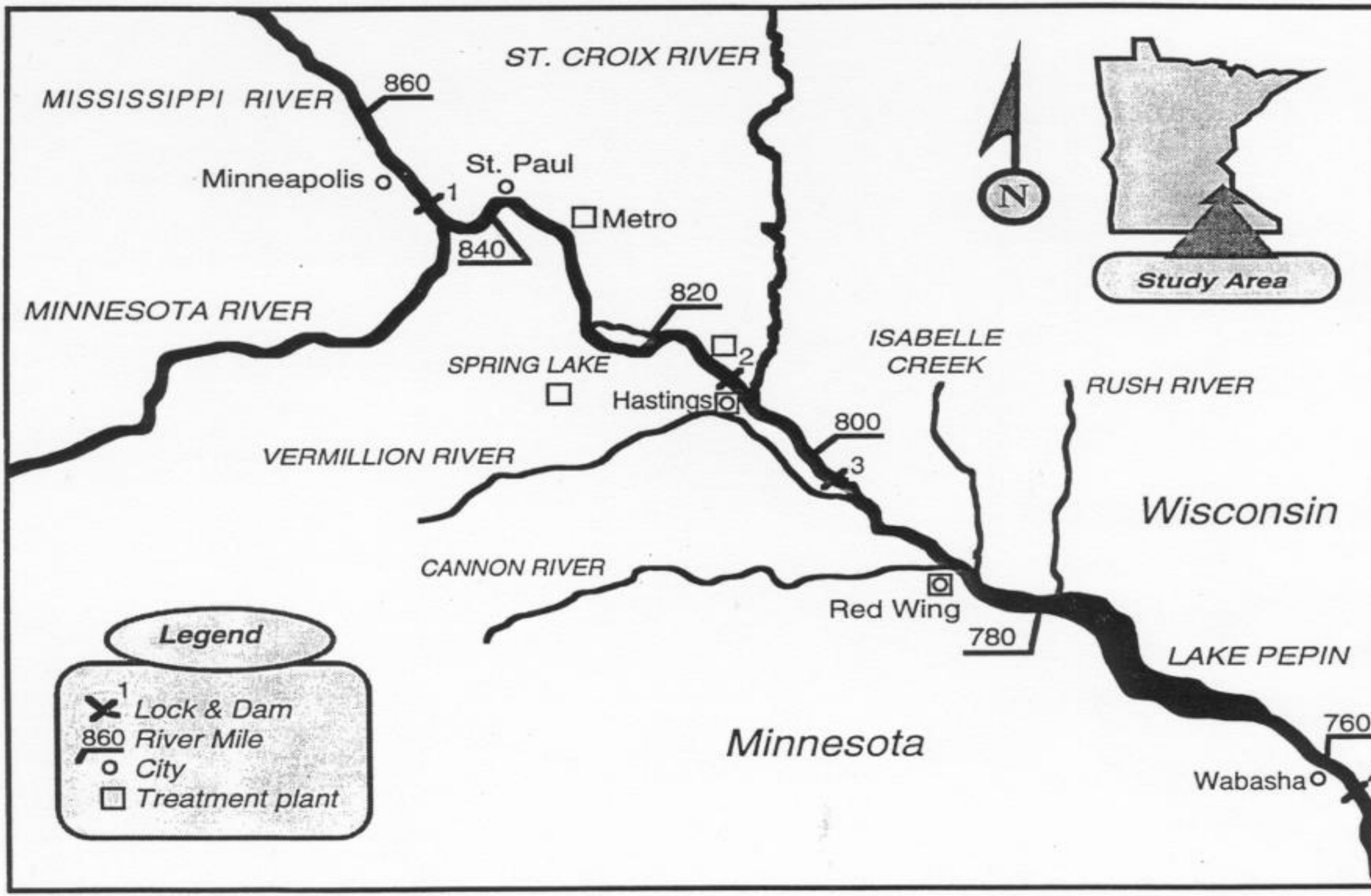




Metro Plant Data from Lung (1998):

Treatment	CBOD$_5$	CBOD$_u$/CBOD$_5$
Primary	101	1.00
Seconday	40.9	2.50
Sec+Nitri	5.63	3.60

Numerical Tagging of Phosphorus in Lake Pepin



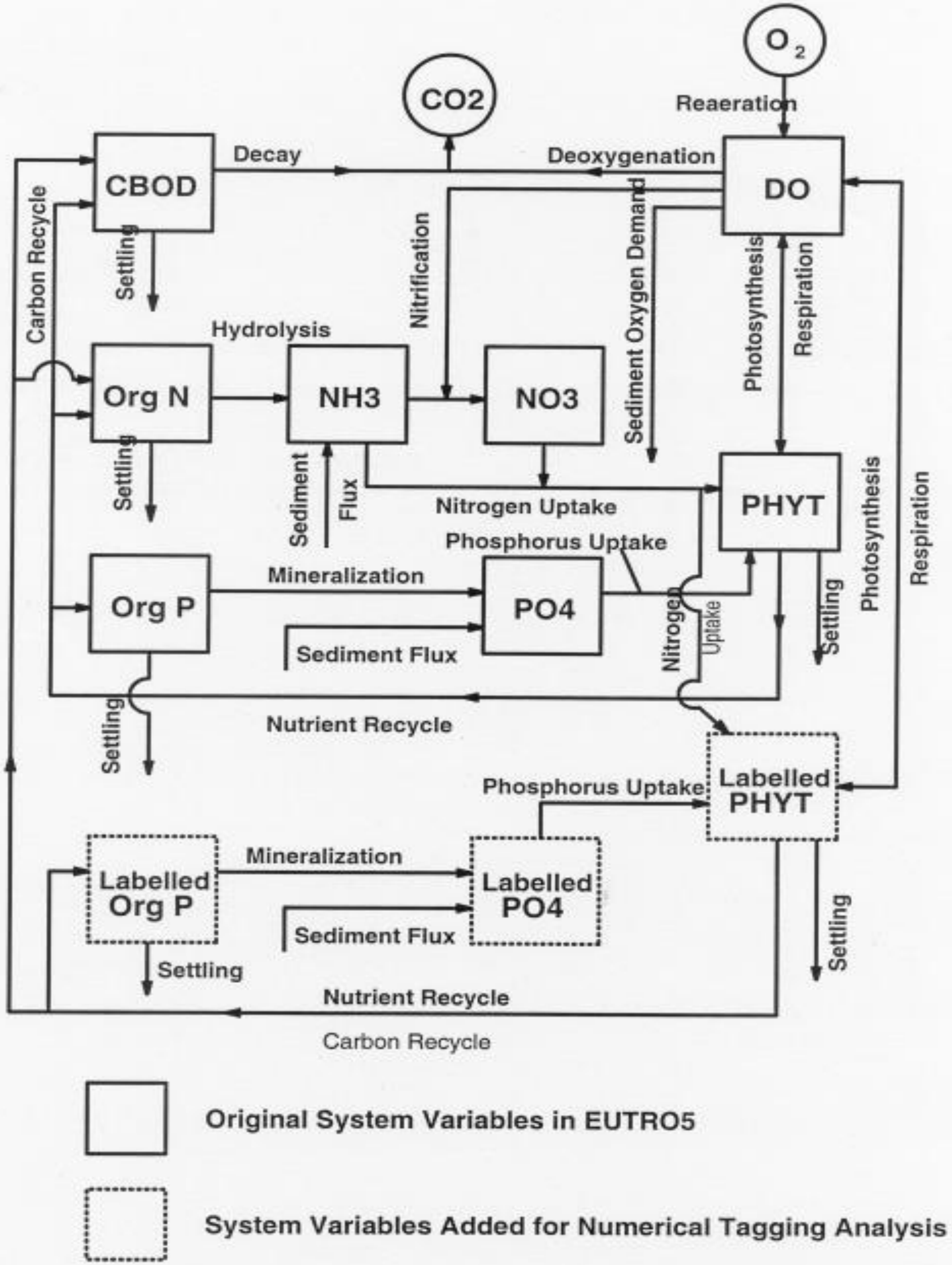
Fate and Transport of Phosphorus from the Metro Plant

- Model (WASP/EUTRO) Results Show That Phosphorus Load Reduction at the Metro Plant Would Have a Minimal Effect on Reducing the Algal Biomass in Lake Pepin.
- To What Extent Is Phosphorus from the Metro Plant Transported to Lake Pepin under Both Existing and Potential Reduced Phosphorus Loading Conditions?
- More Specifically, What Portion of Phosphorus in the Algal biomass in Lake Pepin Is from the Metro Plant?

Numerical Tagging Analysis

- Simple Component Analysis Routinely Performed in BOD/DO Modeling Does Not Work.
- The Eutrophication Model Has Nonlinear Structure for Algal Growth Kinetics (i.e., Temperature, Light, and Nutrient Effects).
- Similar to the $^{32}PO_4$ Technique That Limnologists Use in Tracking Phosphorus in Natural Water Systems by Measuring the Amount of $^{32}PO_4$ in Various Phosphorus Compartments.
- The Numerical Tagging Analysis Requires That the EUTRO Model be Modified to Enable Phosphorus Loads from Individual Sources Such as the Metro Plant to be Numerically Labeled and Tracked Separately from Other Phosphorus Sources.

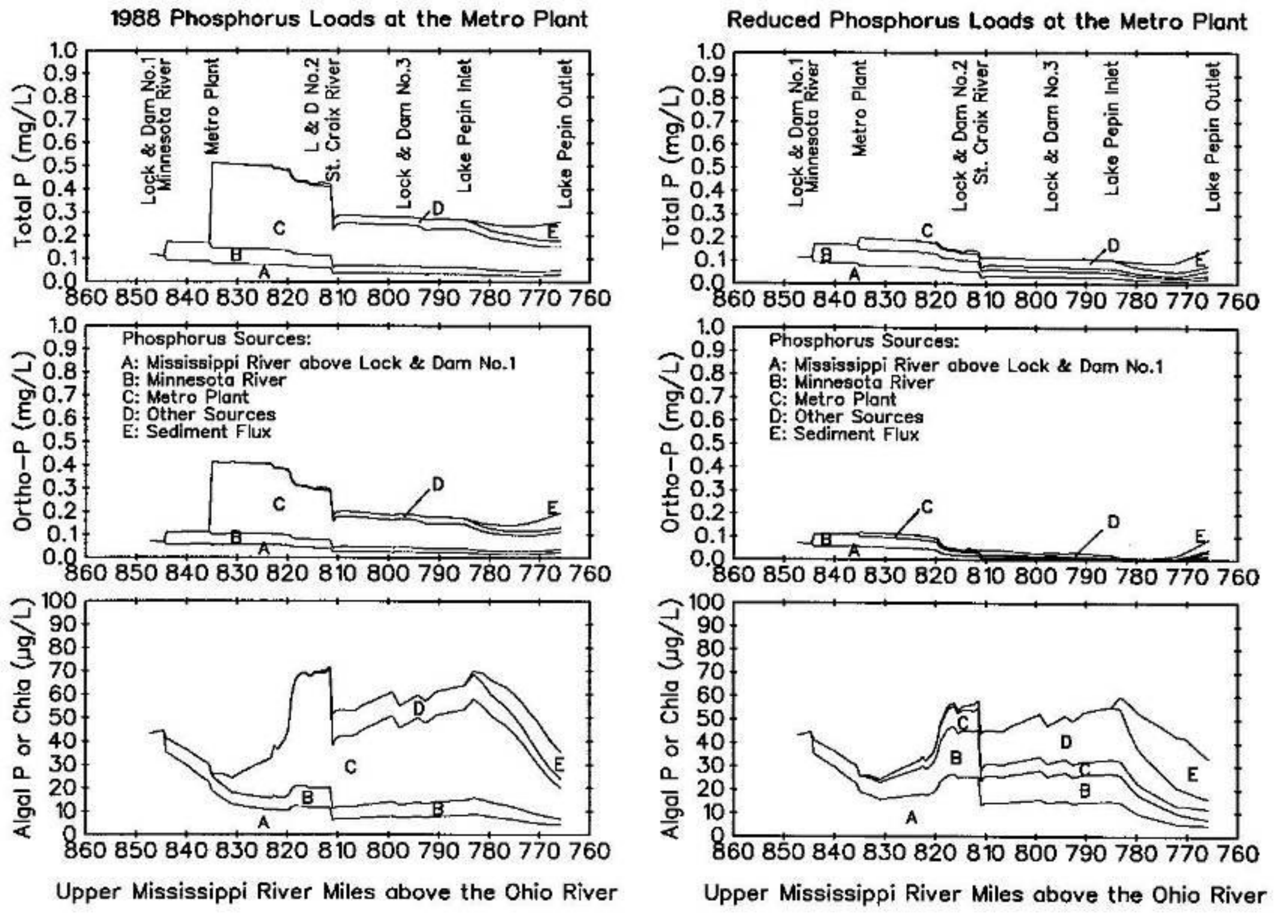
Modified EUTRO5 Kinetics for Numerical Tagging of Lake Pepin



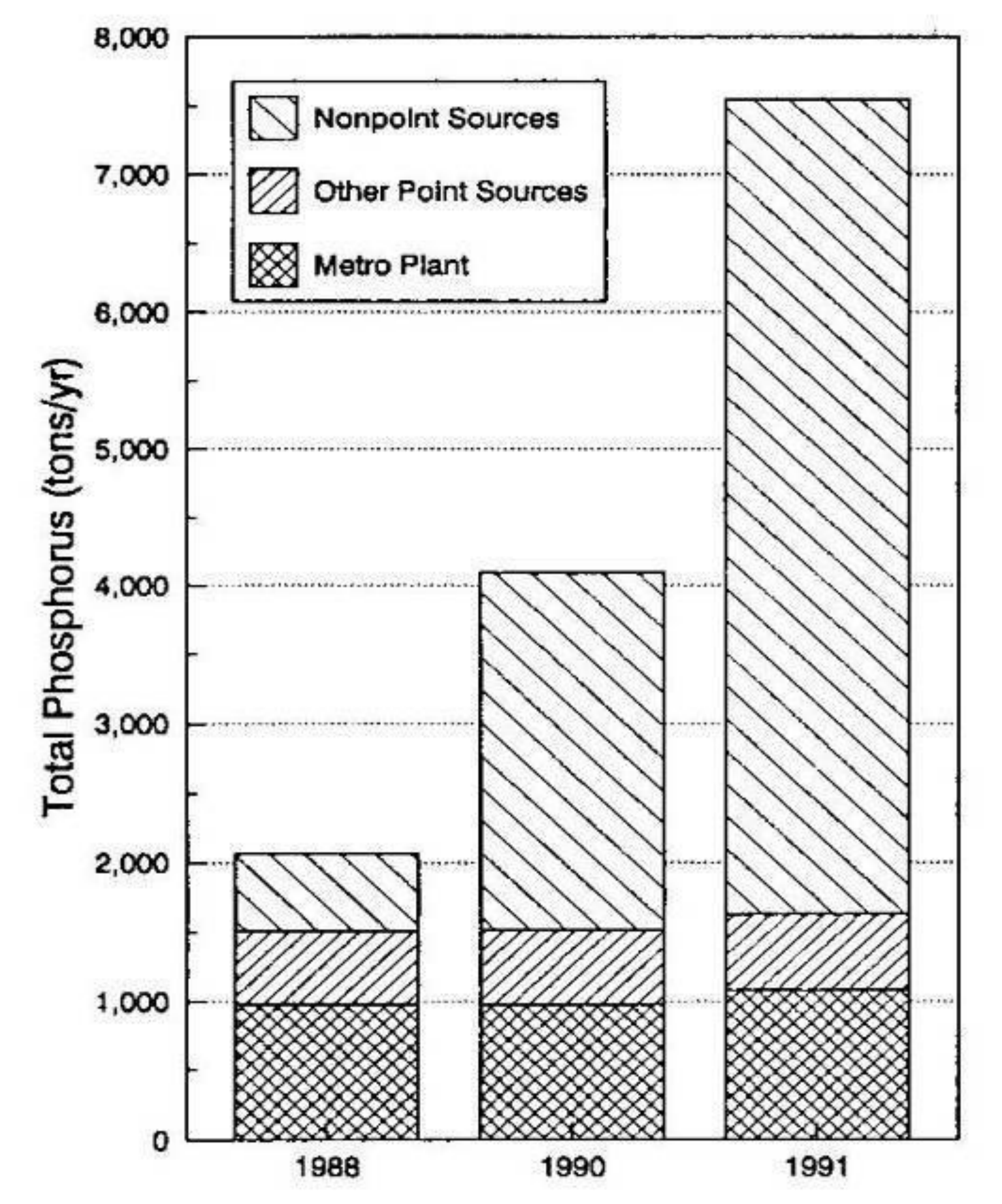
Numerical Tagging Analysis

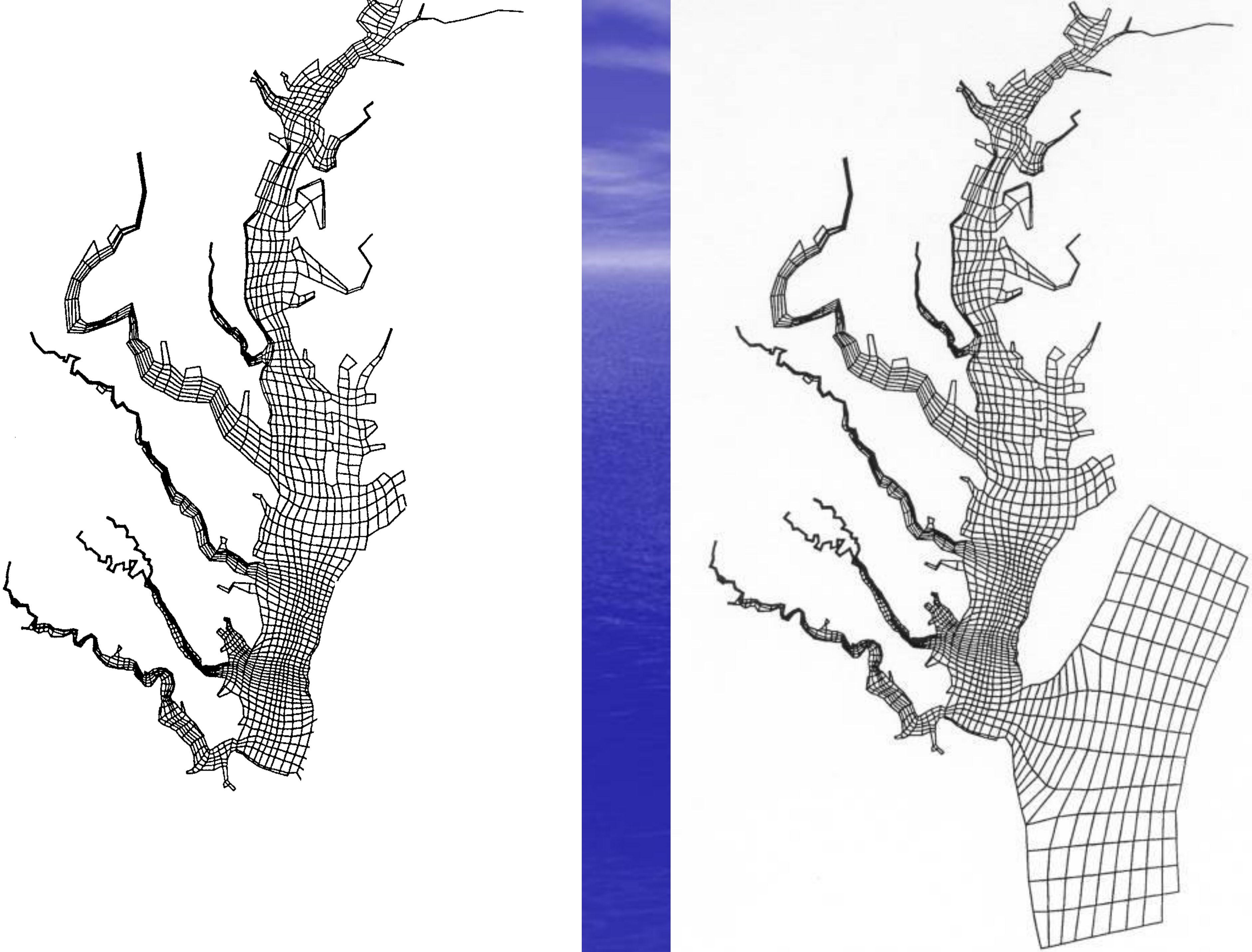
- Additional System Variables: Labeled Orthophosphate, Labeled Nonliving Organic Phosphorus, and Labeled Phytoplankton
- Algal Growth Rates Must Be Calculated Based on the Combined Concentration of Labeled and Unlabeled Orthophosphate
- Labeled Phosphorus Cycles among the Labeled Compartments but Undergoes the Same Rate (Mineralization, Settling, etc.) as Unlabeled Phosphorus
- Only When Calculating the Algal Growth and Phosphorus Uptake Rates Do the Labeled and Unlabeled Systems Need to Communicate and Correctly Proportion the Increase in Algal Biomass and the Decrease in Orthophosphate between the Two Systems

Model Results of Numerical Tagging for Lake Pepin

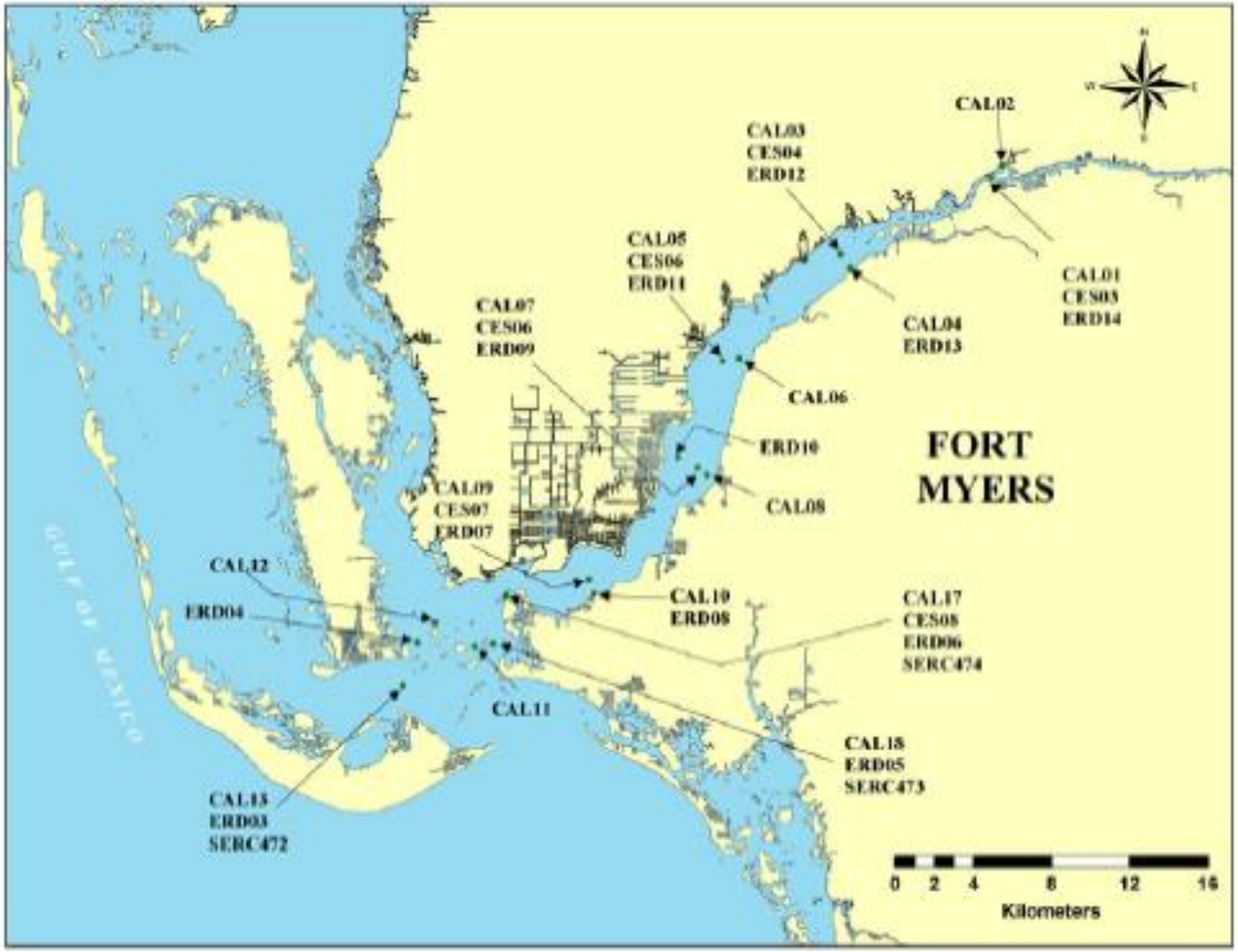


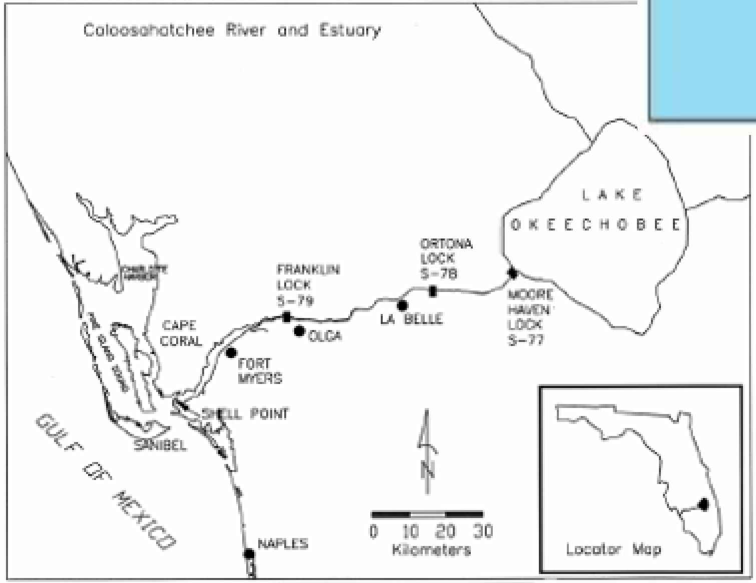
Annual Total Phosphorus Loads to Lake Pepin



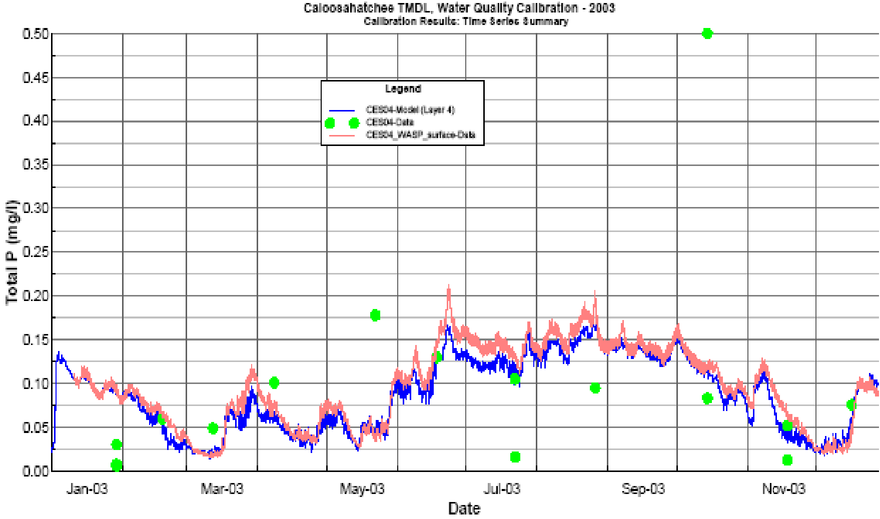


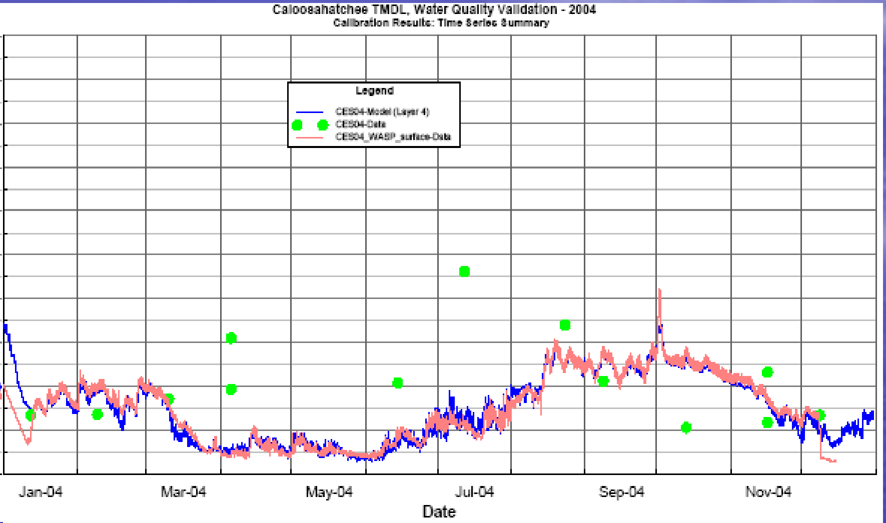
Lake Okeechobee and Caloosahatchee River

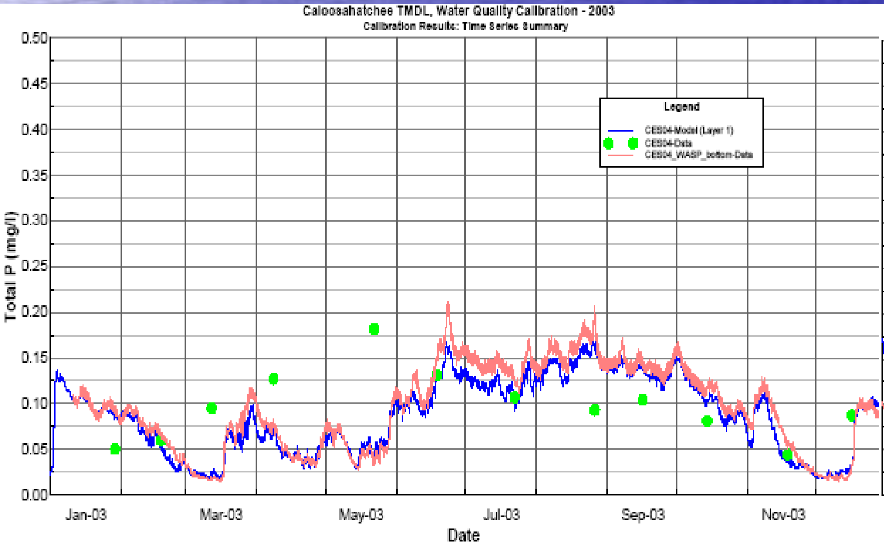


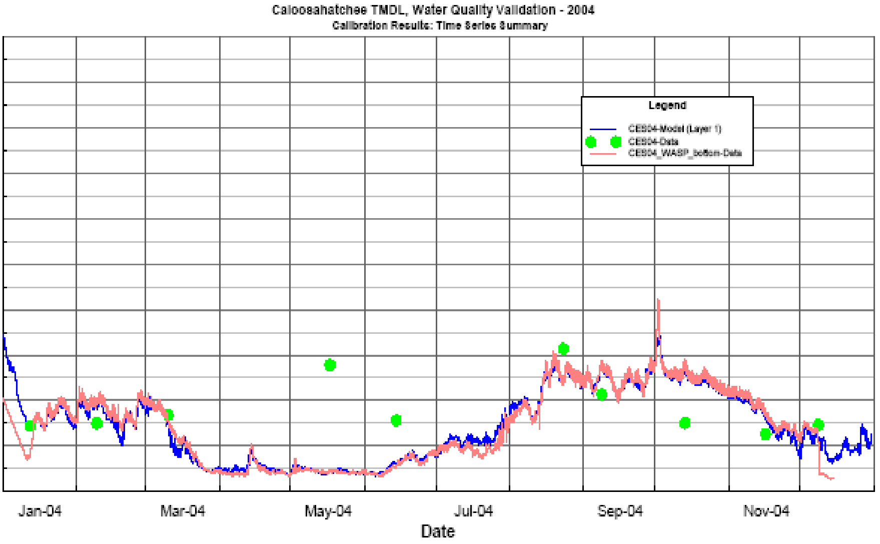


Resetting Initial Conditions – Caloosahatchee River Estuary, FD





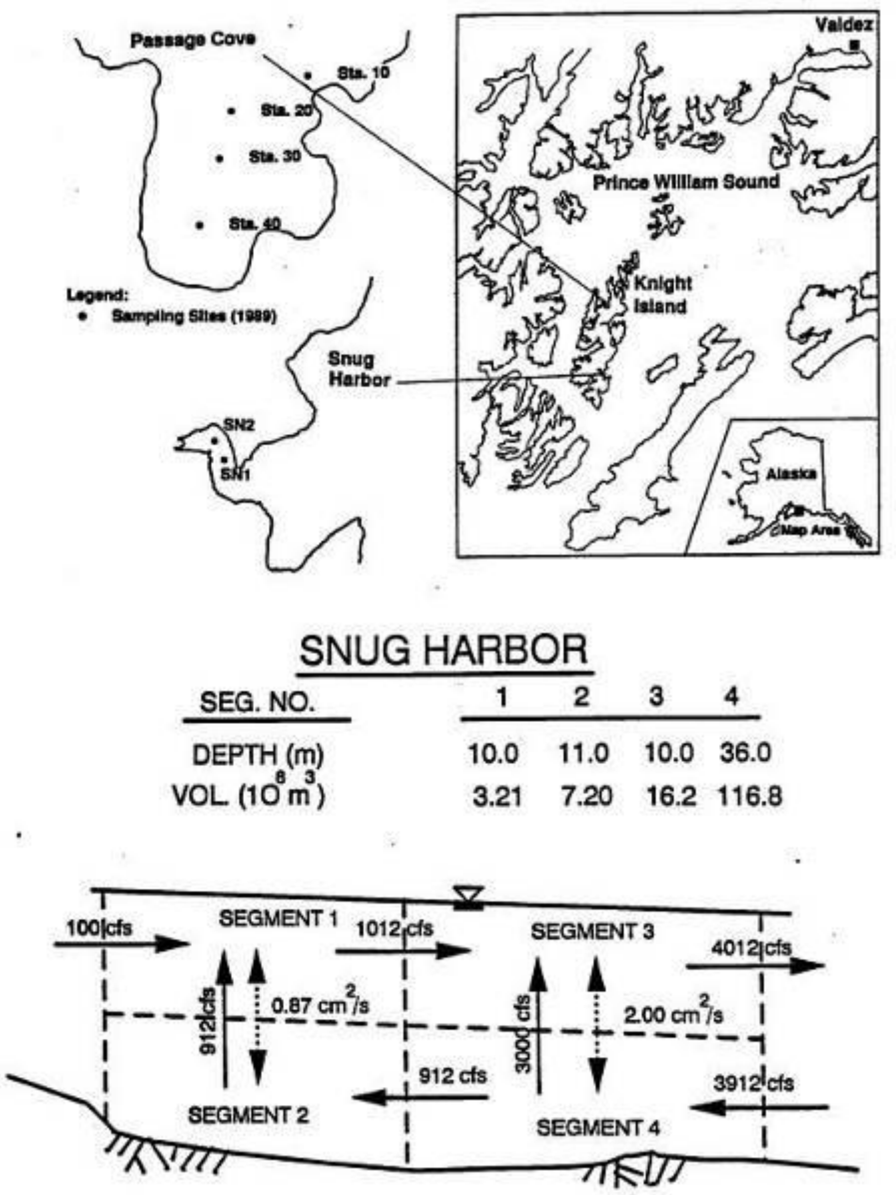




Steady State Applications

EXXON Valdez Oil Spill

1. WASP/EUTRO Model Configured to Simulate Impact of Chemical Applications in Bioremediation following the Oil Spill in 1989
2. Limited Field Data Available
3. Algal Growth Not Predicted Due to Significant Mixing at Open Boundaries



SNUG HARBOR

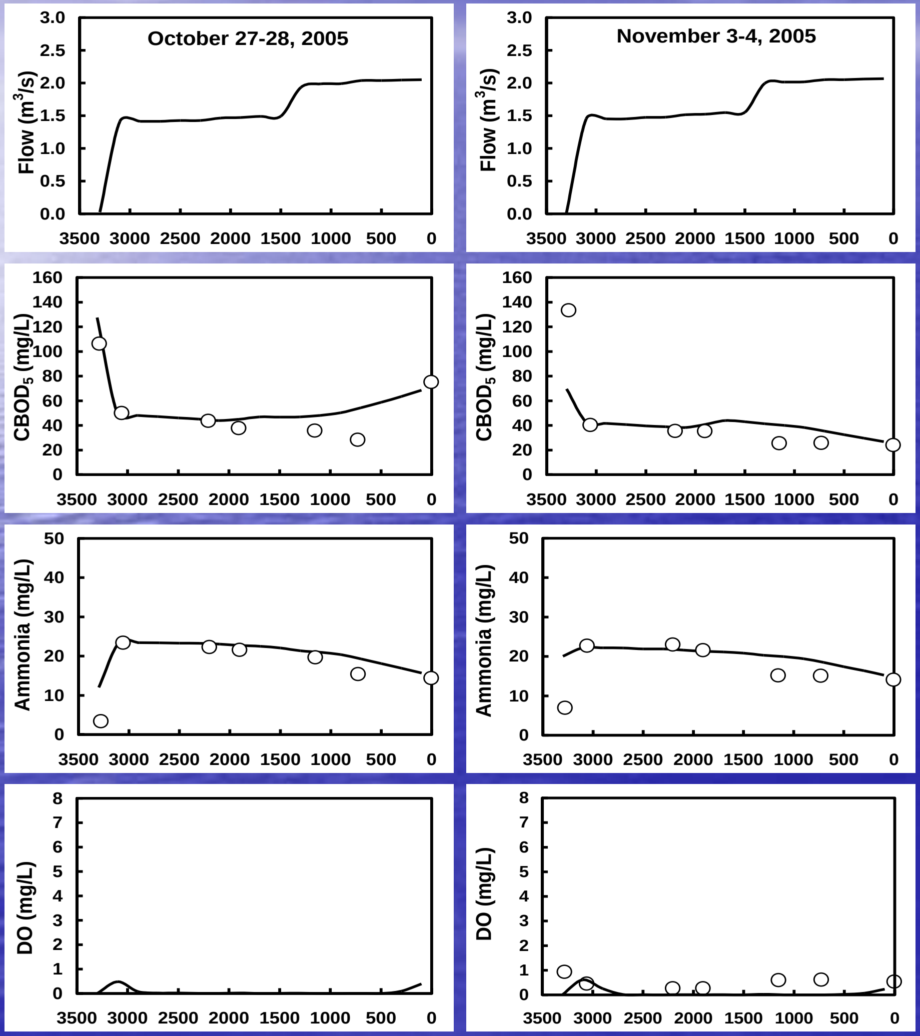
SEG. NO.	1	2	3	4
DEPTH (m)	10.0	11.0	10.0	36.0
VOL. (10^6 m^3)	3.21	7.20	16.2	116.8

Lung et al. (1993) *Journal of Environmental Engineering*, 119(5): 811-824.

Steady State Applications

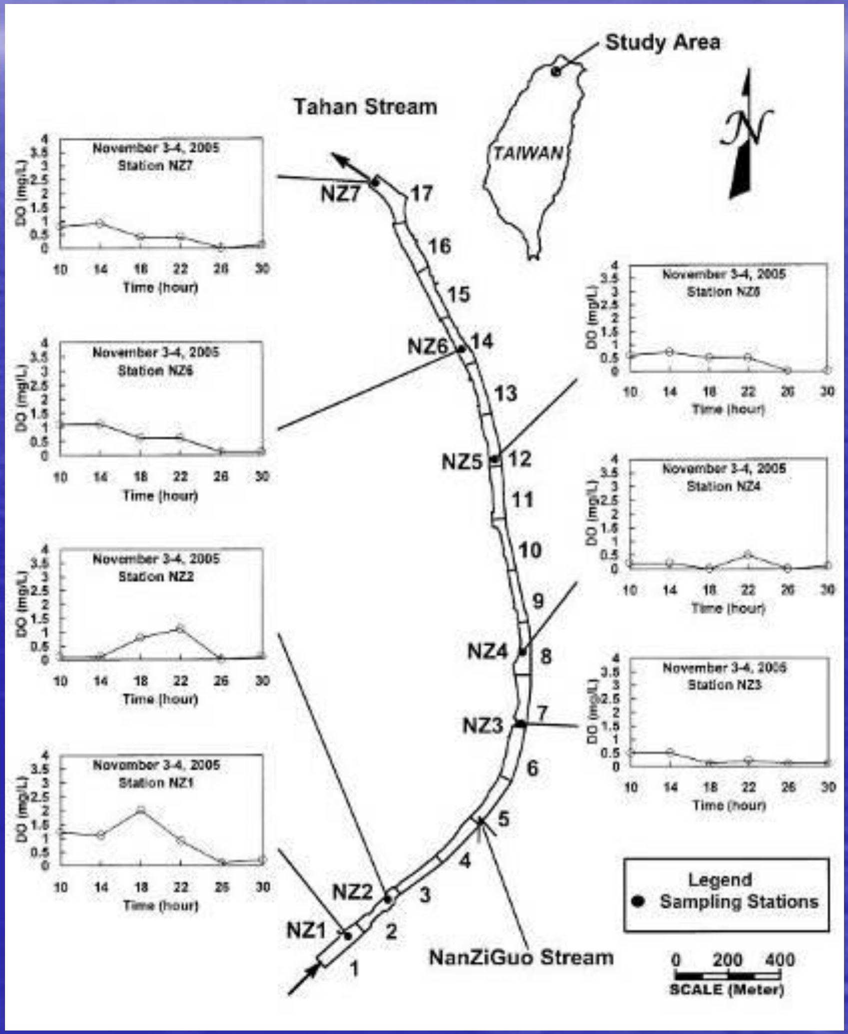
NanZiGuo, Taipei County

Temperature at upstream = 31.3°C Temperature at upstream = 29.8°C

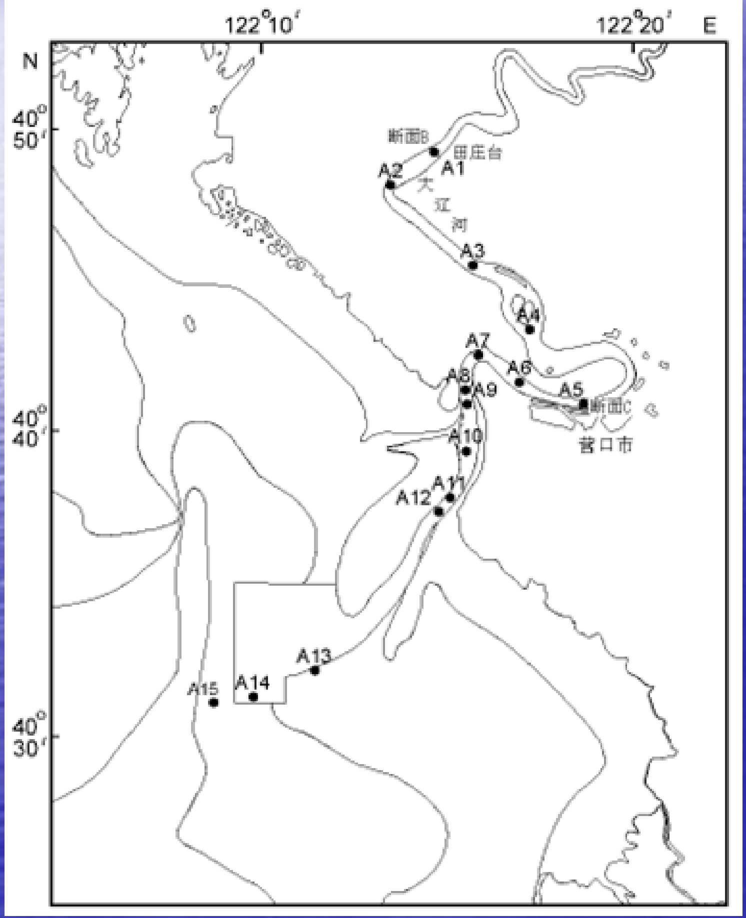


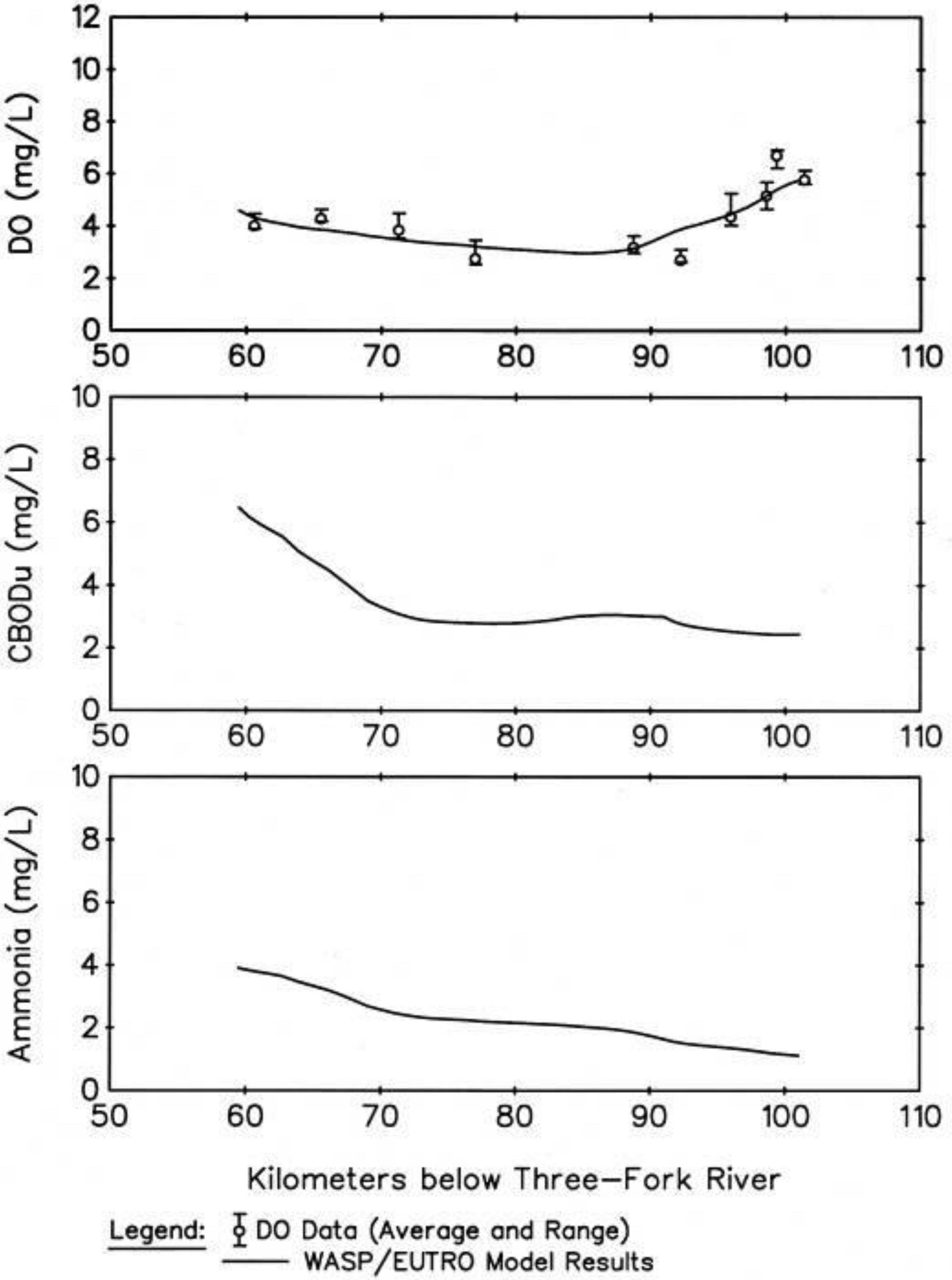
NanZiGuo Stream Meters NanZiGuo Stream Meters

Legend: ○ Observed Data — Water Quality Model Results



BOD/DO Modeling of the Liaohe River Using WASP/EUTRO





Selecting a Model

- Model…Necessary?
- Which One?
- Simple One? Complex One?
- Focus on What?
- Model & Management?
- Model to Public?
- Customized?
- How Do You Know Your Results are Right?

淡水河系水質模式評選原則

適用水體	• 適用淡水河系之河川、支流排放與感潮特性
模擬污染項目	• 具備模擬BOD、DO、SS、NH_3-N之能力
是否包含水理計算	• 水理模式須含斷面、流量、流速、水位等計算
穩態與動態模擬	• 具備動態模擬可演算長期趨勢與變化
程式碼是否公開	• 針對淡水河特性或需求調整演算結構或模組參數 • 版權問題與取得之方式
輸入資料複雜度	• 考量目標水體的資料掌握度，評估模擬結果可信度 • 模擬維度越高，資料量需求越大
已建立完成之水質模式	• 成功運用於淡水河或具相關運用經驗應優先考量

水質模式綜合評析

- WASP為USEPA公開之模式，具備模擬 1-D ~ 3-D動態或穩態下，感潮河段內四項水質項目之功能，模式可擴充性佳，於淡水河之應用經驗豐富。
- QUAL2K同為 USEPA 公開之模式，曾應用於淡水河，可模擬1-D穩態下感潮河段內四項水質項目。
- STREAM僅模擬1-D穩態BOD-DO，因使用解析解，使用者可自行撰寫模式，惟模擬項目少、較不具可擴充性，經簡化後之方程式無法有效模擬感潮河段。
- CE-QUAL-W2為公開之模式，模擬2-D動態或穩態下四項水質項目，惟資料需求大，目前國內較常應用於水庫水體，未曾應用於淡水河。

模式名稱	模擬四項水質項目	水 理計算	演算支排污染負荷量	程式碼是否公開	資料掌握度與複雜度	是否具備穩態與動態模擬	模式可擴充性	是否具成功應用之經驗
WASP5	O	O	O	O	O	O	O	O
QUAL 2K	O	Δ	Δ	O	O	Δ	Δ	Δ
STREAM	X	X	X	O	O	Δ	X	Δ
CE-QUAL W2	O	O	O	O	X	O	O	X

考量計畫需求下，並依淡水河水質水理特性及模式特色，以WASP為最適用模式。

O：完全具備或符合本計畫要求　Δ：尚可符合本計畫之要求　X：較不符合本計畫之要求

WASP5為最適合模式之理由

- ***模式穩定性、強健性與準確性***
  - WASP發展迄今逾25年，歷經諸多國內、外學者檢定驗證，由USEPA公開發行，模式演算具備良好穩定性、強健性與準確性。
  - WASP5內建水理(DYNHYD5)與水質模組(EUTRO & TOXI)，使用者可直接使用，或與外部水理模式耦合(ex. HEC-RAS)，均可達到良好模擬成效。
- ***模式可擴充性***
  - WASP5為免費之公開軟體，取得容易、無版權歸屬問題，使用者可針對需求修改程式碼，具有高度可擴充性。
  - WASP5可進行1-D ~ 3-D之穩態/動態模擬，考量參數及模擬項目眾多，使用上具彈性，可依資料掌握程度漸增進行更高維度及動態之模擬與校、驗證。
- ***於台灣之應用經驗***
  - WASP應用於淡水河系逾15年，期間邀集國、內外學者共同參與模式研發與修正，在地模式完成度高，校、驗證歷程及參數建立完整，針對各項污染整治工作進行情境模擬之結果具可信度，適合應用於河川污染整治與規劃管理之決策依據。

Water Quality Modeling

- To Quantify Exposure Levels (Concentrations) of Contaminants in Water and Sediment Systems
- Field Data are Essential to Model Development, Calibration, and Verification
- Model Prediction Results are Used by Decision Makers in Ecosystem Management

Take-Home Messages

- Modeling, Not Running Models
- Bracketing Uncertainty
- Analyzing Available Data to Understand Existing Conditions
- Offering Range of Results, not Single Numbers

What Would You Do

- If There is No Data ??
- If Data is Not Sufficient ??
- How to Look for Check Points ??