Research Topic

Water Quality & Aquatic Ecosystem Modeling

Weiming Wu, PhD
Professor
Dept. of Civil and Environmental Eng.
Clarkson University
Potsdam, NY 13699, USA

Updated on Oct. 9, 2014

Stream Water Quality, Ecosystem and Ecotoxicology Modeling

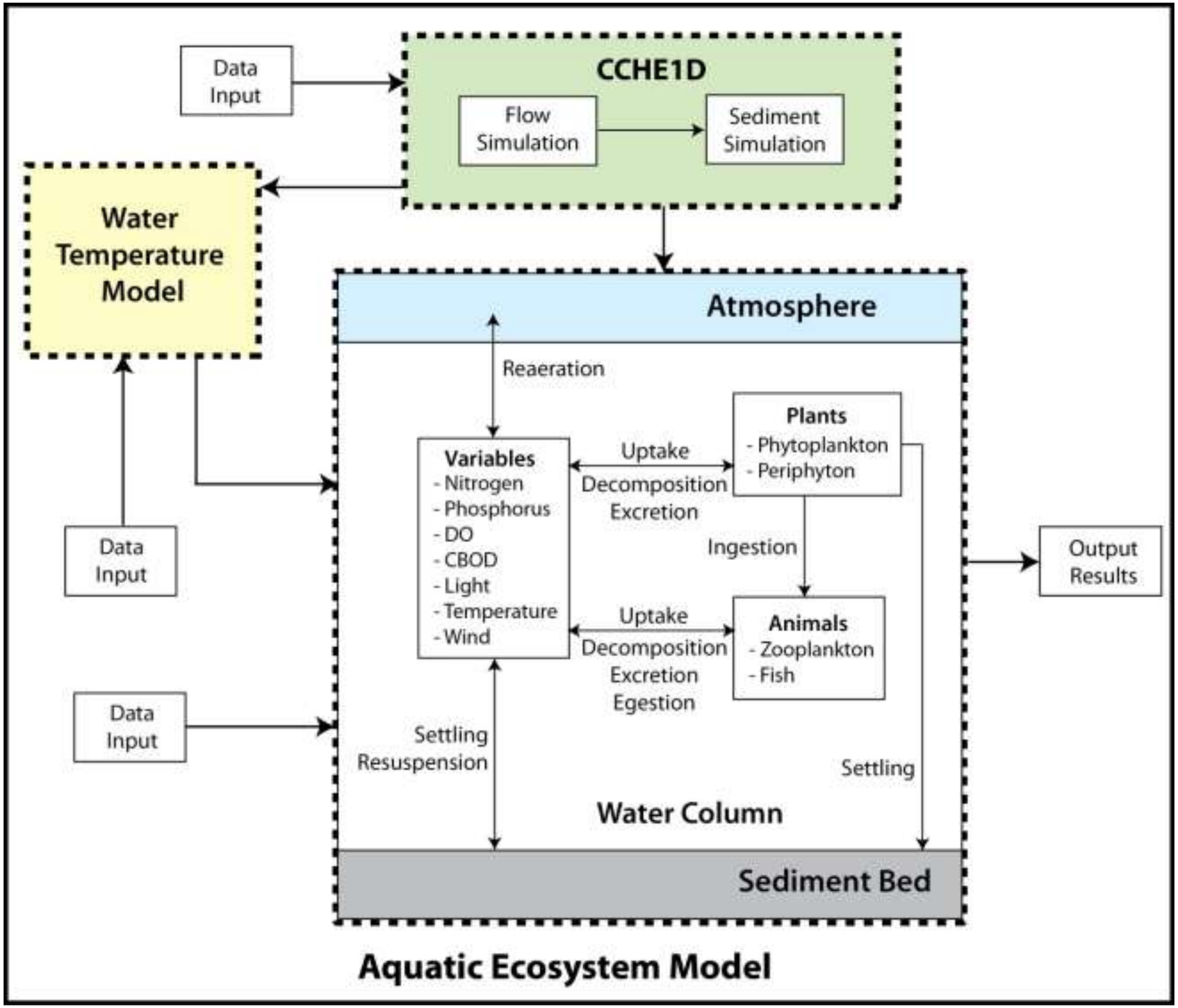
Podjanee Inthasaro's Dissertation Topic (2010)

Supervised by Weiming Wu

Model Features

- Water temperature model
- Water quality and aquatic ecosystem model
  - Dissolved oxygen (DO)
  - Biological oxygen demand (BOD),
  - Nitrogen (ON, NH_3, and NO_3),
  - Phosphorus (OP and PO_4),
  - Non-conservative substance,
  - Four-trophic level food web (phytoplankton, zooplankton, forage fish, and predatory fish)
- Aquatic ecotoxicology model

Conceptual framework of the CCHE1D water quality and aquatic ecosystem model



Water Temperature Model

1-D heat transport equation:

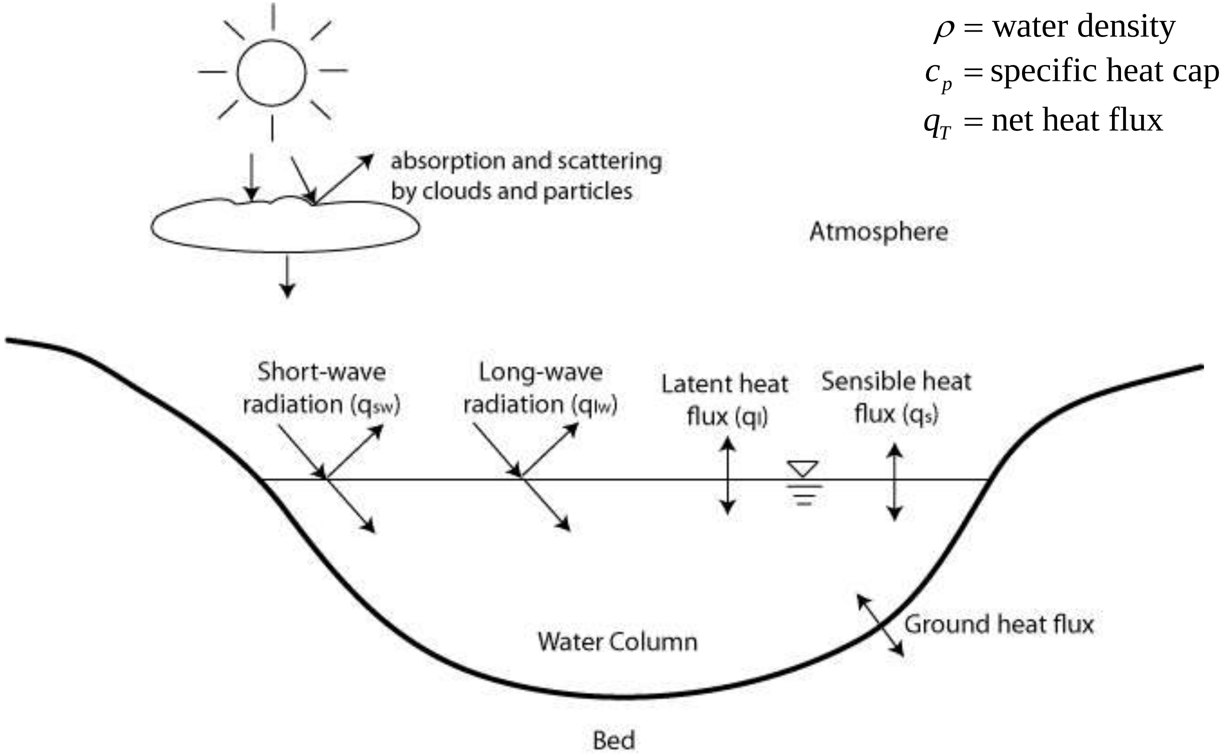
$$\frac{\partial(AT)}{\partial t}+\frac{\partial(QT)}{\partial x}=\frac{\partial}{\partial x}\left(E_T A\frac{\partial T}{\partial x}\right)+\frac{Bq_T}{\rho c_p}$$

where E_T = longitudinal diffusivity of heat

ρ = water density

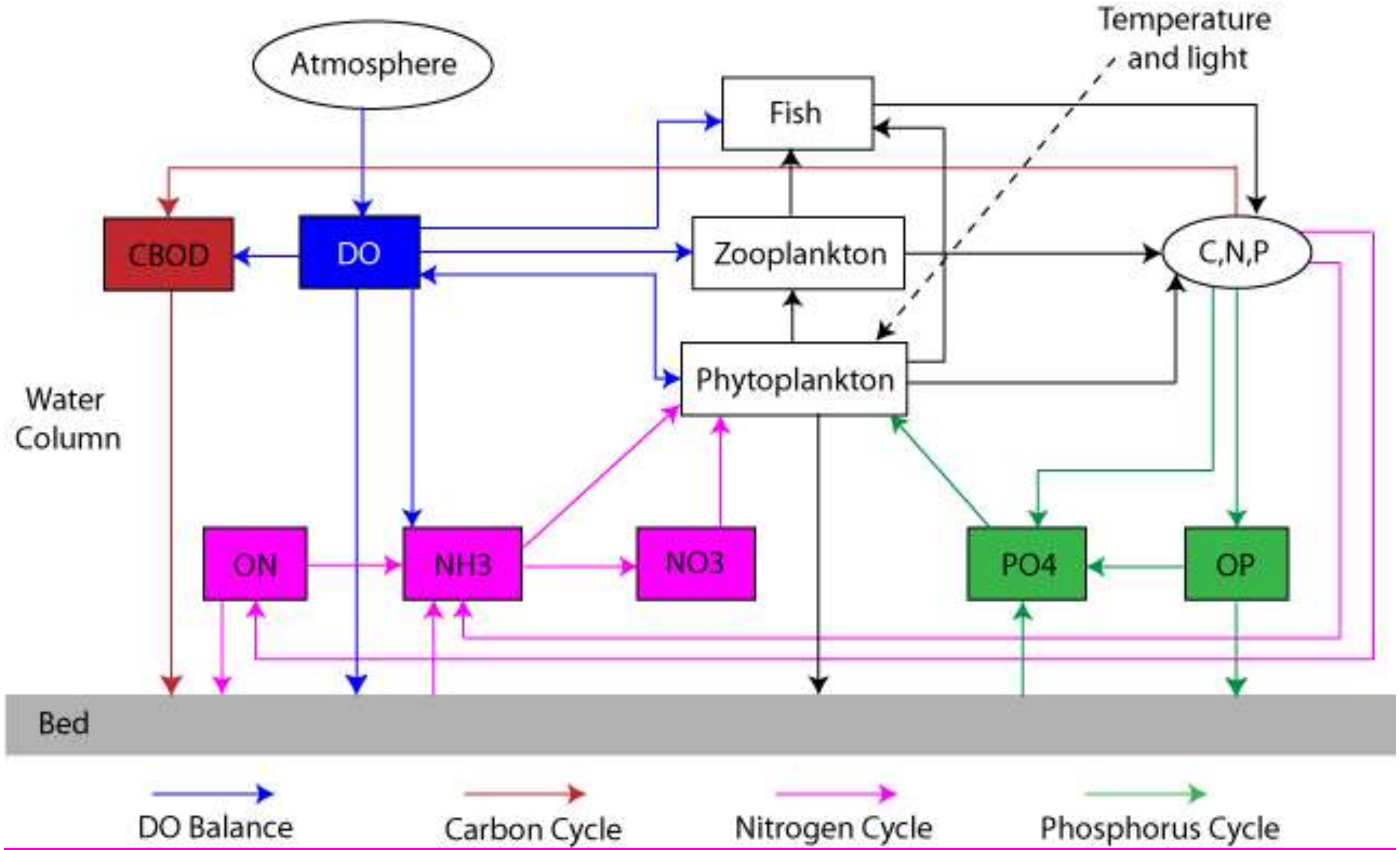
c_p = specific heat capacity

q_T = net heat flux



Major heat fluxes in the water temperature model

Kinetic Processes in Water Column



Constituents and state variables

The interactions of water quality variables and biotic compartments are based on laws of chemistry and bio-chemistry.

Water Quality and Aquatic Ecosystem Model

- Simulation of the fate and transport of constituents under either steady or unsteady flow conditions
- The transport equation described by the following advection-dispersion equation

$$\frac{\partial(AC)}{\partial t} + \frac{\partial(\alpha QC)}{\partial x} - \frac{\partial}{\partial x}\left(E_L A \frac{\partial C}{\partial x}\right) = S_c A$$

where C = concentration of a constituent

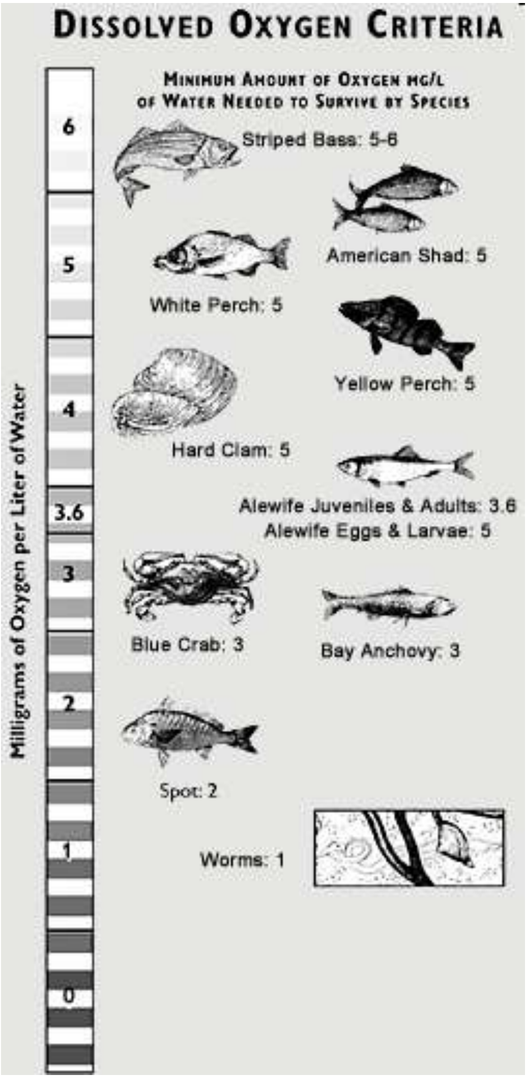
E_L = longitudinal dispersion coefficient

α = fish velocity coefficient

$S_c = \frac{dC}{dt}$ is the net source term for each constituent due to biochemical and physical changes and/or due to lateral input to the channel by runoff

Dissolved Oxygen (DO)

- Dissolved oxygen analysis measures the amount of gaseous oxygen (O_2) dissolved in an aqueous solution.
- Oxygen plays an important role in aquatic ecosystems.
- It is essential for living organisms and controls many chemical and biological reactions through the oxidation process.
- It can be removed from or added to water by various physical, chemical, and biological reactions.



http://www.chesapeakebay.net

Dissolved Oxygen (cont'd)

- The kinetic processes of DO are described by

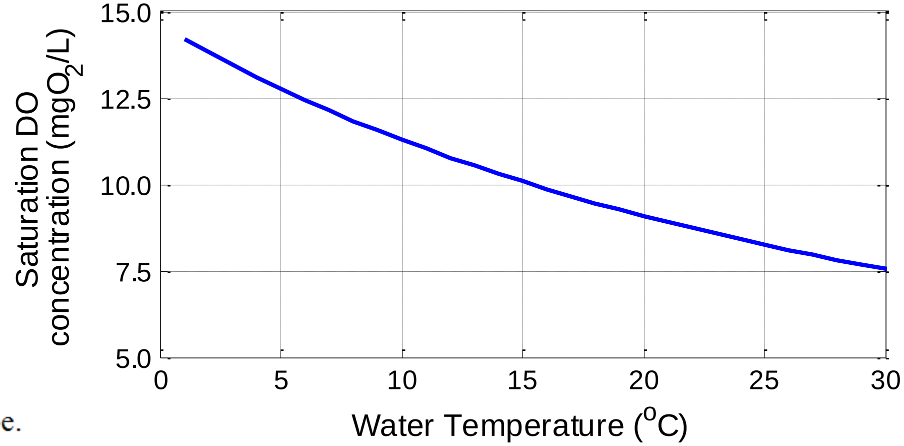
$$\frac{dC_{DO}}{dt} = \overbrace{\left(\frac{32}{12}+\frac{48}{14}\alpha_{NC}\left(1-p_{NH_3}\right)\right)K_{ag}C_a}^{\text{Phytoplankton Growth}} - \overbrace{\frac{32}{12}\sum_{i\in\{a,z,f,p\}}K_{ir}C_i}^{\text{Respiration}} + \overbrace{K_{RE}\theta_{RE}^{T-20}\left(C'_{DO}-C_{DO}\right)}^{\text{Reareation}}$$

$$-\underbrace{K_{BOD}\lambda_{BOD}\theta_{BOD}^{T-20}C_{BOD}}_{\text{Decomposition}} - \underbrace{\frac{64}{14}K_{NH_3}\lambda_{NH_3}\theta_{NH_3}^{T-20}C_{NH_3}}_{\text{Nitrification}} + \underset{\text{Sediment oxygen demand}}{\underline{\frac{S_{SOD}}{h}}}$$

Investigators	Formulas for K_{RE} (day^{-1})[a]
Modified USACE[b]	$5.58U^{0.607}h^{-1.689}$
O'Connor-Dobbins (1958)	$3.93U^{0.50}h^{-1.50}$
Churchill (1962)	$5.02Uh^{-1.67}$
Krenket and Orlob (1962)	$173(SU)^{0.404}h^{-0.66}$
Owen and Gibbs (1964)	$5.32U^{0.67}h^{-1.85}$
Langbein and Durum (1967)	$5.14Uh^{-1.33}$
Caldwallader and McDonnell (1969)	$186(SU)^{0.5}h^{-1.0}$
Padden and Gloyna (1971)	$4.55U^{0.703}h^{-1.054}$

[a] U is the flow velocity (m/s), h is the water depth (m), and S is the friction slope.

[b] The equation is suggested by Rounds et al. (1999).



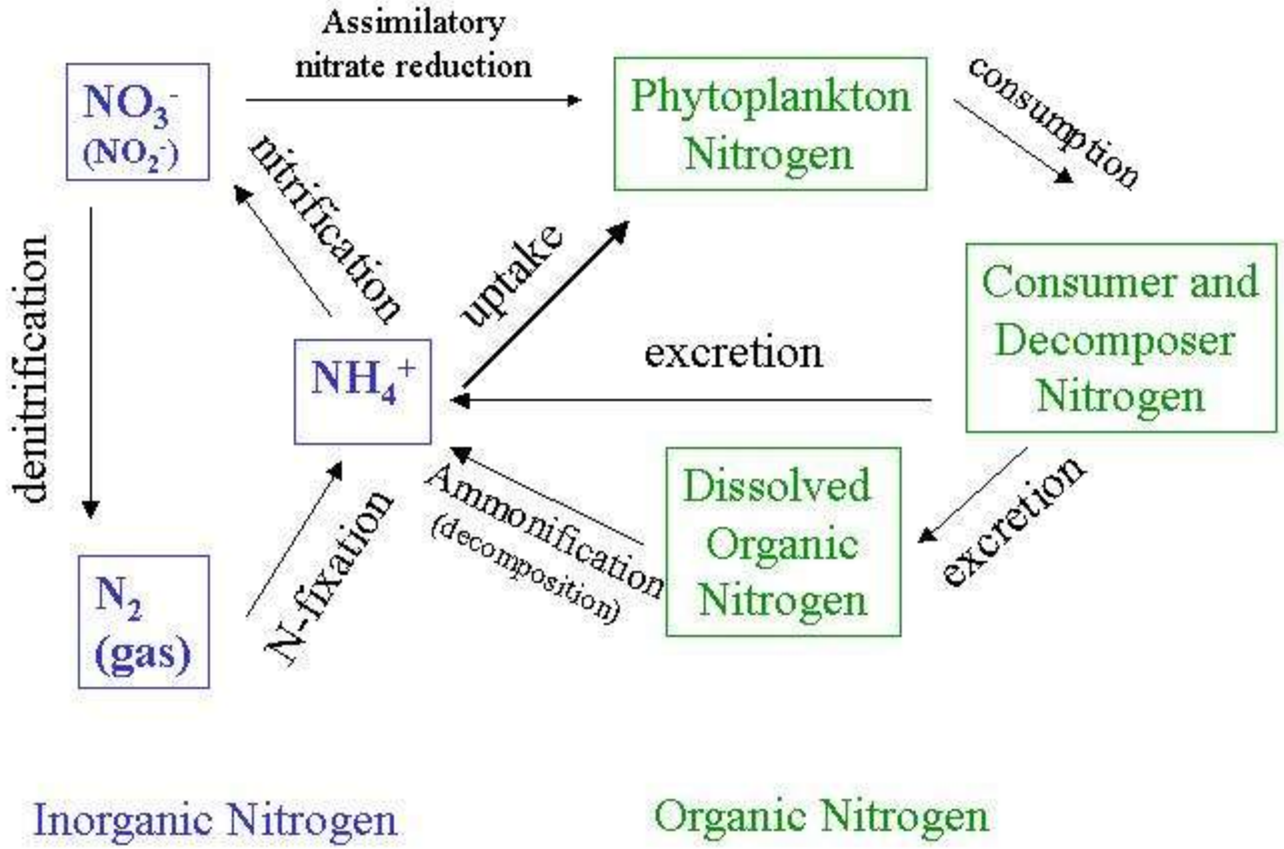
Biological Oxygen Demand (BOD)

- BOD is one of the common water quality indicators.
- It is a measurement of the amount of oxygen required to stabilize organic matter in the water.
- The rate of oxygen consumption is affected by temperature, the presence of certain kinds of microorganisms, and the type of organic and inorganic material in the water.

$$\frac{dC_{BOD}}{dt} = \overbrace{\frac{32}{12}K_{am}C_a + \frac{32}{12}\sum_{i\in\{z,f,p\}}\left(K_{im}+K_{ie}+K_{id}\right)C_i}^{\text{Mortality, Excretion, Defecation}} - \overbrace{K_{BOD}\lambda_{BOD}\theta_{BOD}^{T-20}C_{BOD}}^{\text{Decomposition}}$$

$$\underbrace{-\frac{5}{4}\frac{32}{14}K_{NO_3}\lambda_{NO_3}\theta_{NO_3}^{T-20}C_{NO_3}}_{\text{Nitrification}} + \underbrace{\frac{\omega_{BOD}}{h}f_{PBOD}C_{BOD}}_{\text{Settling}}$$

Aquatic Nitrogen Cycle



NO_3^-
(NO_2^-)

Assimilatory nitrate reduction

Phytoplankton Nitrogen

consumption

Consumer and Decomposer Nitrogen

nitrification

uptake

excretion

NH_4^+

denitrification

N_2 (gas)

N-fixation

Ammonification (decomposition)

Dissolved Organic Nitrogen

excretion

Inorganic Nitrogen

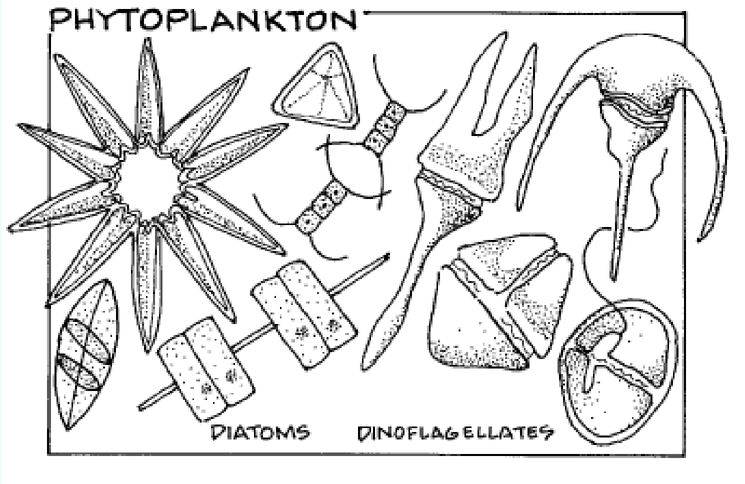
Organic Nitrogen

Phosphorus Cycle

- Phosphorus in natural water can be divided in several ways.
  - Soluble reactive phosphorus (SRP), orthophosphate, or soluble inorganic phosphorus
  - Particulate organic phosphorus
  - Nonparticulate organic phosphorus
  - Particulate inorganic phosphorus
  - Nonparticulate inorganic phosphorus

Phytoplankton

- Autotroph
- Groups of phytoplankton: diatoms, cyanobacteria, and dinoflagellates
- Macronutrients: nitrate, phosphate or silicic acid
- Habitat: at or near water surface
- The kinetic processes of phytoplankton are calculated as



$$\frac{dC_a}{dt} = \left(\underset{\text{Photosynthesis}}{K_{ag}} - \underset{\text{Respiration}}{K_{ar}} - \underset{\text{Excretion}}{K_{ae}} - \underset{\text{Mortality}}{K_{am}} \right) C_a - \underbrace{\sum_{i\in\{z,f,p\}} K_{ig}\, f_{ai} C_i}_{\text{Predation}} - \underset{\text{Settling}}{\frac{\omega_a}{h} C_a}$$

Phytoplankton Processes

Photosynthesis:

$$K_{ag} = K_{ag,\max} f_N \, f_L \, f_T \, f'_{ag}$$

Nutrient limitation factor:

$$f_N = \min\left(\frac{C_{NH_3} + C_{NO_3}}{h_N + C_{NH_3} + C_{NO_3}}, \frac{C_{PO_4}}{h_P + C_{PO_4}} \right)$$

Depth-averaged light limitation factor:

$$f_L = \frac{1}{\gamma h} \ln\left(\frac{h_L + I_0}{h_L + I_0 e^{-\lambda h}} \right)$$

Temperature rate modifier (Cerco & Cole, 1995):

$$f_T = \exp\left(-KT_{g1} \left(T - T_{opt} \right)^2 \right) \quad \text{when} \quad T \le T_{opt}$$

$$f_T = \exp\left(-KT_{g2} \left(T_{opt} - T \right)^2 \right) \quad \text{when} \quad T > T_{opt}$$

Respiration:

$$K_{ar} = K_{ar,\max} \theta_a^{T-20}$$

Mortality:

$$K_{am} = \left(1 + f'_{am} \right) K_{am,\max} \theta_a^{T-20}$$

Grazing of Predator on Prey

Predator Grazing rate: $K_{ig} = K_{ig,\max} \lambda_i f_T f'_{ig}$

Saturation-feeding kinetic factor:

$$\lambda_i = \frac{\sum_j (p_{ij} C_j) - \mu_i}{h_i + \sum_j (p_{ij} C_j)}$$

where

μ_i is the threshold food concentration,

h_i is the half-saturation food concentration.

Table 5.5 Preference consumption of the UHR food web model.

Species	Detritus	Phytoplankton	Zooplankton	Forage Fish	Predatory Fish
Zooplankton	0.15	0.85	-	-	-
Forage Fish	0.15	0.25	0.5	0.1	-
Predatory Fish	0.025	0.175	0.25	0.85	0.15

Zooplankton

- Zooplankton includes protozoa, small crustaceans, jellyfish and worm.
- Zooplankton is a heterotrophic component that drifts in the water column
- Zooplankton feeds on bacterioplankton, phytoplankton, other zooplankton, and detritus.
- Zooplankton dynamics is calculated by

$$\frac{dC_z}{dt} = \left(\underset{\text{Grazing}}{K_{zg}} - \underset{\text{Defecation}}{K_{zd}} - \underset{\text{Respiration}}{K_{zr}} - \underset{\text{Excretion}}{K_{ze}} - \underset{\text{Mortality}}{K_{zm}} \right) C_z - \underbrace{\sum_{i\in\{f,p\}} K_{ig} f_{i,z} C_i}_{\text{Predation}}$$

Fish Dynamics

- Fish is divided into two groups: forage fish (f) and predatory fish (p).
- Simple food chain with a single class is considered in the model.
- The dynamic processes of each group are described as

$$\frac{dC_f}{dt} = \left(\underset{\text{Grazing}}{K_{fg}} - \underset{\text{Respiration}}{K_{fr}} - \underset{\text{Excretion}}{K_{fe}} - \underset{\text{Mortality}}{K_{fm}} - \underset{\text{Defecation}}{K_{fd}} - \underset{\text{Gamete Loss}}{K_{fa}} + \underset{\text{Reproduction}}{K_{fre}} \right) C_f - \underbrace{K_{pg} f_{fp} C_p}_{\text{Predation}}$$

$$\frac{dC_p}{dt} = \left(\underset{\text{Grazing}}{K_{pg}} - \underset{\text{Respiration}}{K_{pr}} - \underset{\text{Excretion}}{K_{pe}} - \underset{\text{Mortality}}{K_{pm}} - \underset{\text{Defecation}}{K_{pd}} - \underset{\text{Gamete Loss}}{K_{pa}} + \underset{\text{Reproduction}}{K_{pre}} \right) C_p$$

Contaminant Fate and Transport

- The physicochemical model includes the mechanisms of
  - sorption/desorption interaction between dissolved and particulate contaminants,
  - volatilization,
  - microbial decay processes,
  - diffusive exchange of the dissolved contaminant between bed sediment and the overlying water column and between layers of the bed sediment itself,
  - transport of the contaminant via advective and dispersive processes,
  - external inputs of the contaminant, and
  - uptake and depuration of the contaminant due to aquatic organisms.

Contaminant Fate and Transport

- The 1-D governing equation for the fate and transport of a contaminant in water column is given as

$$\frac{1}{A}\left[\frac{\partial\left(AC_{tw}\right)}{\partial t}+\frac{\partial\left(QC_{tw}\right)}{\partial x}-\frac{\partial}{\partial x}\left(E_L A\frac{\partial C_{tw}}{\partial x}\right)\right]=q_{tw}+S_{tw}+\frac{J_{dbw}}{h}+\frac{q_{t,ex}}{h}$$

where

C_{tw} is the total concentration of contaminant in water column,

q_{tw} is the total loading rate of contaminant,

S_{tw} is the source term fluxes due to physical, chemical and biological reactions,

J_{dbw} is the vertical diffusion fluxes between water column and bed surface layer,

$q_{t,ex}$ is the exchange rates of contaminant due to sedimentation.

- The source term is computed by

$$S_{tw}=-\underset{\text{Hydrolysis}}{S_h}-\underset{\text{Photolysis}}{S_p}-\underset{\text{Biodegradation}}{S_b}-\underset{\text{Volatilization}}{S_v}-\underbrace{\sum_{i\in\{a,z,f,p\}}S_i}_{\text{Biotic Organisms}}$$

Aquatic Bioaccumulation

- The contaminant concentrations at various trophic levels of the aquatic food web vary according to the following mechanisms:
  - direct uptake of the dissolved contaminant from water,
  - food web accumulation of the contaminant resulting from consumption of contaminated prey,
  - depuration of the contaminant due to all loss pathways, and
  - growth and respiration of the organisms.

$$\frac{\partial\left(AC_{ti}\right)}{\partial t}+\frac{\partial\left(\alpha QC_{ti}\right)}{\partial x}-\frac{\partial}{\partial x}\left(E_L A\frac{\partial C_{ti}}{\partial x}\right)=S_{ti}A$$

where

C_{ti} is the concentration of contaminant associated with biotic organism in unit volumeof water

$S_{ti}=\dfrac{dC_{ti}}{dt}$ is the net source term for the contaminant rate change due to biotic organism.

Kinetic Source Terms for Contaminant/Food-Chain Interactions

The dynamic processes of concentration of contaminant in phytoplankton per unit volume of water is modeled as

$$\frac{dC_{ta}}{dt} = \underbrace{K_{a1}C_{dw}C_{a}}_{\text{Uptake}} - \underbrace{K_{a2}C_{ta}}_{\text{Depuration}} - \left(\underset{\text{Excretion}}{K_{ae}} + \underset{\text{Mortality}}{K_{am}} \right) C_{ta} - \underbrace{\sum_{i \in \{z,f,p\}} \left(K_{ig} f_{ai} C_{i} \right) \nu_{a}}_{\text{Predation}}$$

For higher trophic levels, the input of contaminant due to ingestion of contaminated food plays an important role. The rate of change in chemical concentration is determined by

$$\frac{dC_{tz}}{dt} = \underbrace{K_{z1}C_{dw}}_{\text{Uptake}} + \underbrace{K_{zg}e_{zg}C_{ta}}_{\text{Consumption}} - \underbrace{\left(K_{z2} + K_{zm}\right)C_{tz}}_{\text{Elimination}} - \underbrace{\sum_{i \in \{f,p\}} \left(f_{zi} K_{ig} C_{i} \right) \nu_{z}}_{\text{Predation}}$$

Aquatic Ecotoxicology

Biomass loss due to acute toxicity can be estimated based on the internal concentration of the toxicant in the biotic organism (Park & Clough, 2004)

$$IC_{i50} = BCF_i \times LC_{i50}$$

where

IC_{i50} is the internal concentration that cause 50% mortality,

BCF_i is the time-dependent bioconcentration factor,

LC_{i50} is the concentration of toxicant in water that causes 50% mortality (mg/L).

The lethal internal concentration of toxicant for a given exposure period can be expressed as

$$C_{i50} = \frac{IC_{i50}\left(1 - e^{-K_{i2}t_1}\right)}{1 - e^{-K_{i2}t_2}}$$

where

C_{i50} is the time-varying tissue-base concentration that cause 50% mortality,

K_{i2} is the elimination rate constant,

t_1 is the exposure time in toxicity determination,

t_2 is the elapsed since the beginning of exposure to toxicant.

The ratio of chronic to acute concentrations is

$$r_{ap} = \frac{EC_{ap50}}{LC_{a50}}.$$

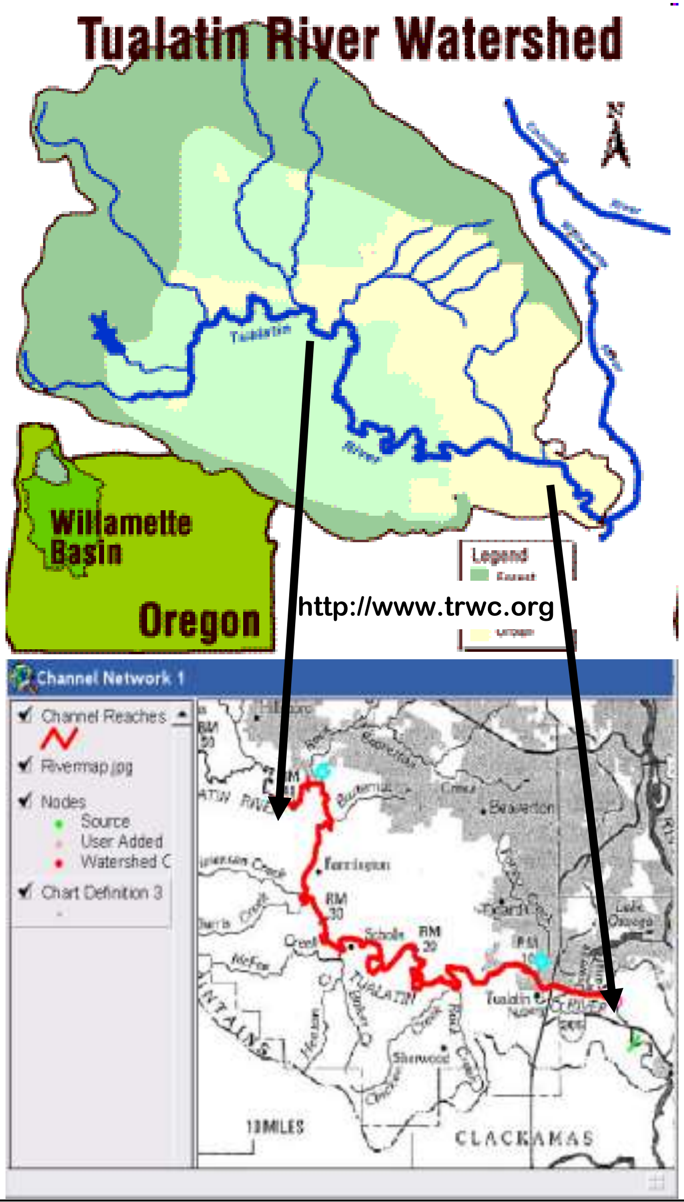
where EC_{ap50} is the external concentration of toxicant at which there is a 50% reduction in photosynthesis.

The reduction factor for photosynthesis can be calculated by (Park & Clough, 2004)

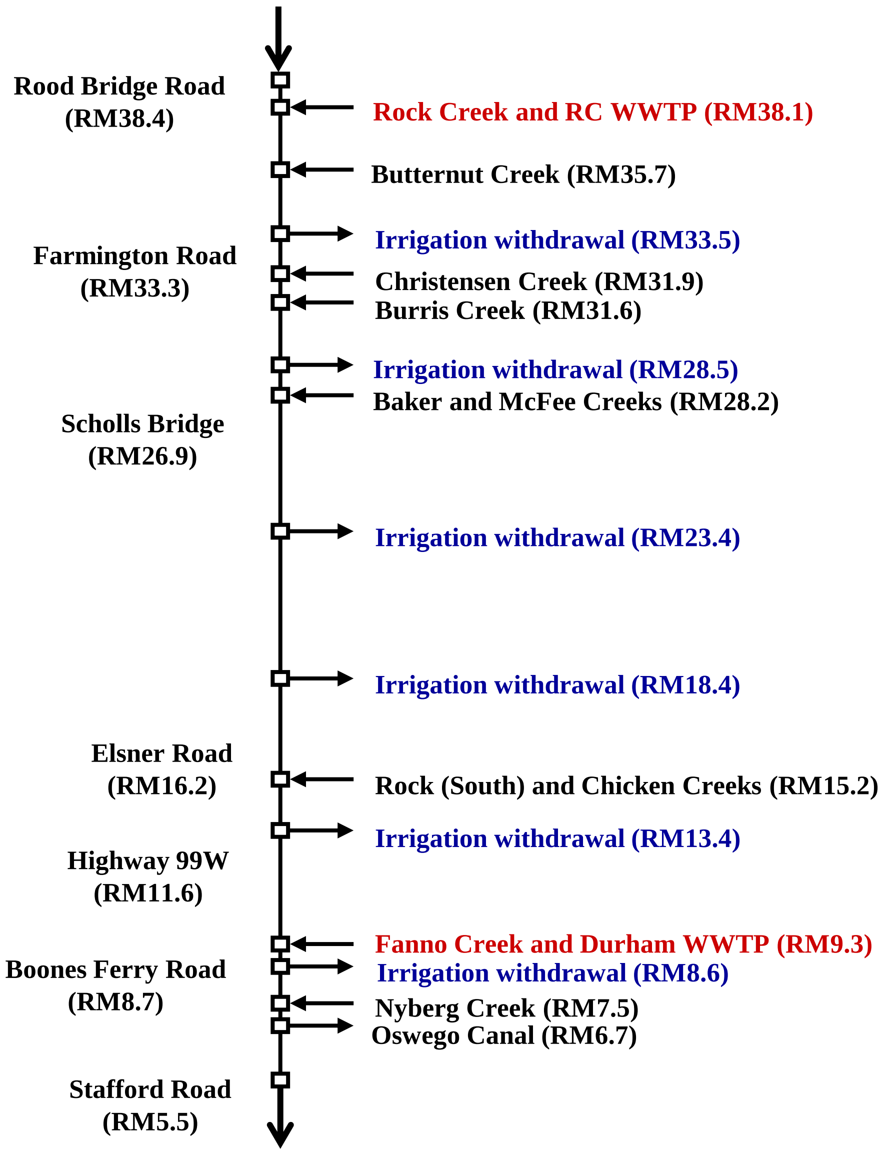
$$f'_{ag} = \exp\left(-\frac{v_a}{C_{a50} r_{ap}}\right)^{\frac{1}{K_s}}.$$

The reduction factors for growth and gamete loss in animals are determined in a similar manner.

Tualatin River, Oregon



http://www.trwc.org



Rood Bridge Road (RM38.4)

Rock Creek and RC WWTP (RM38.1)

Butternut Creek (RM35.7)

Irrigation withdrawal (RM33.5)

Farmington Road (RM33.3)

Christensen Creek (RM31.9)

Burris Creek (RM31.6)

Irrigation withdrawal (RM28.5)

Baker and McFee Creeks (RM28.2)

Scholls Bridge (RM26.9)

Irrigation withdrawal (RM23.4)

Irrigation withdrawal (RM18.4)

Elsner Road (RM16.2)

Rock (South) and Chicken Creeks (RM15.2)

Irrigation withdrawal (RM13.4)

Highway 99W (RM11.6)

Fanno Creek and Durham WWTP (RM9.3)

Irrigation withdrawal (RM8.6)

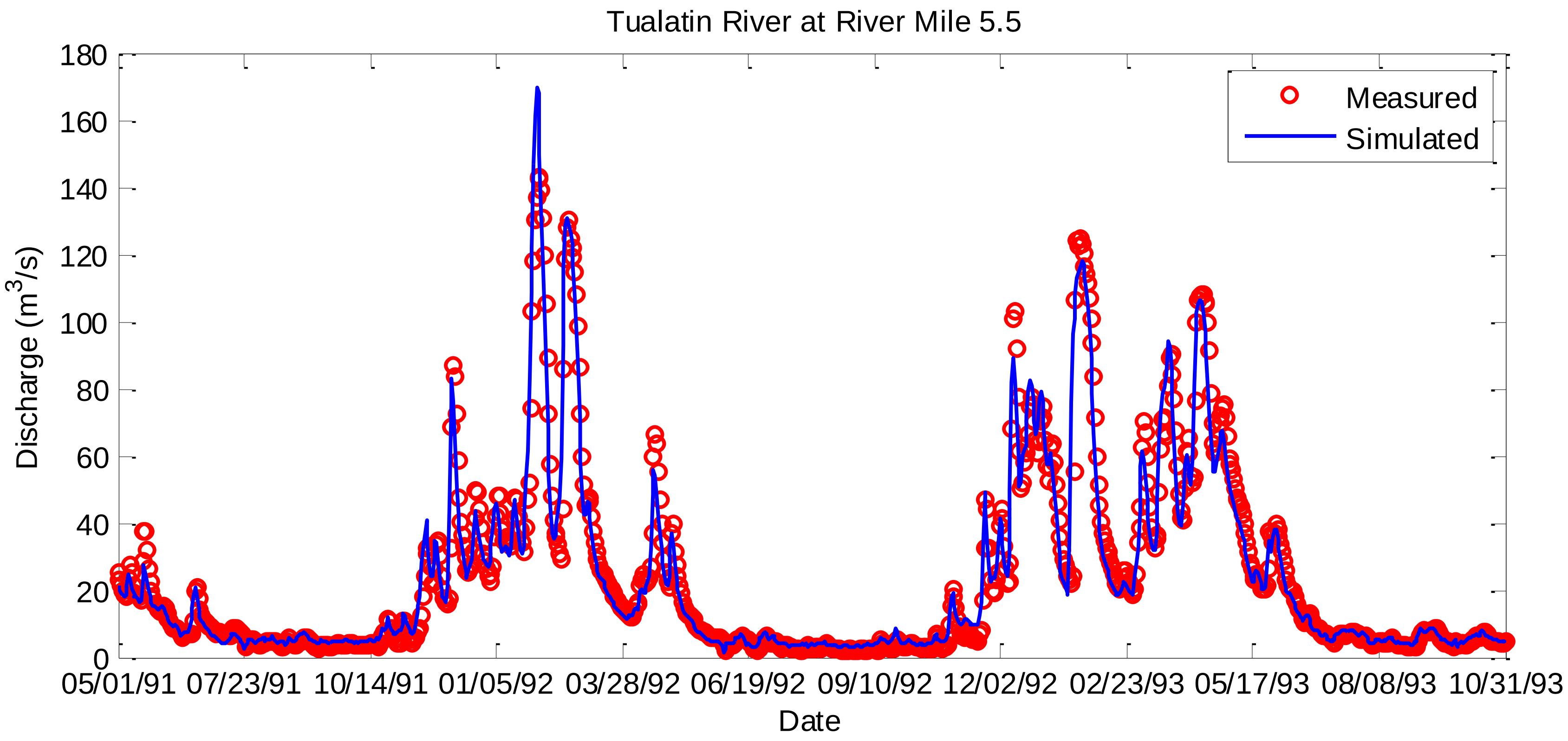
Boones Ferry Road (RM8.7)

Nyberg Creek (RM7.5)

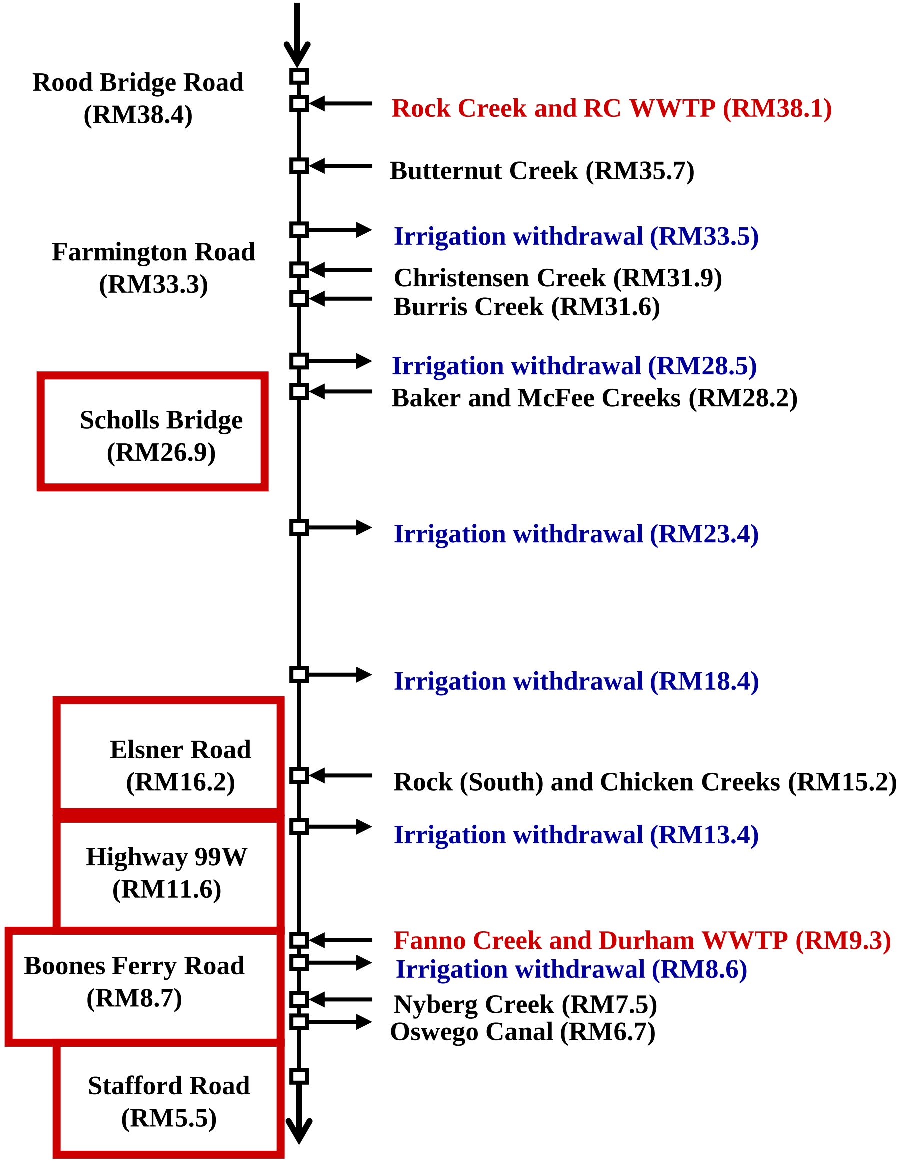
Oswego Canal (RM6.7)

Stafford Road (RM5.5)

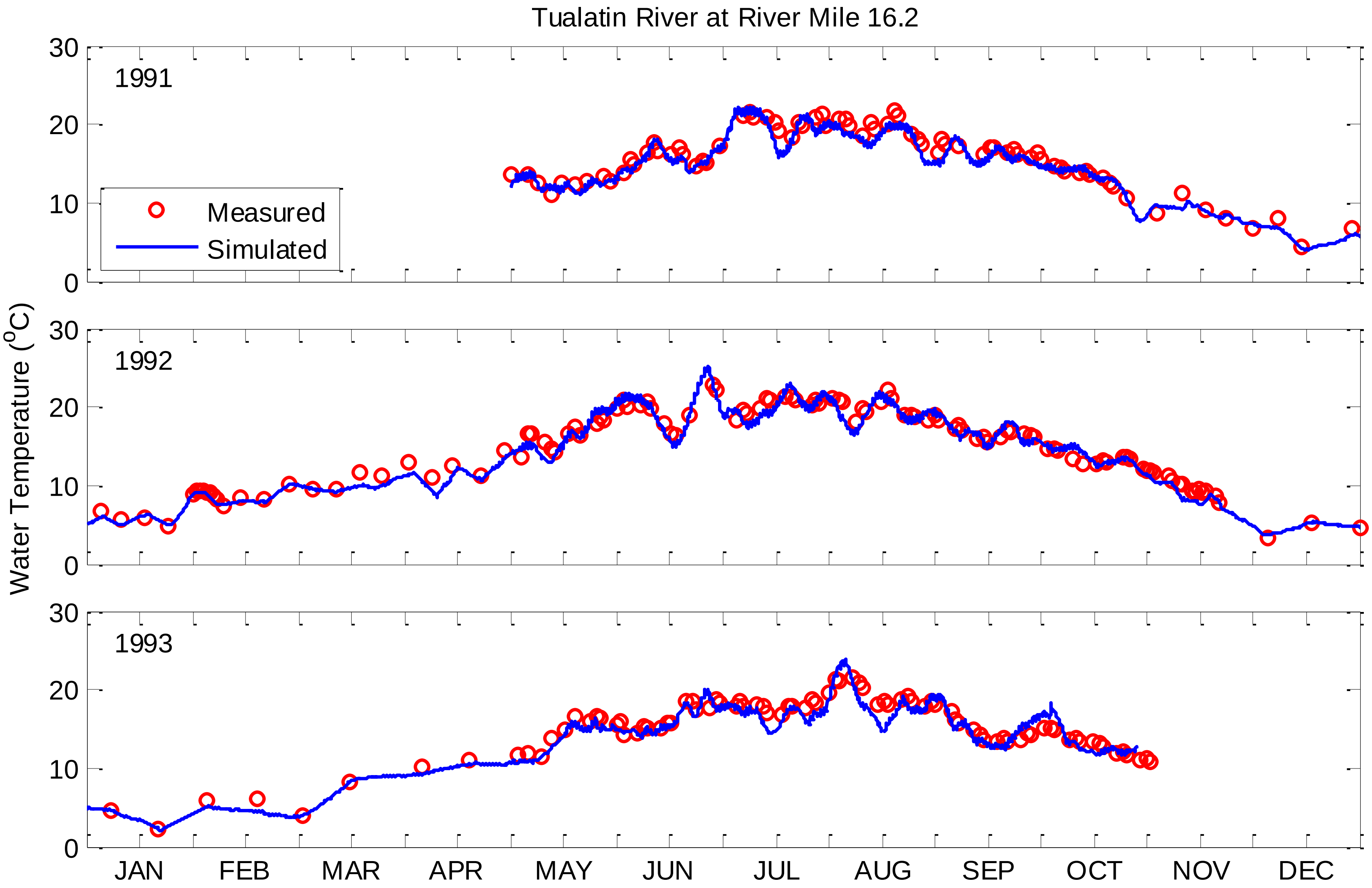
Flow Simulation

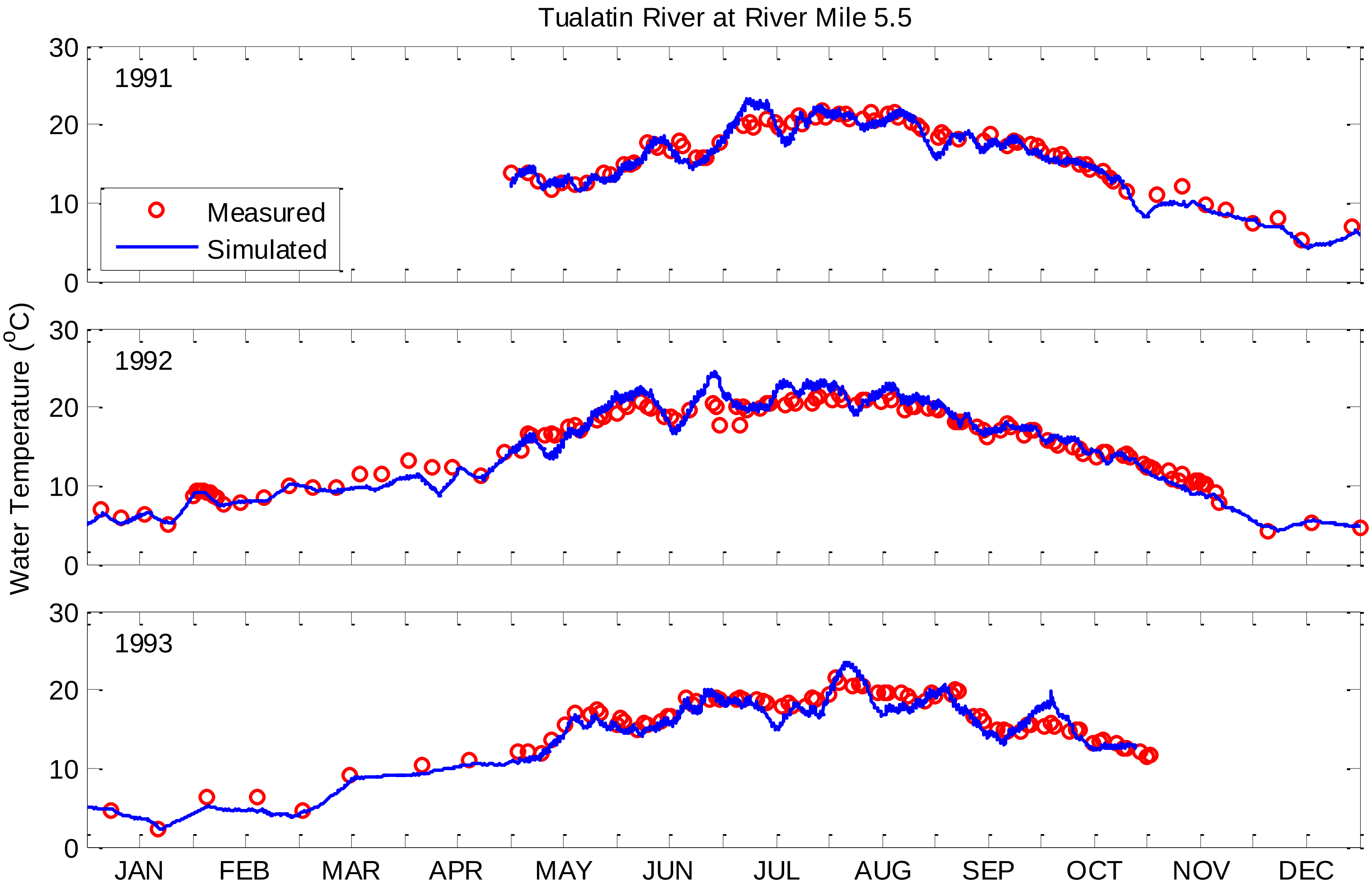


Water Temperature



Water Temperature




Tualatin River at River Mile 5.5
Water Temperature (^oC)
1991
1992
1993
Measured
Simulated
0
10
20
30
JAN
FEB
MAR
APR
MAY
JUN
JUL
AUG
SEP
OCT
NOV
DEC

Water Quality

- The water quality in the approximately 50 km long reach from RM38.4 to RM5.5 of the Tualatin River is modeled from May 1991 until October 1993.
- Eight water quality parameters: chloride, ON, NH_3, NO_3, OP, PO_4, BOD, and DO are simulated.
- Phytoplankton and zooplankton biomasses are modeled in this study.
- The simulation domain is represented by 132 cross-sections. Each cross-section is divided into 11 panels.
- The time step for the water quality simulation is 15 minutes.

Data Inputs and Model Parameters

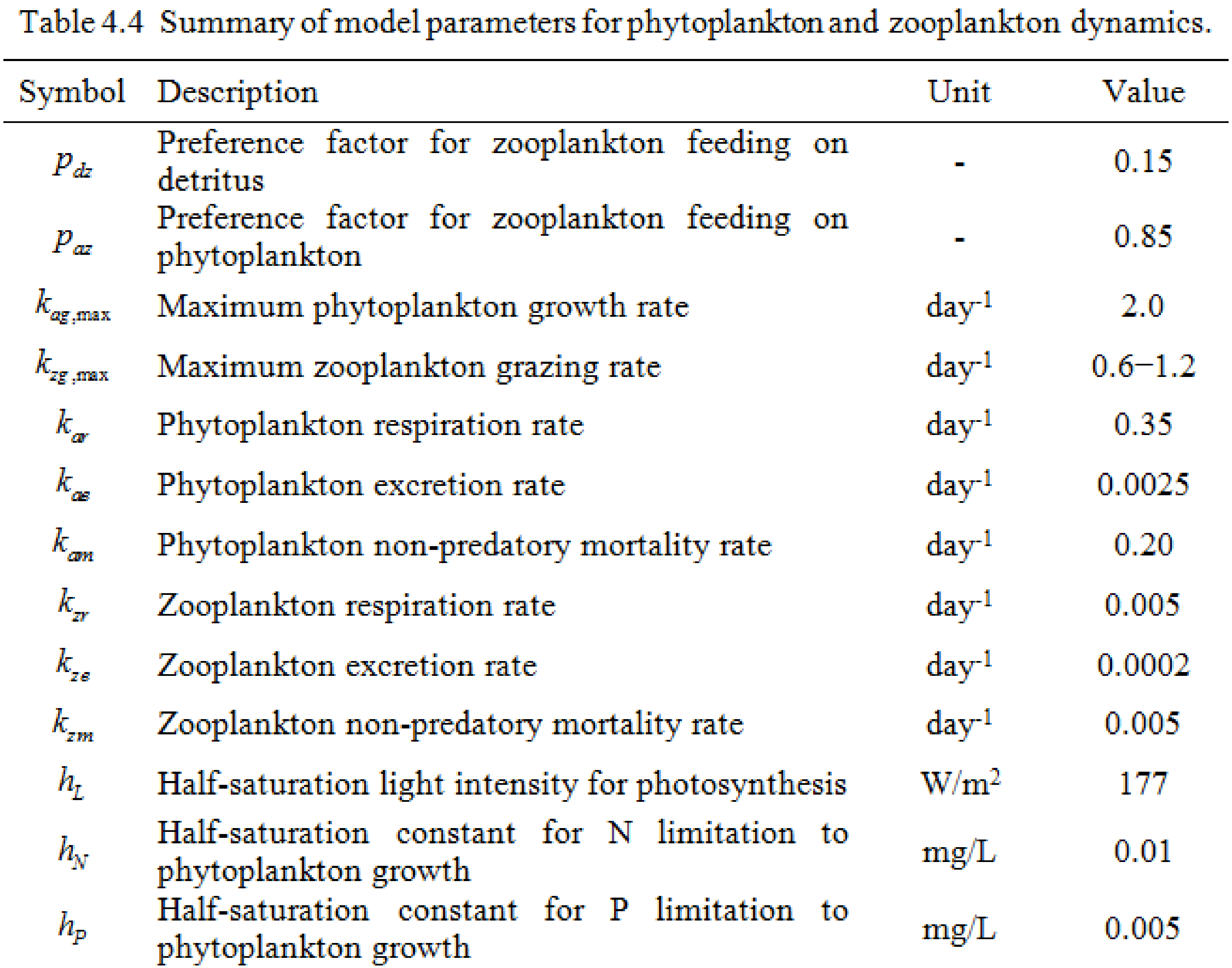
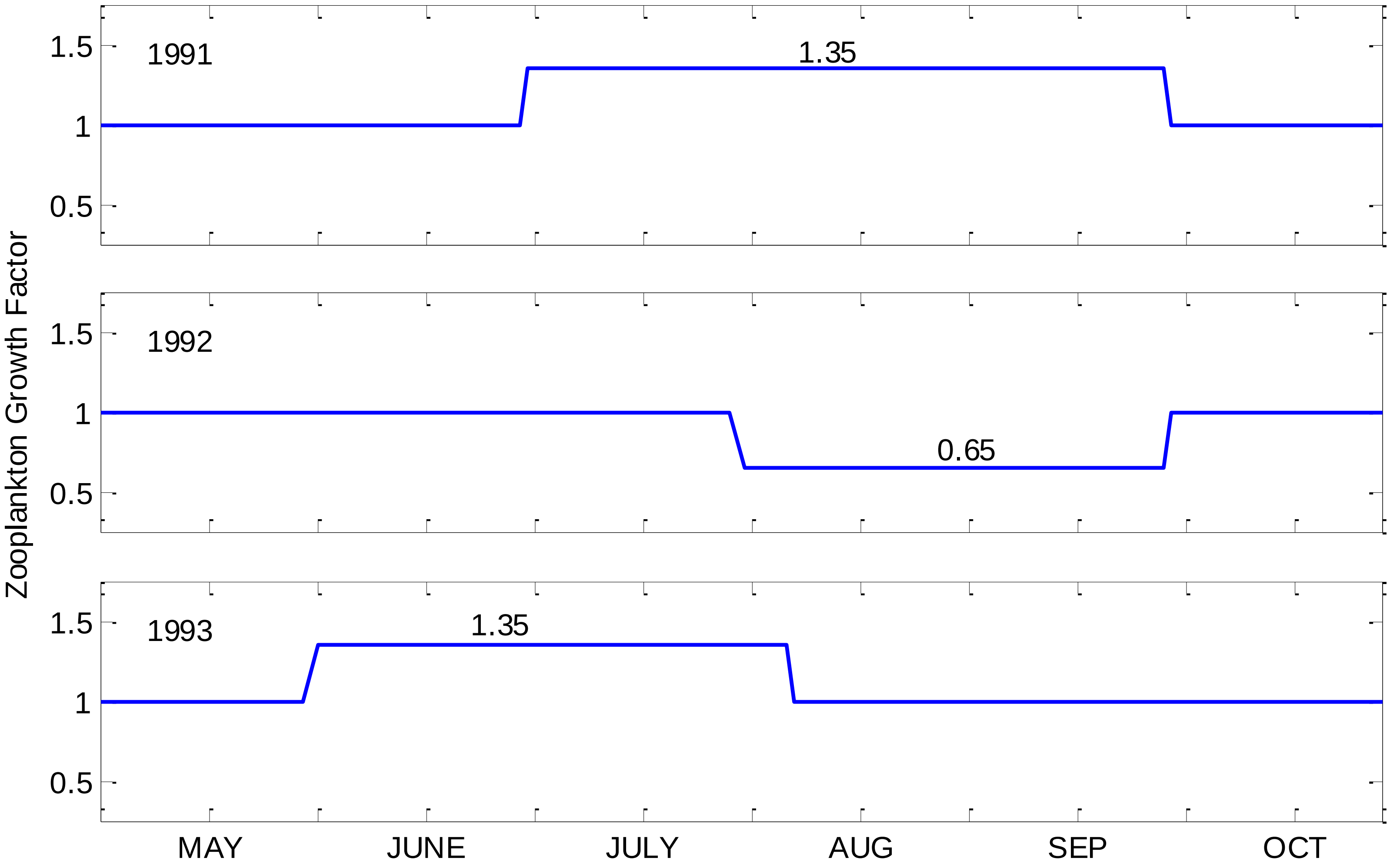


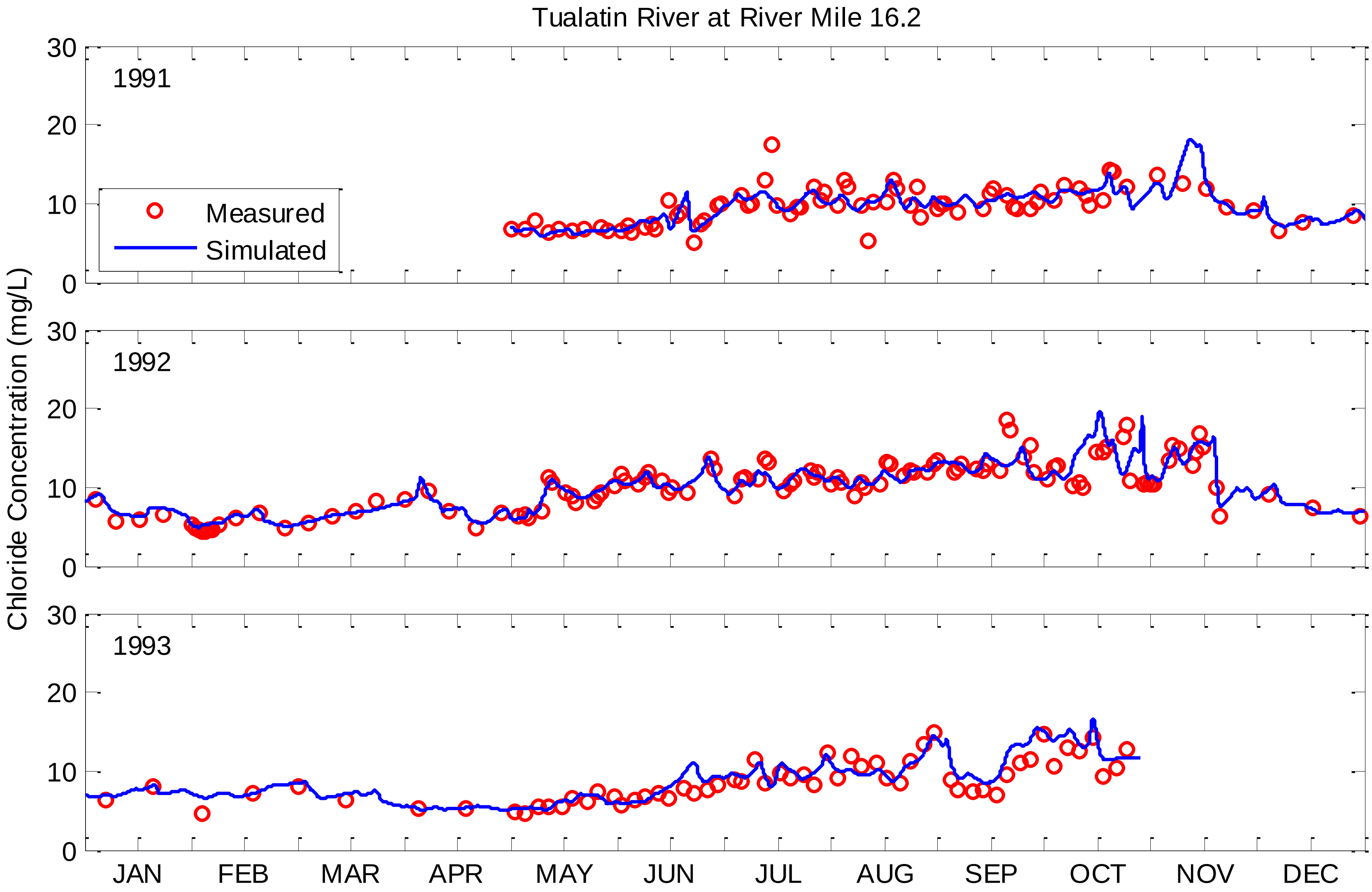
Table 4.4 Summary of model parameters for phytoplankton and zooplankton dynamics.

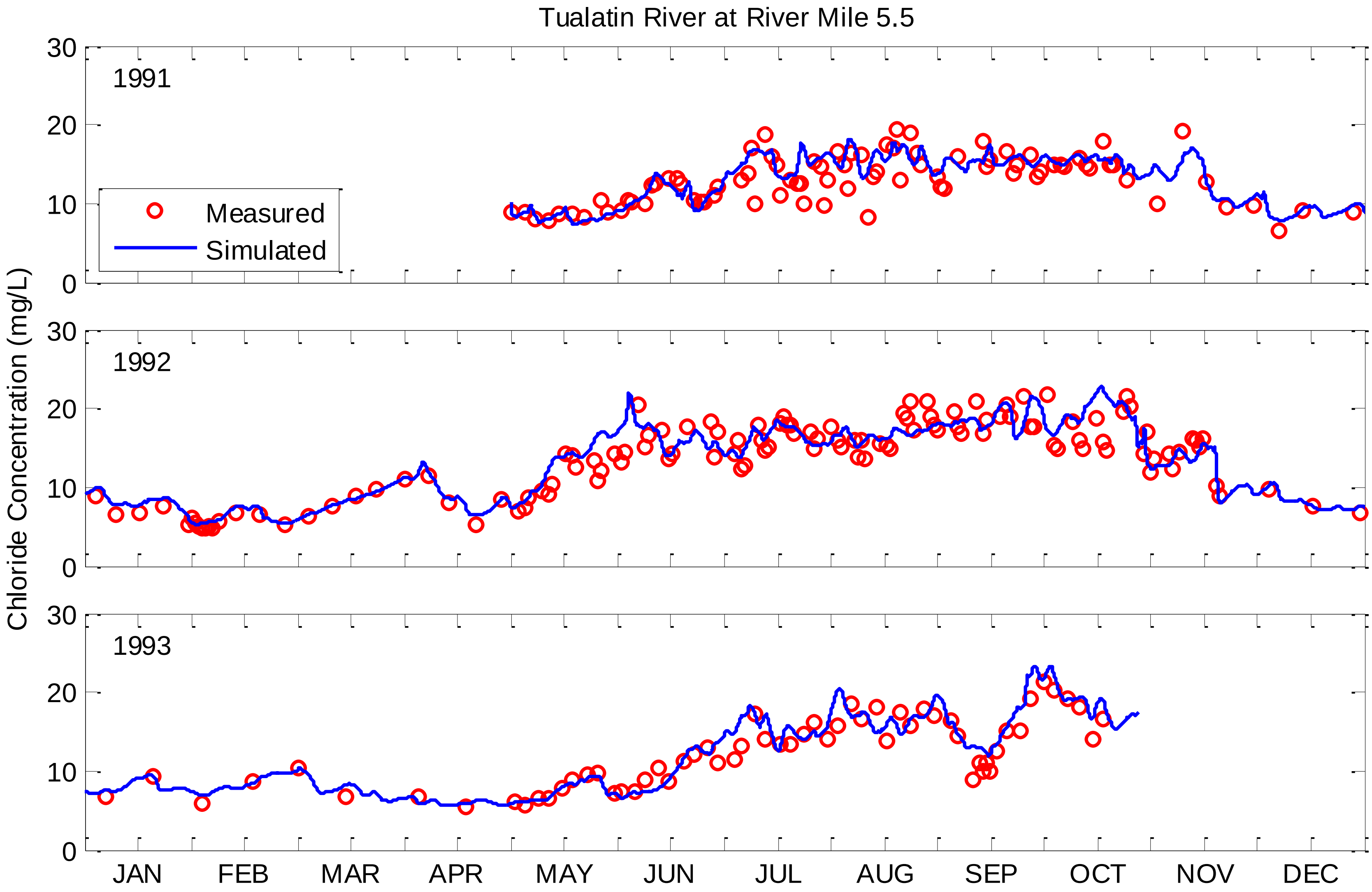
Symbol	Description	Unit	Value
p_{dz}	Preference factor for zooplankton feeding on detritus	-	0.15
p_{az}	Preference factor for zooplankton feeding on phytoplankton	-	0.85
$k_{ag,\max}$	Maximum phytoplankton growth rate	day^{-1}	2.0
$k_{zg,\max}$	Maximum zooplankton grazing rate	day^{-1}	0.6−1.2
k_{ar}	Phytoplankton respiration rate	day^{-1}	0.35
k_{ae}	Phytoplankton excretion rate	day^{-1}	0.0025
k_{am}	Phytoplankton non-predatory mortality rate	day^{-1}	0.20
k_{zr}	Zooplankton respiration rate	day^{-1}	0.005
k_{ze}	Zooplankton excretion rate	day^{-1}	0.0002
k_{zm}	Zooplankton non-predatory mortality rate	day^{-1}	0.005
h_L	Half-saturation light intensity for photosynthesis	W/m^2	177
h_N	Half-saturation constant for N limitation to phytoplankton growth	mg/L	0.01
h_P	Half-saturation constant for P limitation to phytoplankton growth	mg/L	0.005

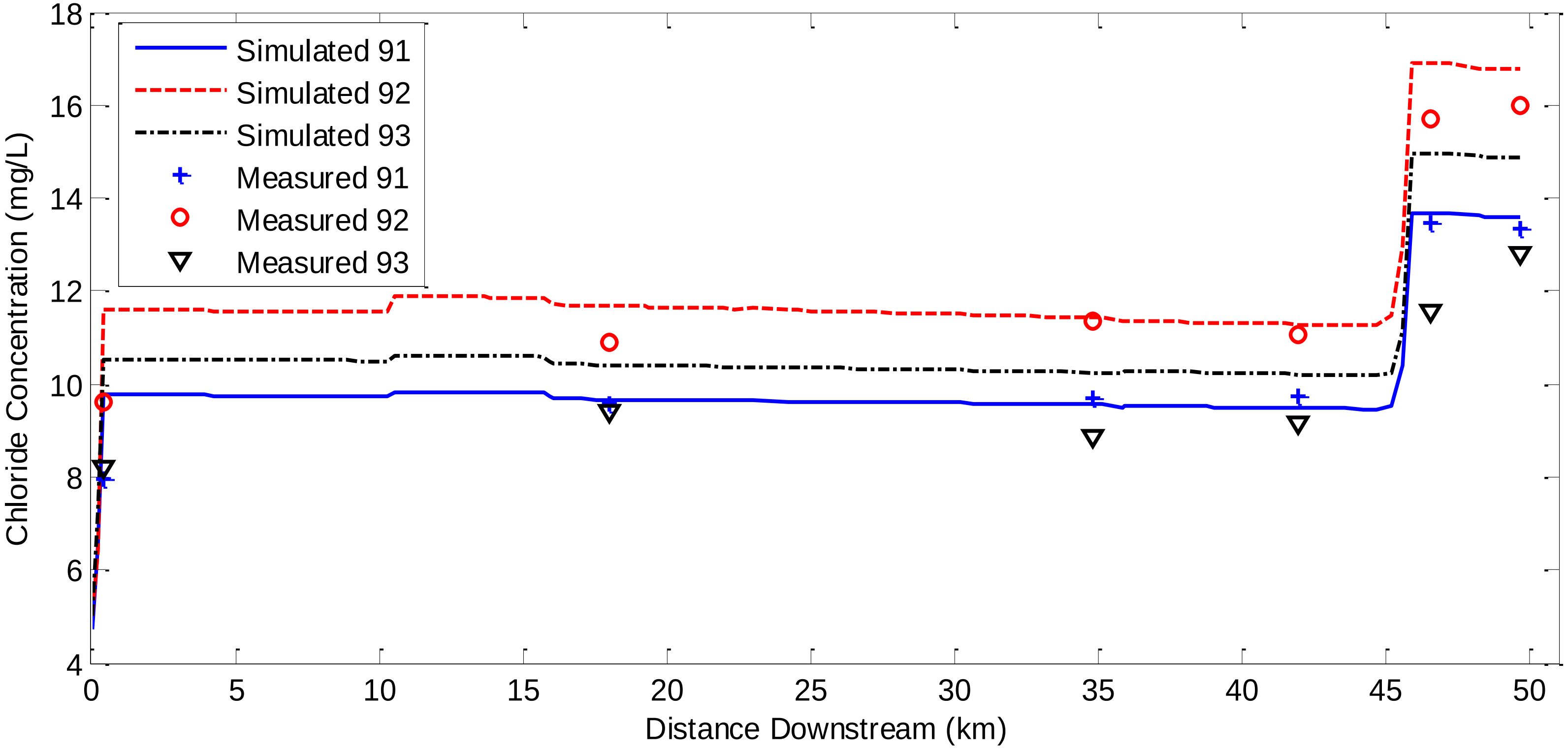
Zooplankton Growth Factor



Chloride Concentration

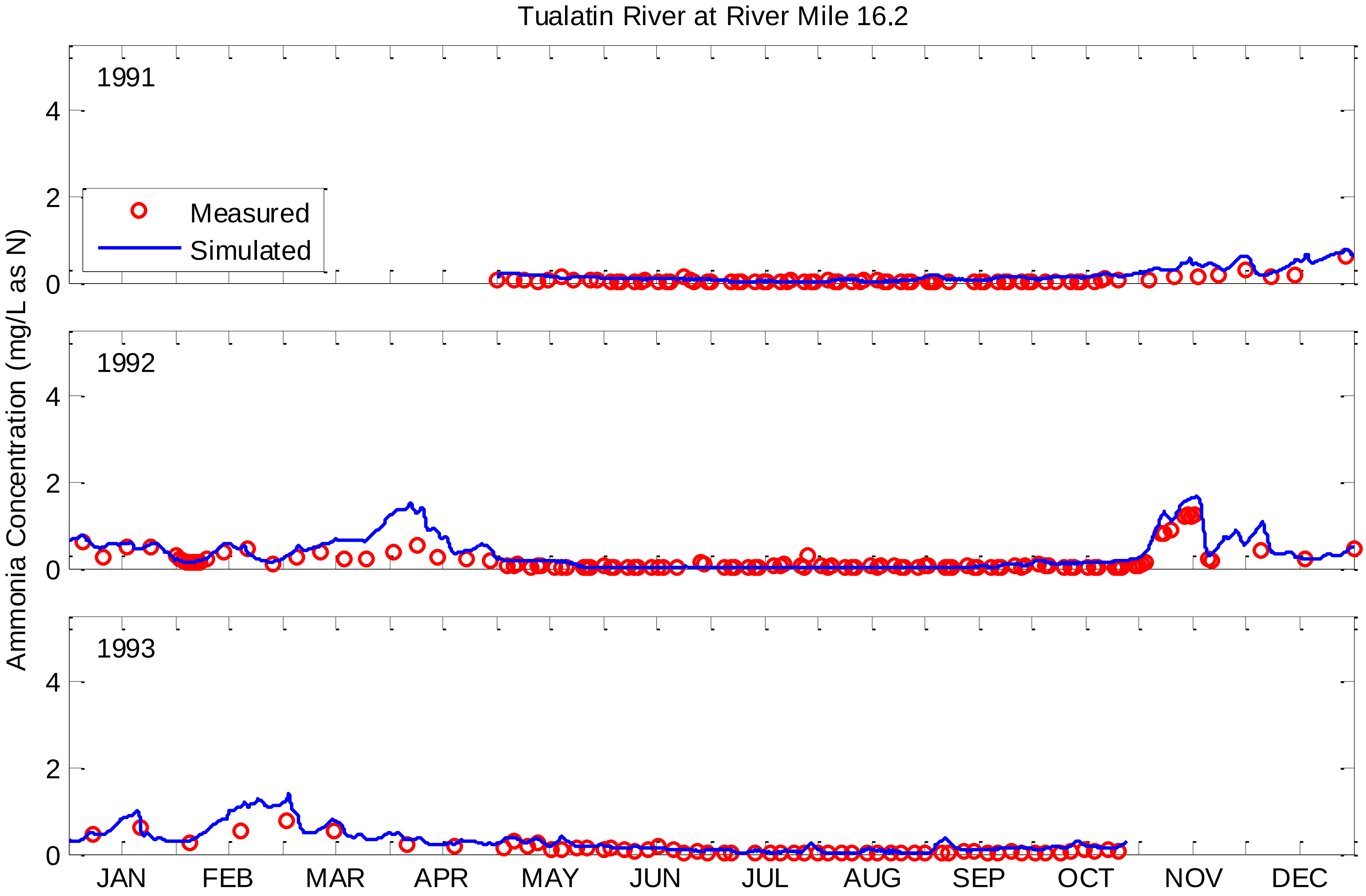


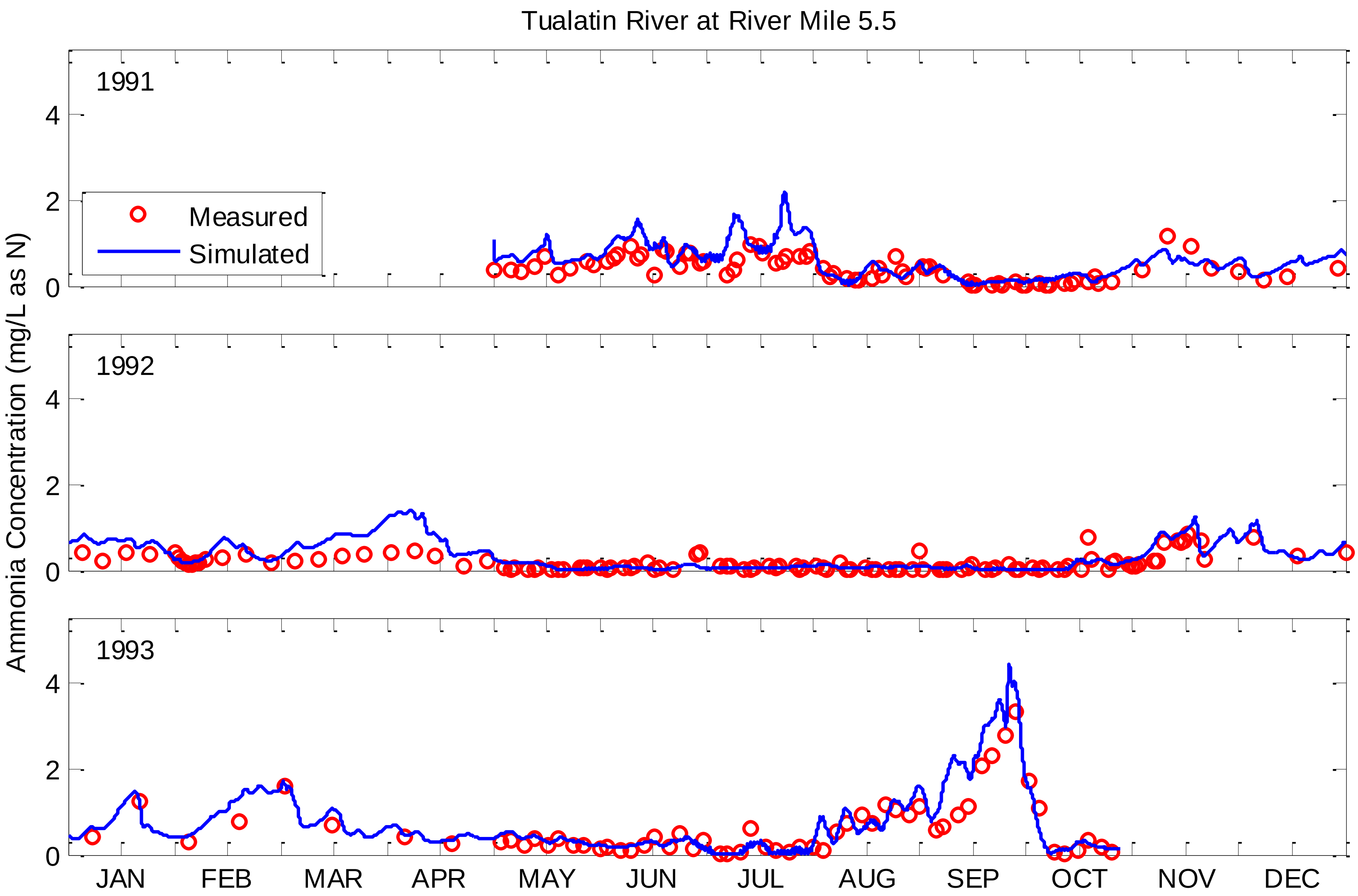

Tualatin River at River Mile 5.5
Chloride Concentration (mg/L)
1991
1992
1993
Measured
Simulated
0
10
20
30
JAN
FEB
MAR
APR
MAY
JUN
JUL
AUG
SEP
OCT
NOV
DEC



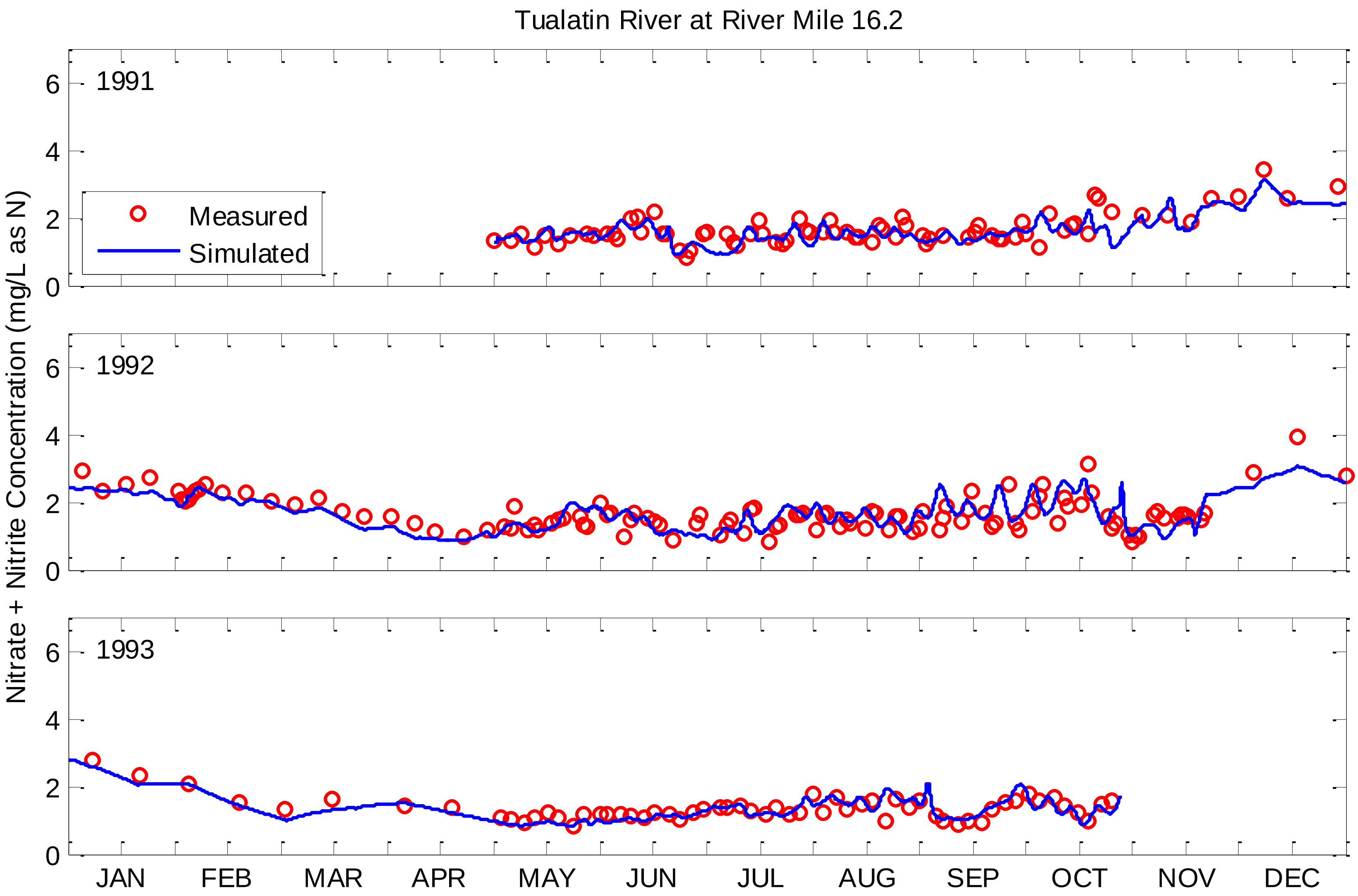
Comparison of the measured and simulated mean chloride concentrations during May–October

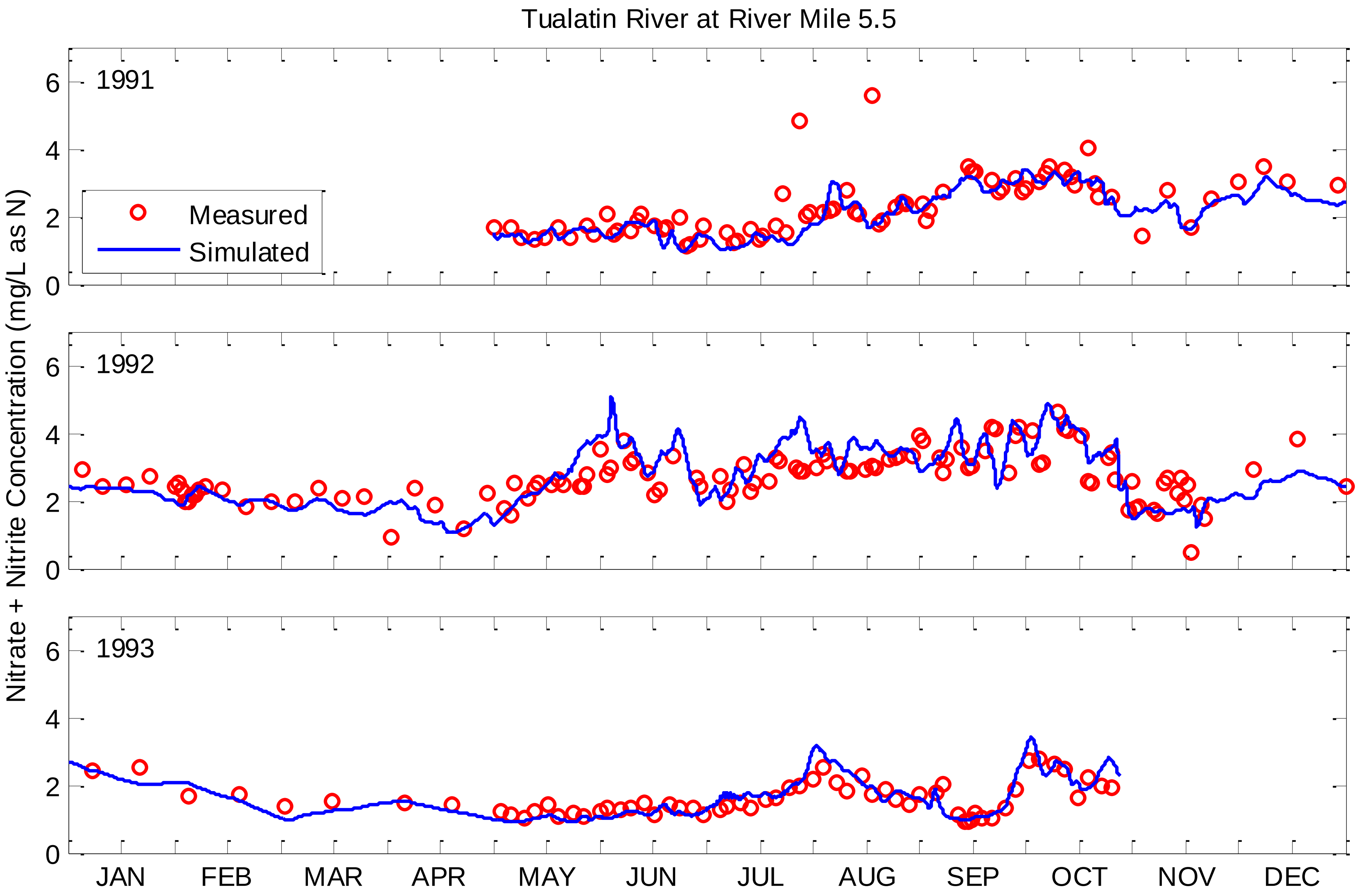
Ammonia Concentration



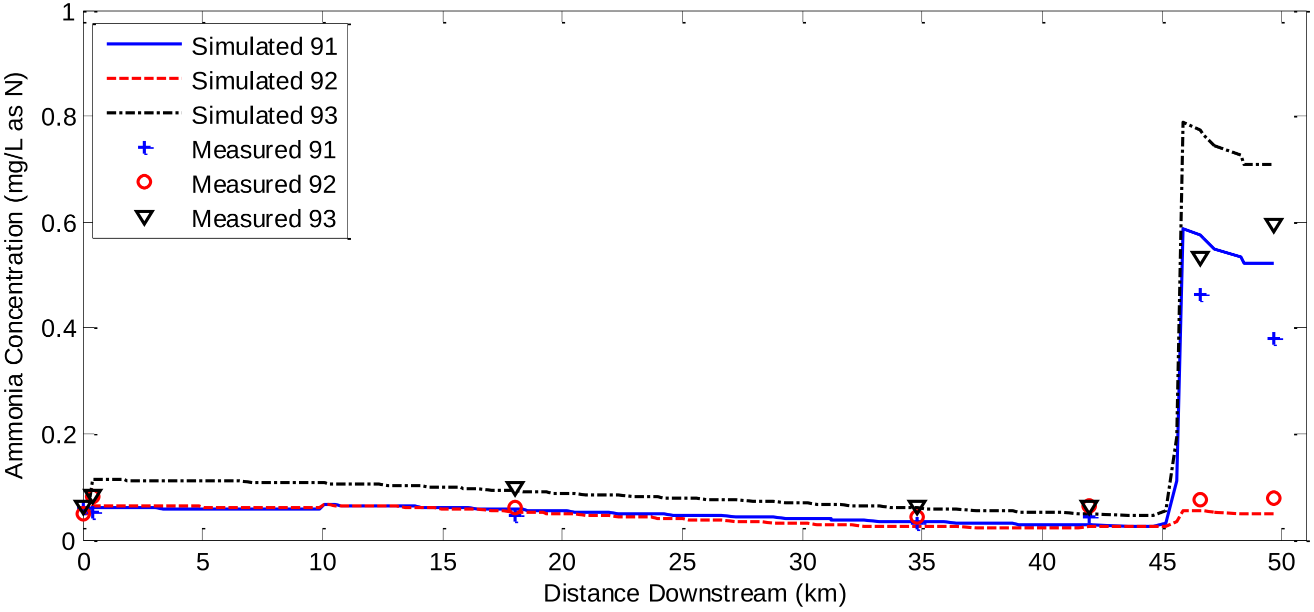

Tualatin River at River Mile 5.5
Ammonia Concentration (mg/L as N)
1991
1992
1993
Measured
Simulated
0
2
4
JAN
FEB
MAR
APR
MAY
JUN
JUL
AUG
SEP
OCT
NOV
DEC

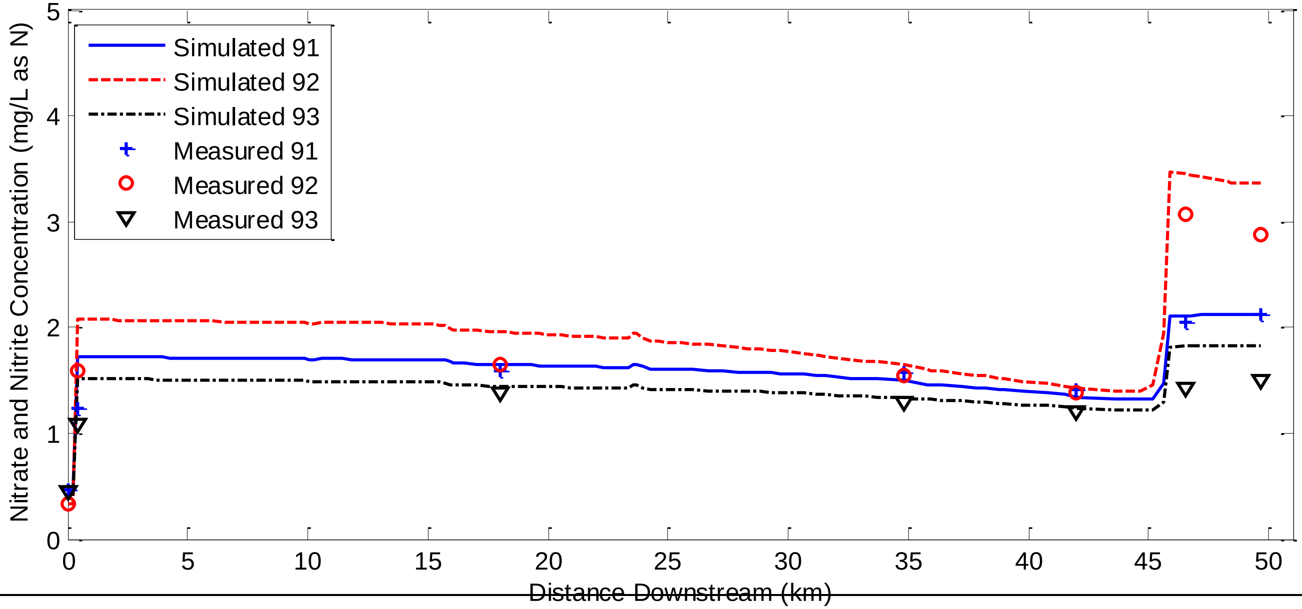
Nitrate + Nitrite Concentration



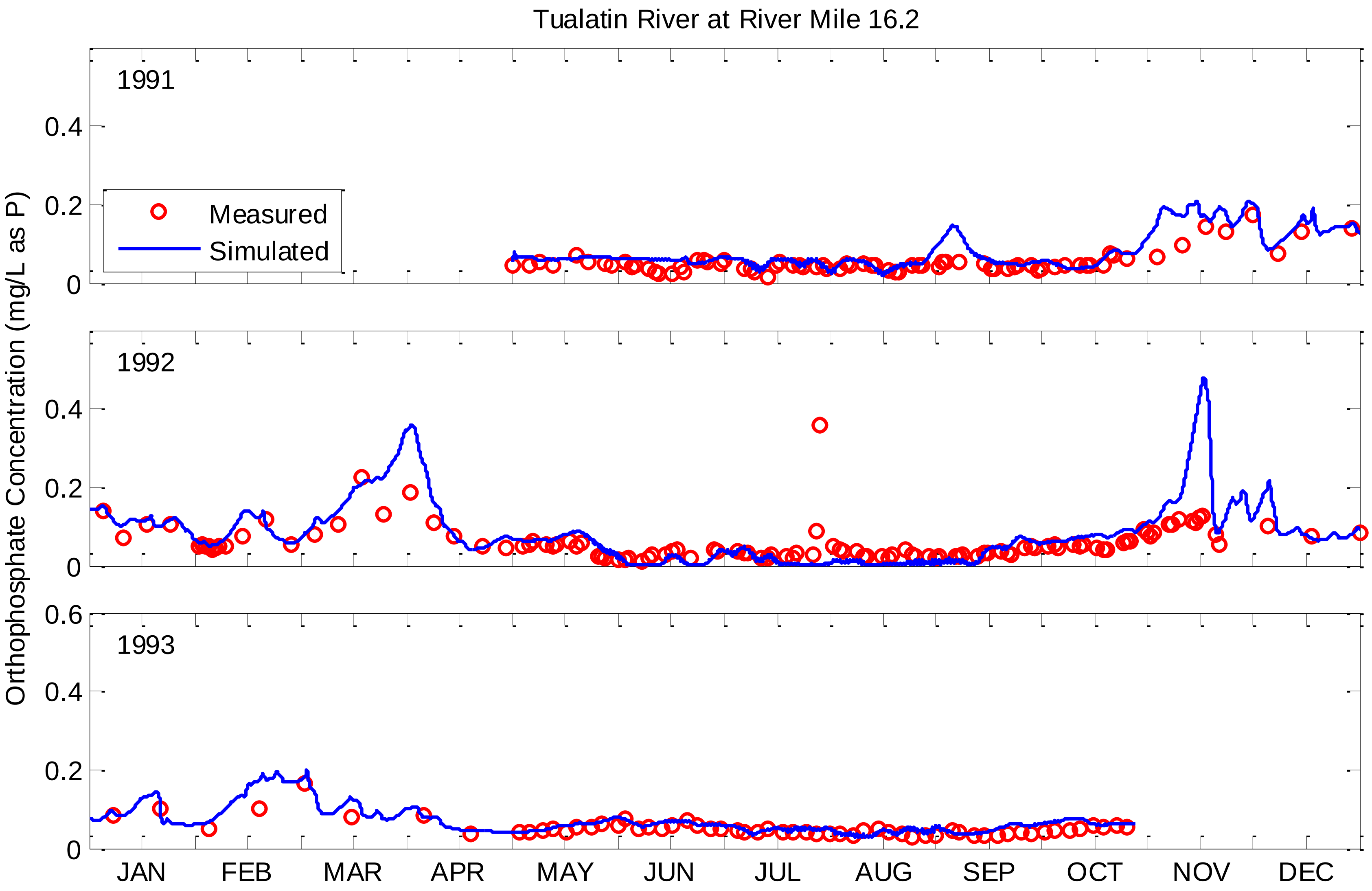

Tualatin River at River Mile 5.5
Nitrate + Nitrite Concentration (mg/L as N)
1991
1992
1993
Measured
Simulated
0
2
4
6
JAN
FEB
MAR
APR
MAY
JUN
JUL
AUG
SEP
OCT
NOV
DEC

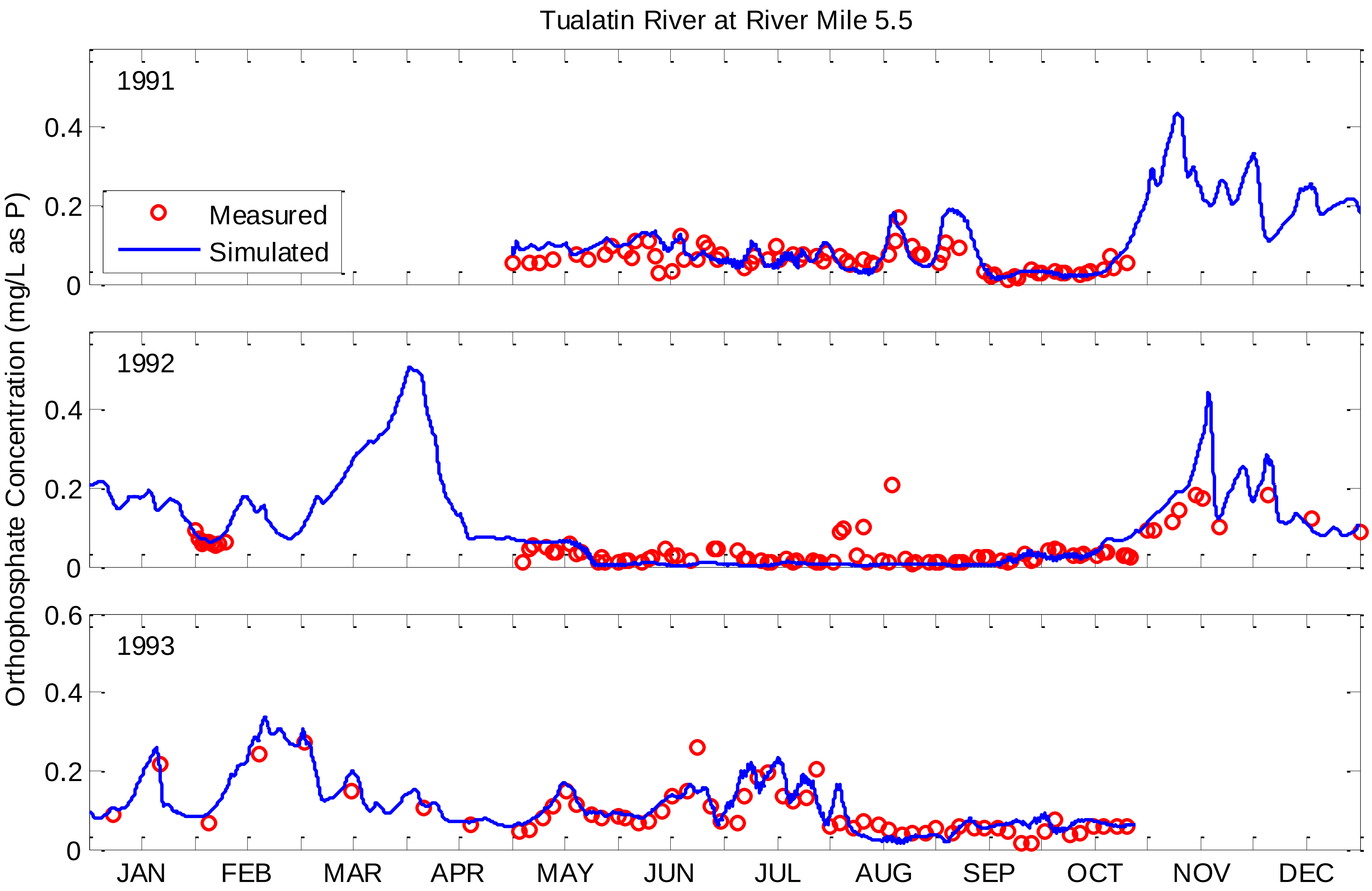
Mean Nitrogen Concentration during May–October

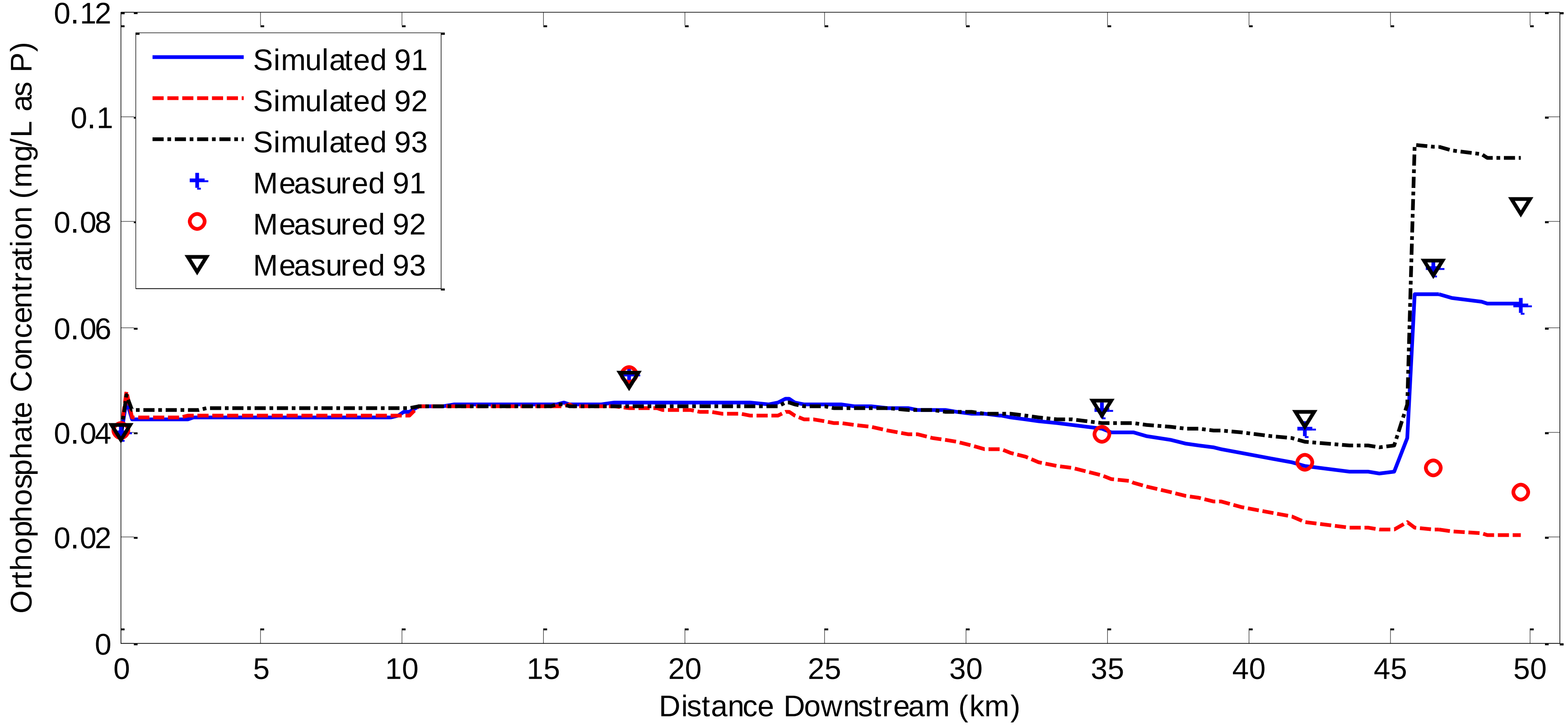




Phosphate Concentration

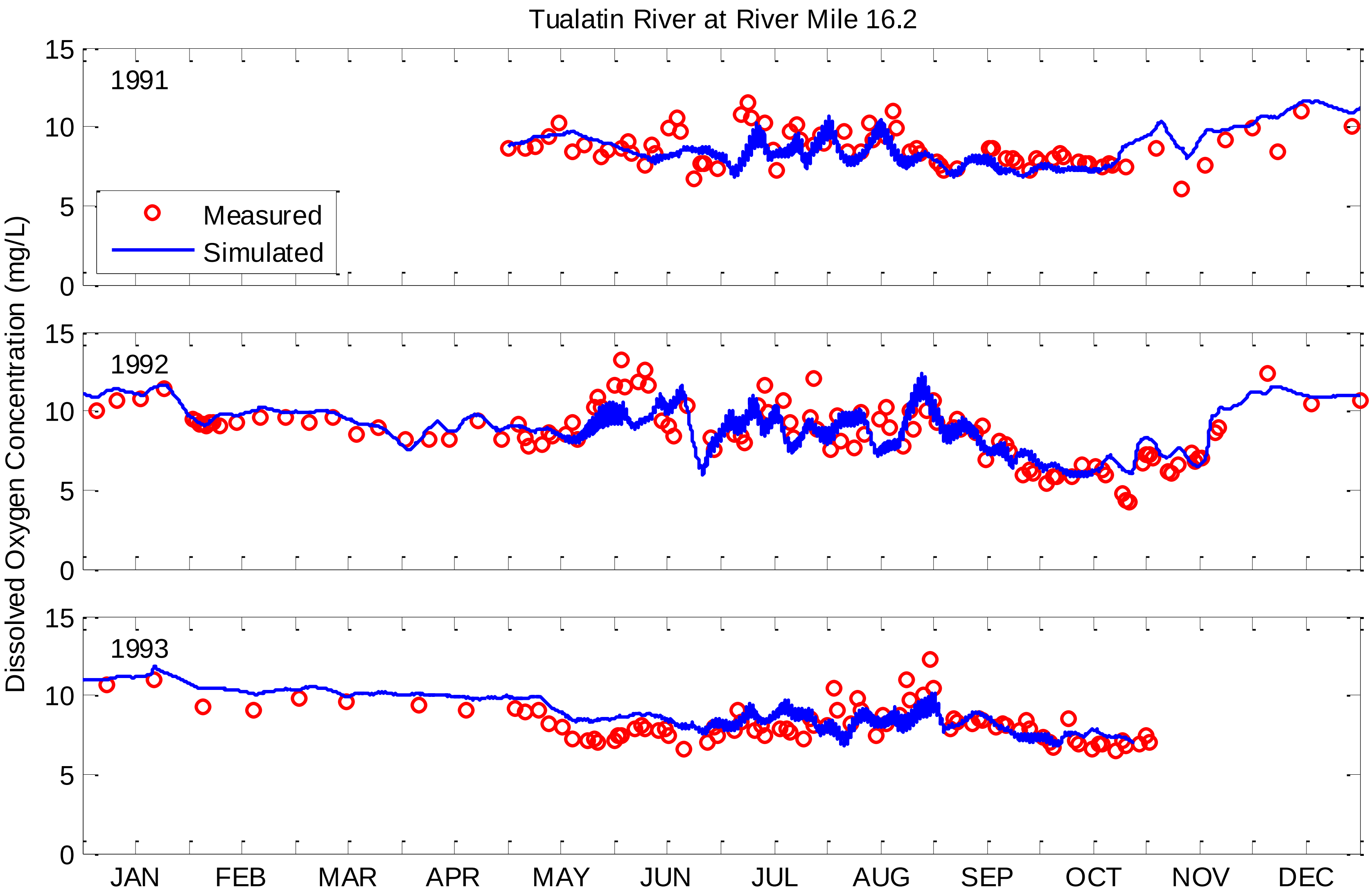


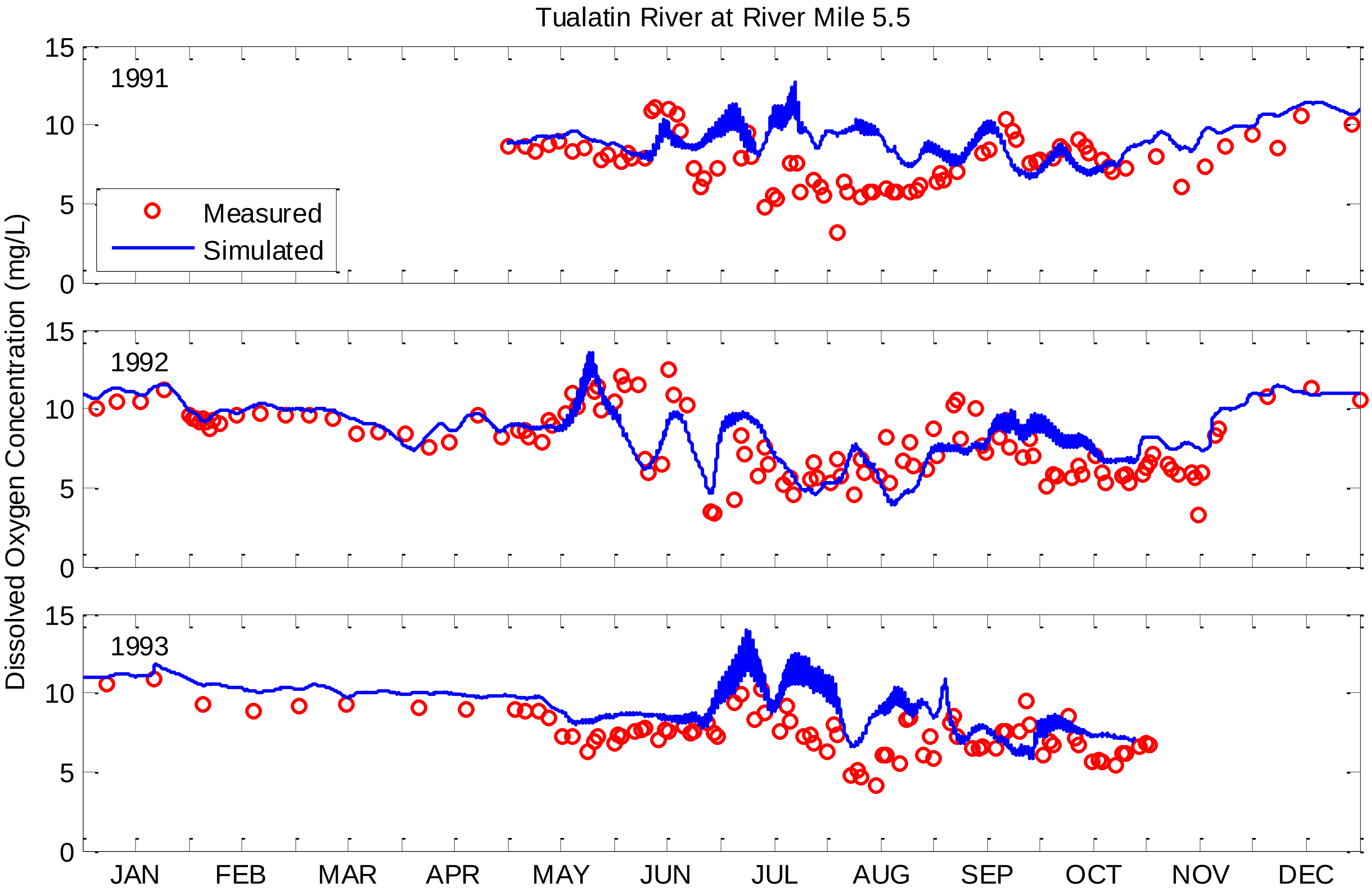

Tualatin River at River Mile 5.5
Orthophosphate Concentration (mg/L as P)
1991
1992
1993
Measured
Simulated
0
0.2
0.4
0.6
JAN
FEB
MAR
APR
MAY
JUN
JUL
AUG
SEP
OCT
NOV
DEC



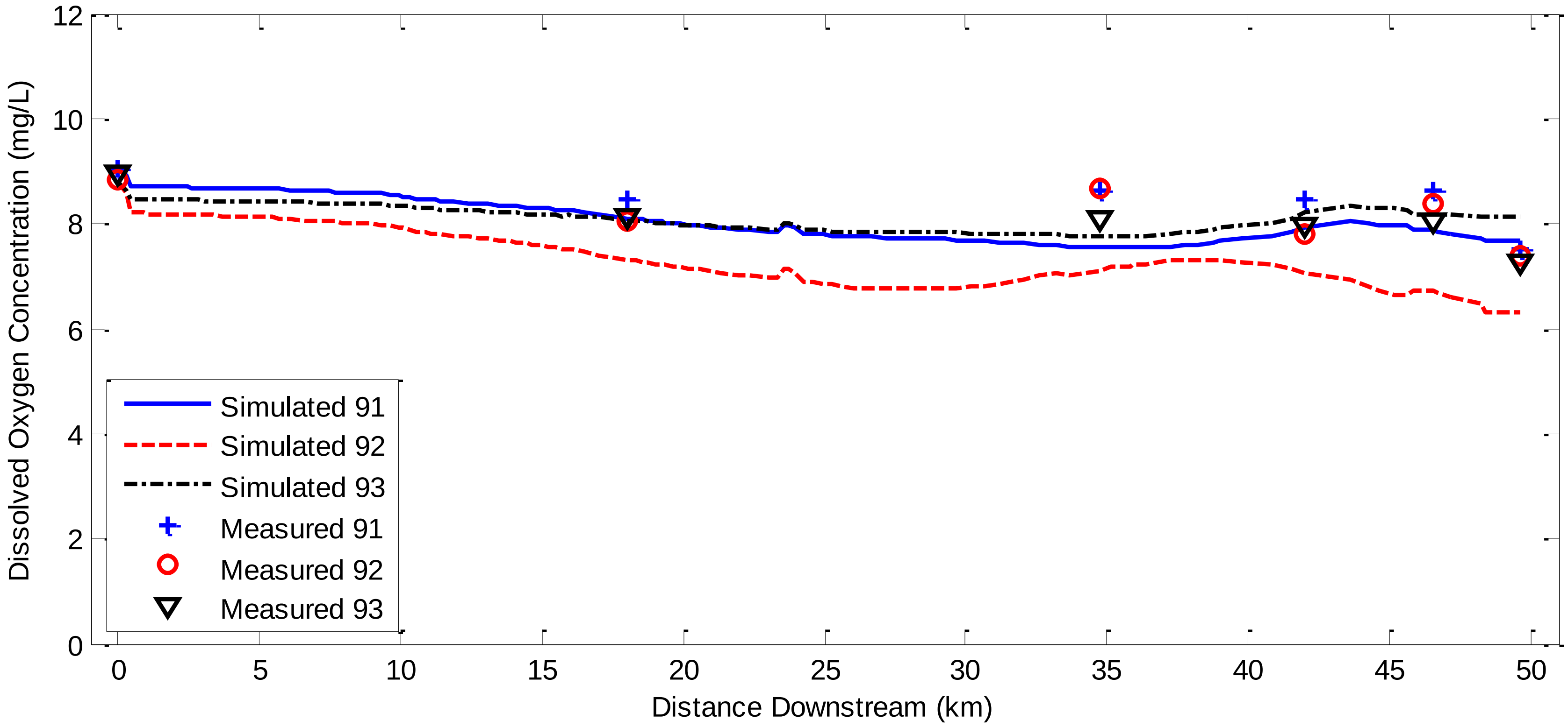
Comparison of the measured and simulated mean phosphate concentrations during May–October

DO Concentration



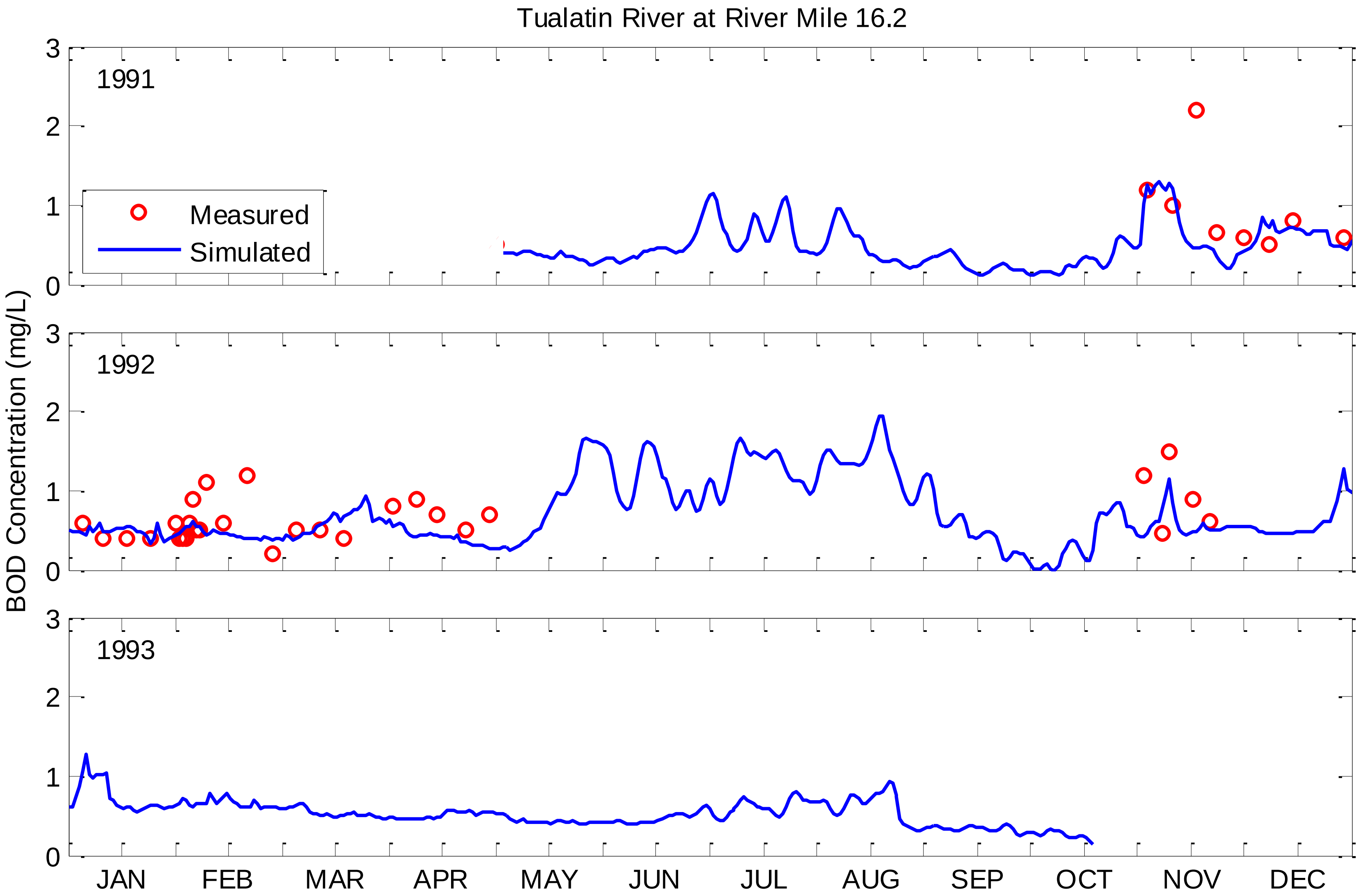


Tualatin River at River Mile 5.5
Dissolved Oxygen Concentration (mg/L)
1991
1992
1993
Measured
Simulated
0
5
10
15
JAN
FEB
MAR
APR
MAY
JUN
JUL
AUG
SEP
OCT
NOV
DEC

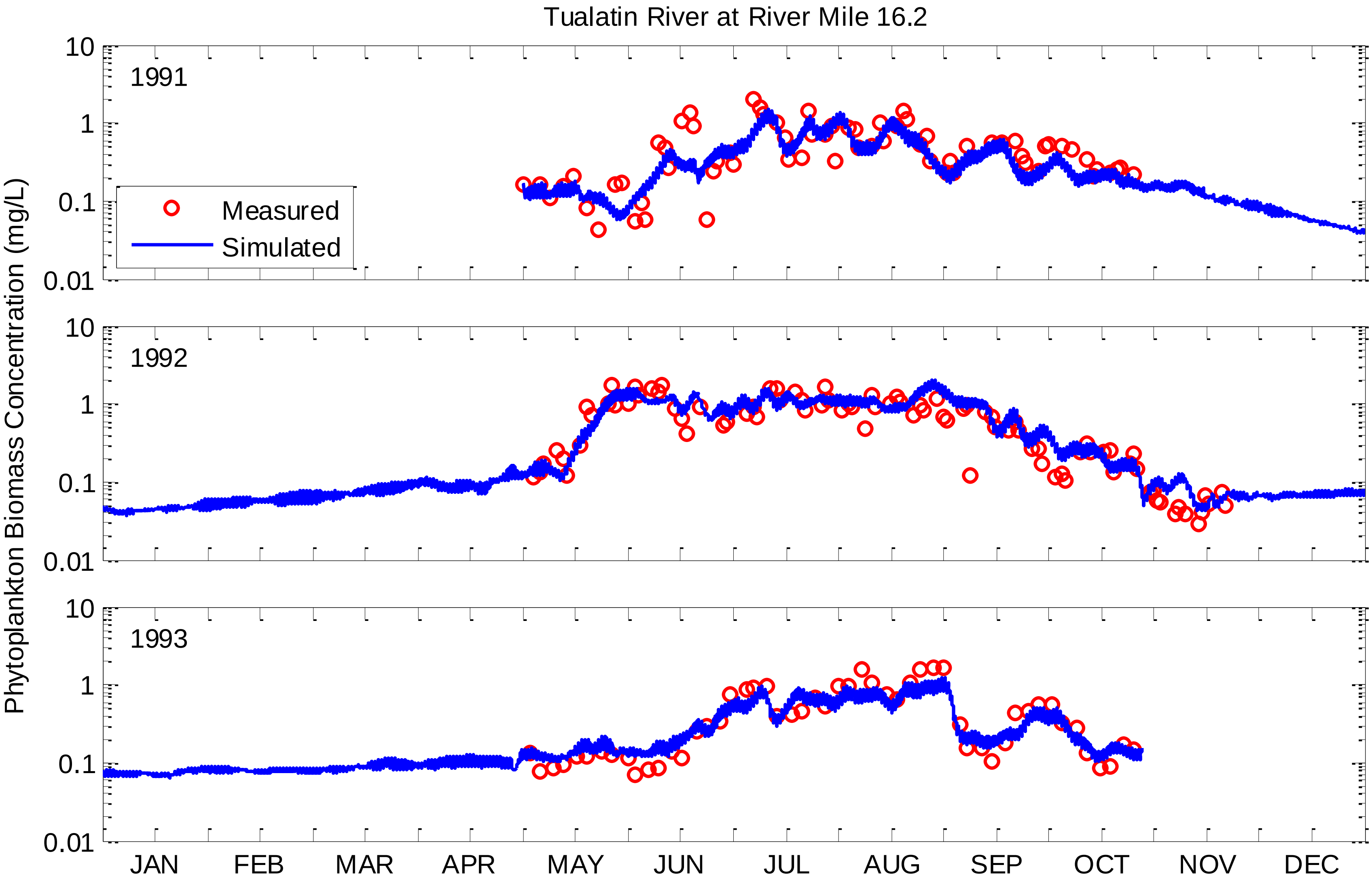


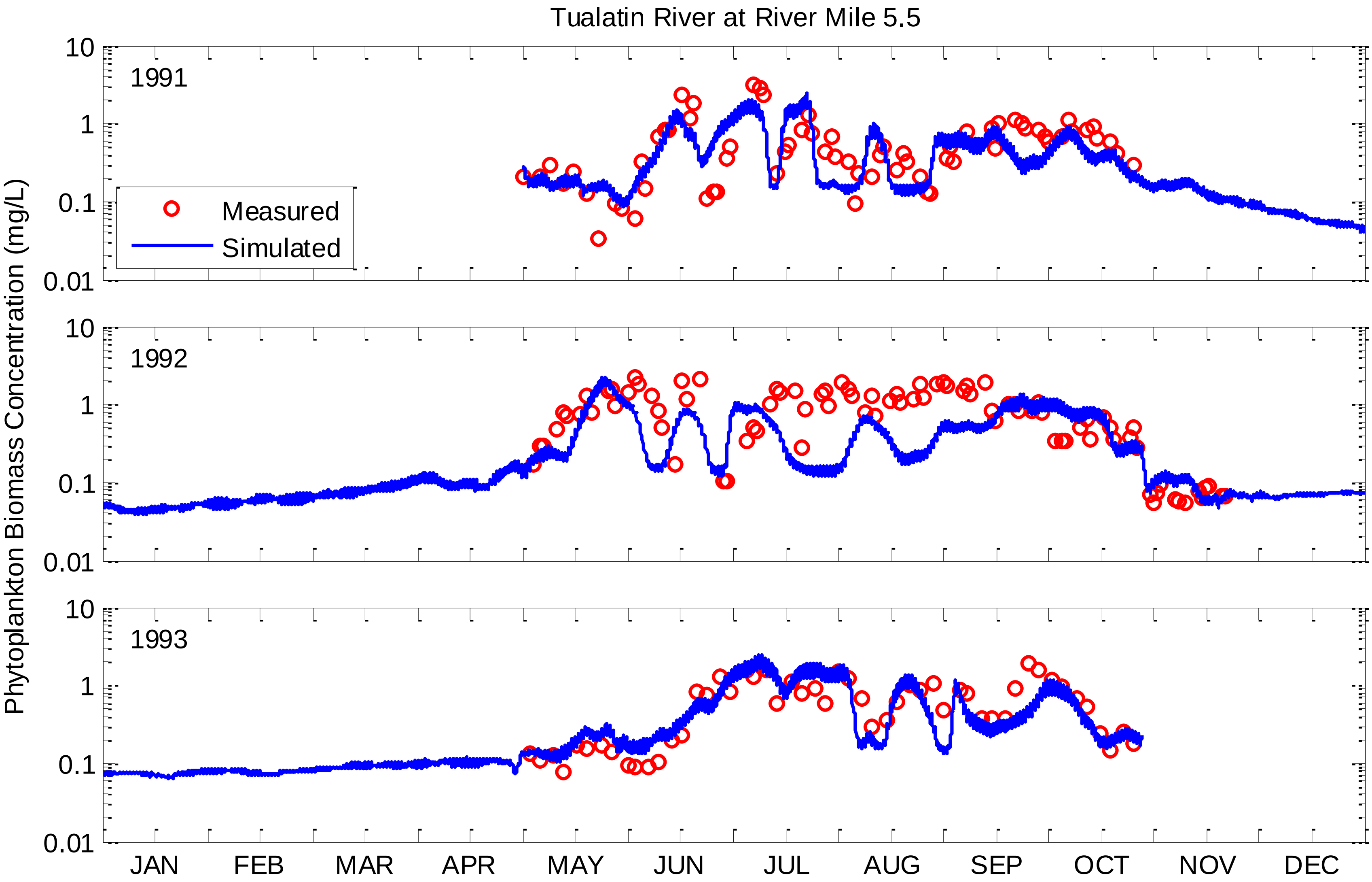
Comparison of the measured and simulated mean DO concentrations during May-October

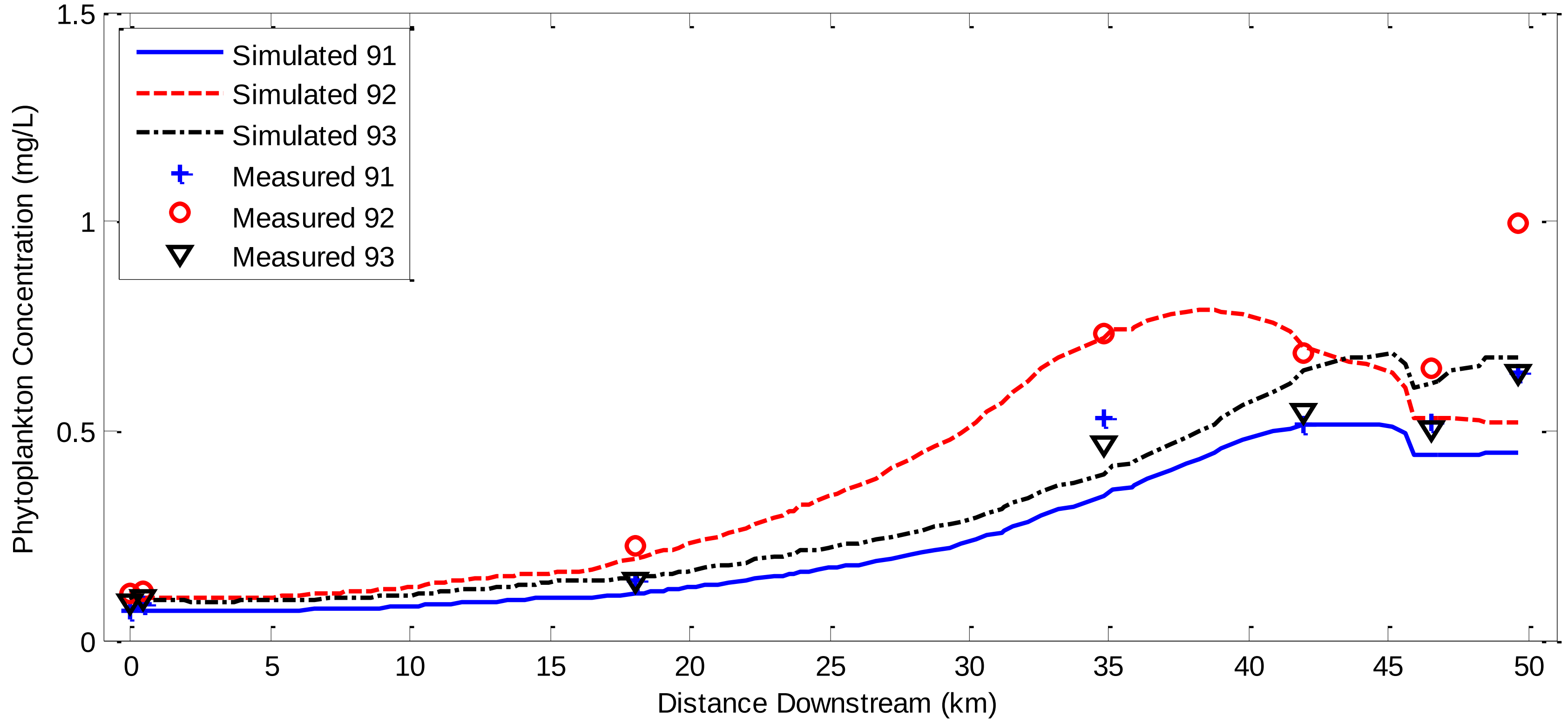
BOD Concentration



Phytoplankton Biomass Concentration

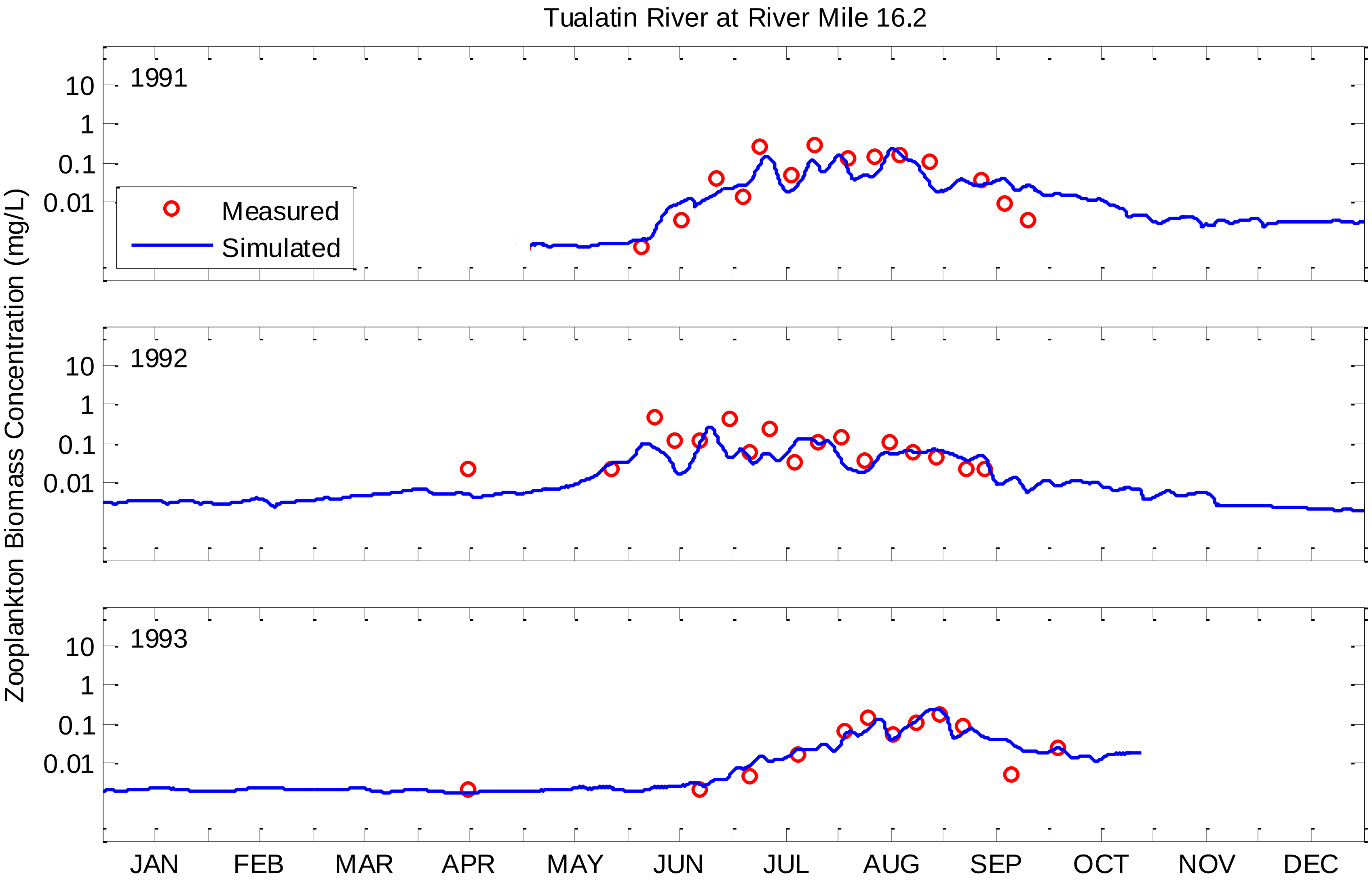


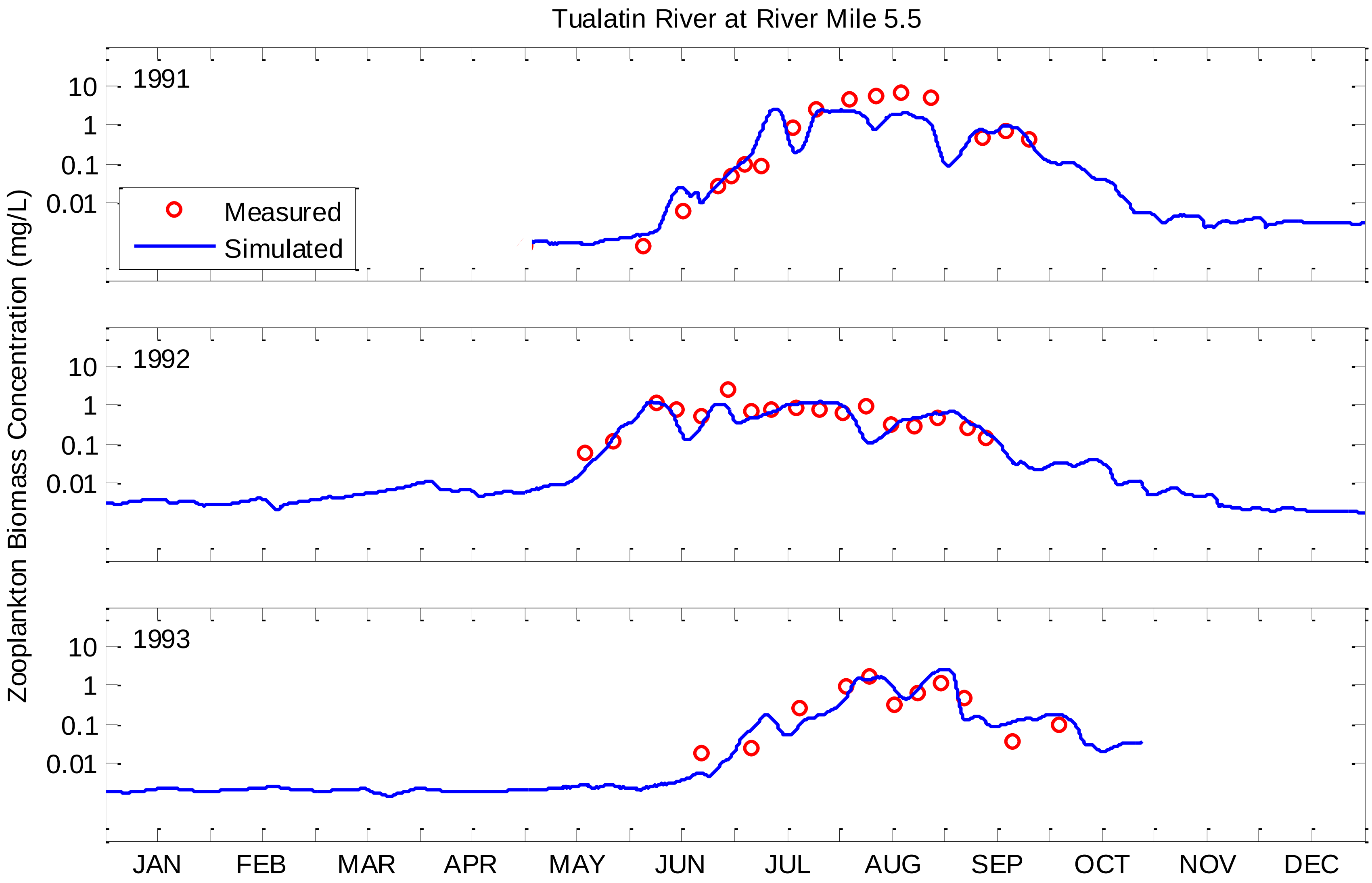

Tualatin River at River Mile 5.5
Phytoplankton Biomass Concentration (mg/L)
10
1
0.1
0.01
1991
1992
1993
Measured
Simulated
JAN
FEB
MAR
APR
MAY
JUN
JUL
AUG
SEP
OCT
NOV
DEC



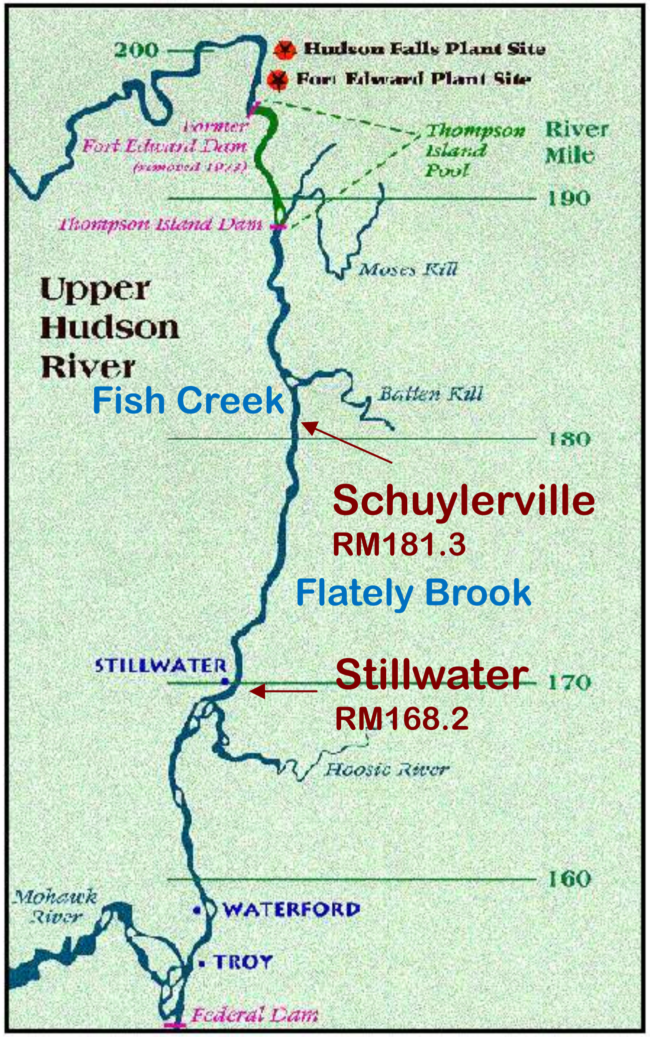
Comparison of the measured and simulated mean phytoplankton concentrations during May–October

Zooplankton Biomass Concentration




Tualatin River at River Mile 5.5
Zooplankton Biomass Concentration (mg/L)
1991
1992
1993
10
1
0.1
0.01
Measured
Simulated
JAN
FEB
MAR
APR
MAY
JUN
JUL
AUG
SEP
OCT
NOV
DEC

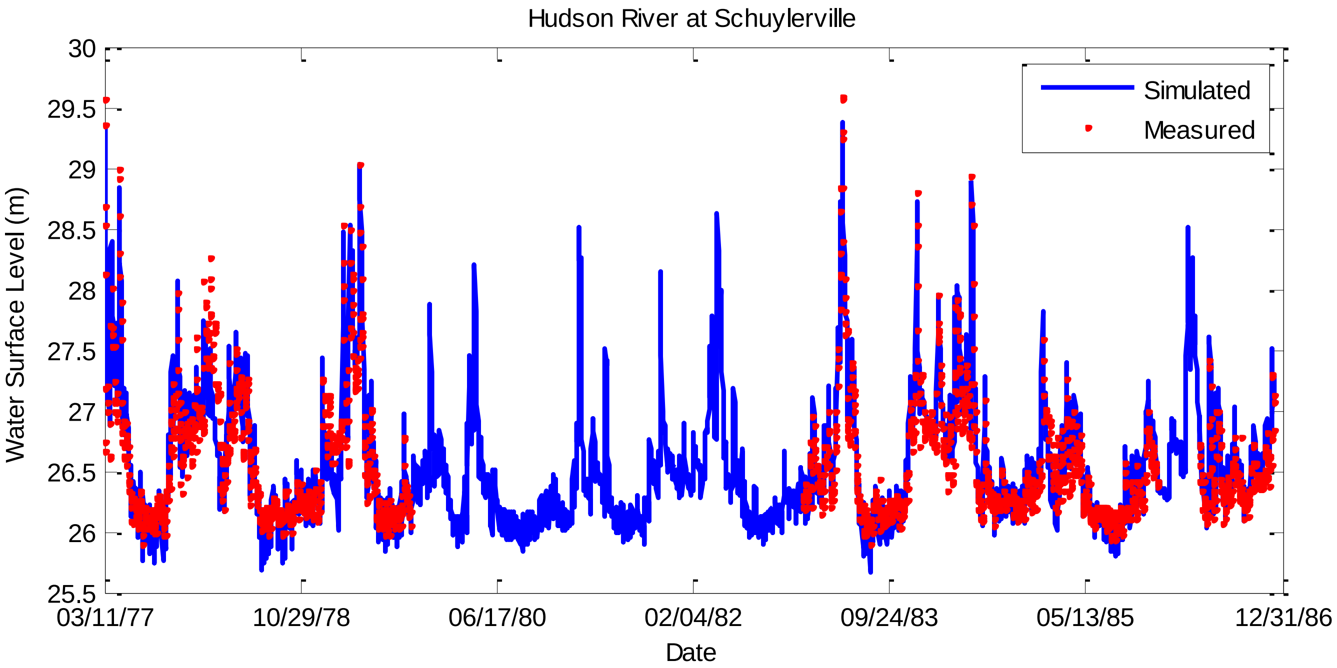
Hudson River, New York



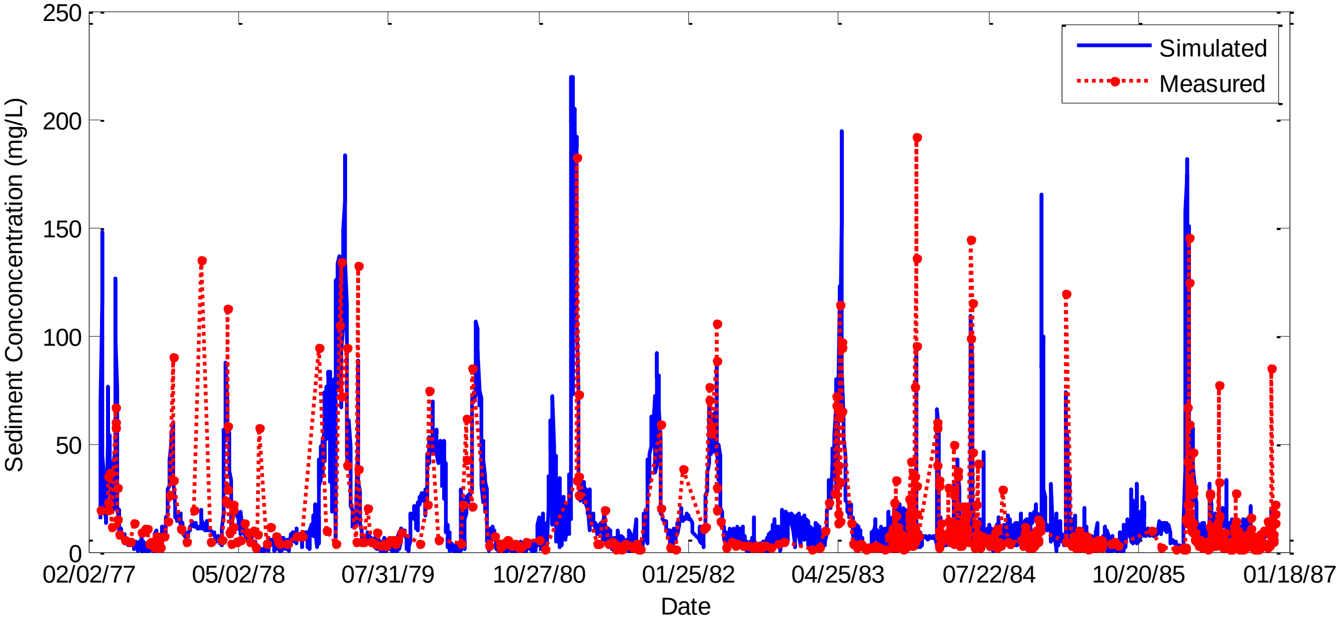
http://www.dec.ny.gov/images/wildlife_images/ex02.gif

- US EPA Superfund site (1983)
- 200-mile reach from Hudson Falls to Battery
- Upper Hudson River (UHR) and Lower Hudson River (LHR)
- PCBs accumulation
- GE company (1947-1977)
  - Hudson Falls
  - Fort Edward
- Simulation Domain: Schuylerville to Stillwater (163 cross-sections)
- Simulation Period: 1977-1983

Hydrodynamic Results

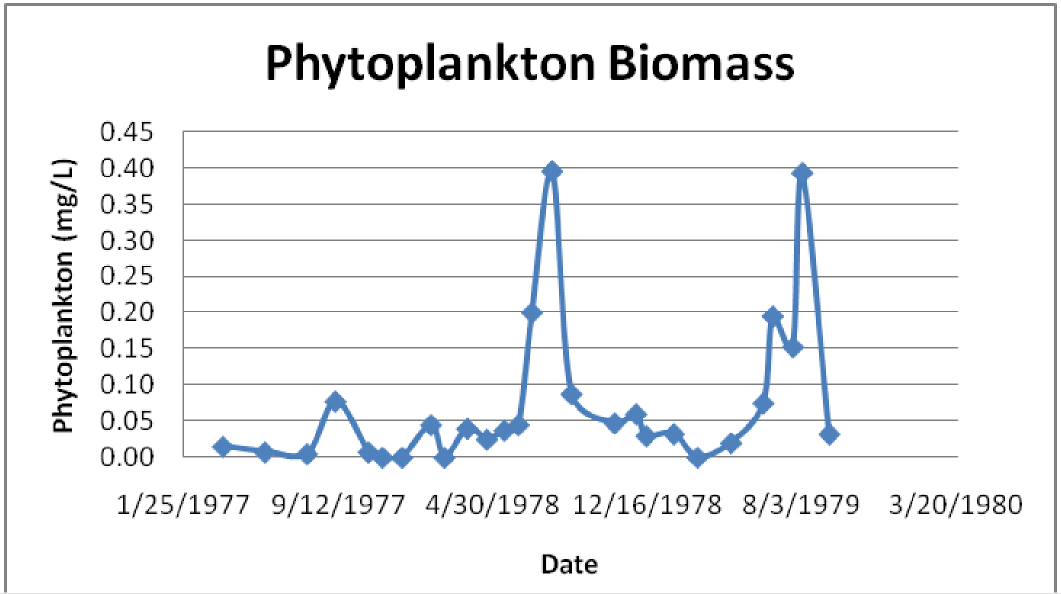


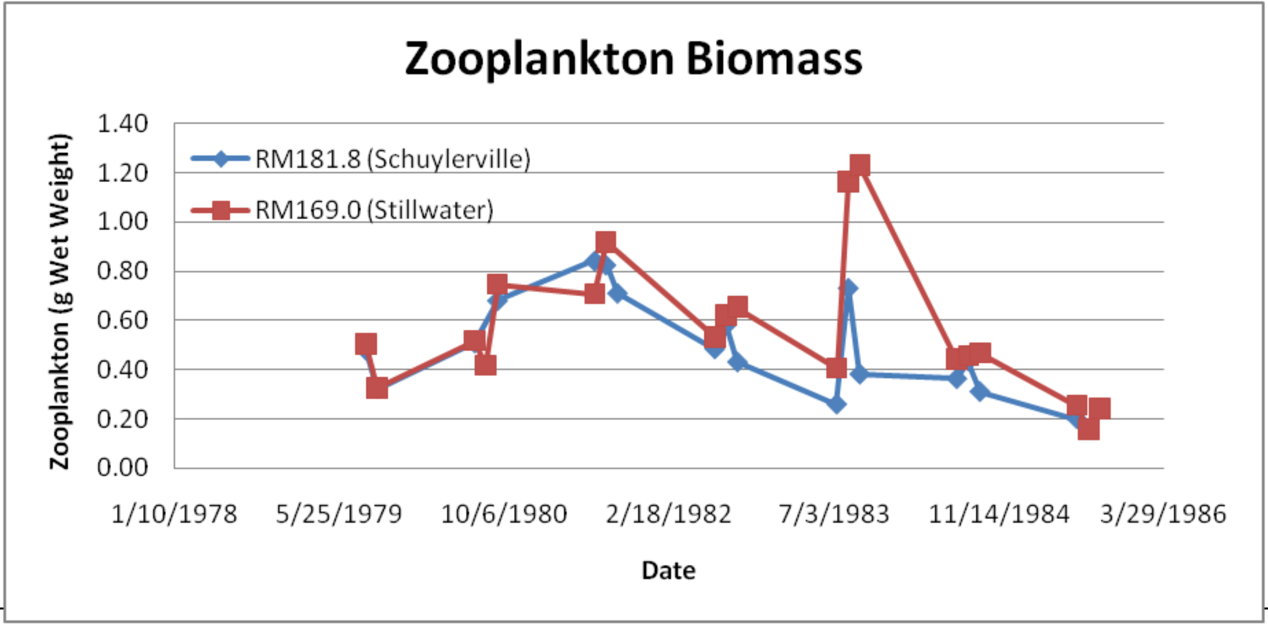
WSL

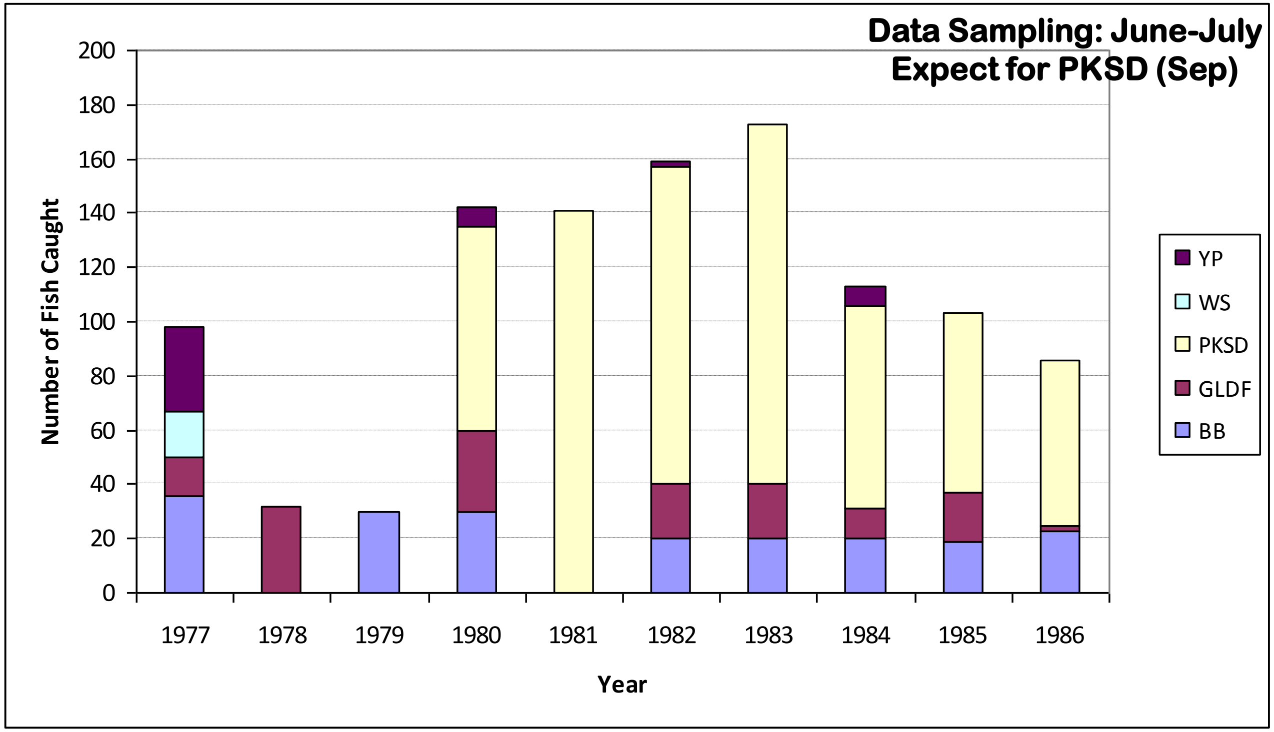


Sediment

Phytoplankton and Zooplankton







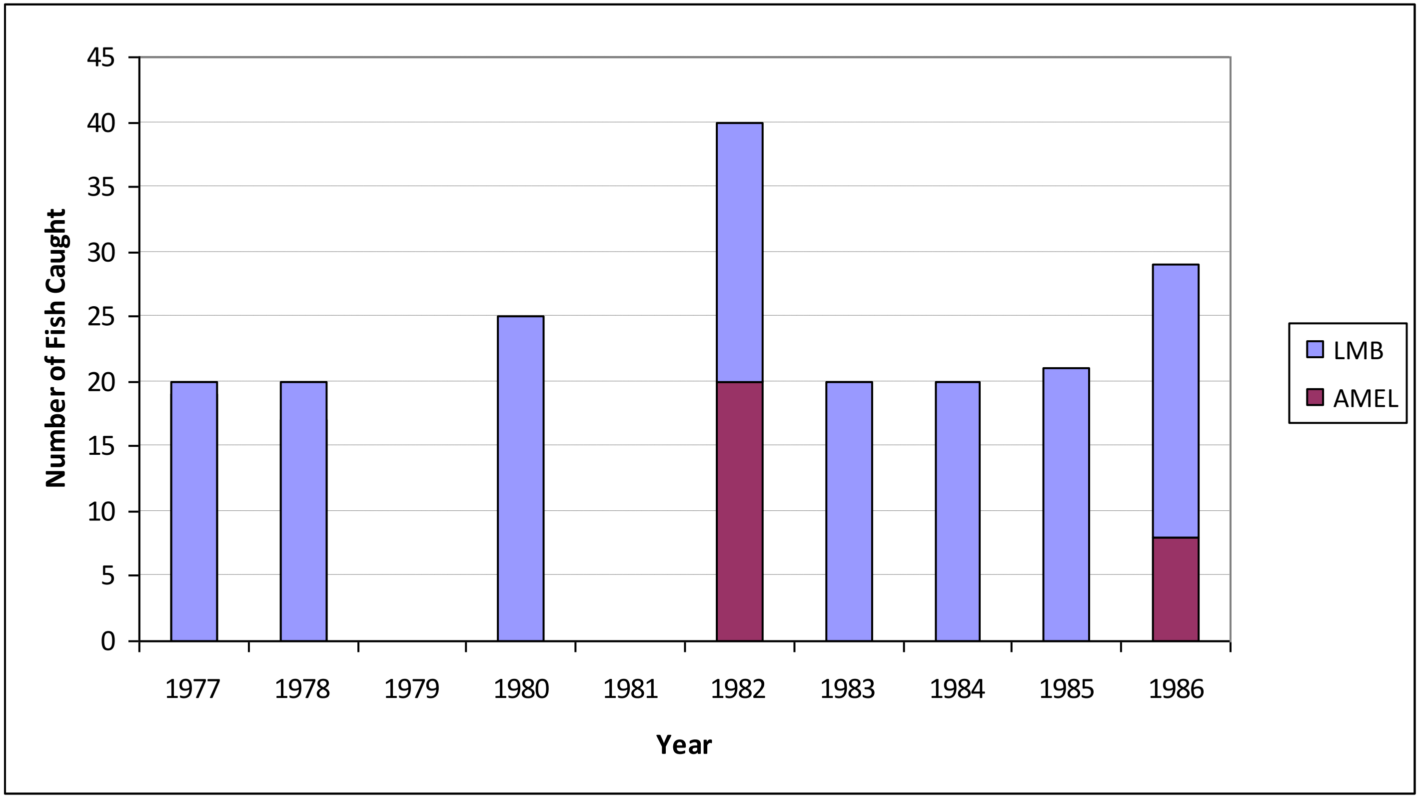
YP: Yellow Perch

WS: White sucker

BB head

Number of fish classified by weight

Fish	Fish weight (g)						Total
	<200	200-400	400-600	600-800	800-1000	>1000	
BB	19	98	71	10	0	0	198
GLDF	18	60	37	23	7	1	146
PKSD	732	0	0	0	0	0	732
WS	0	8	9	0	0	0	17
YP	42	5	0	0	0	0	47
Total	811	171	117	33	7	1	1140



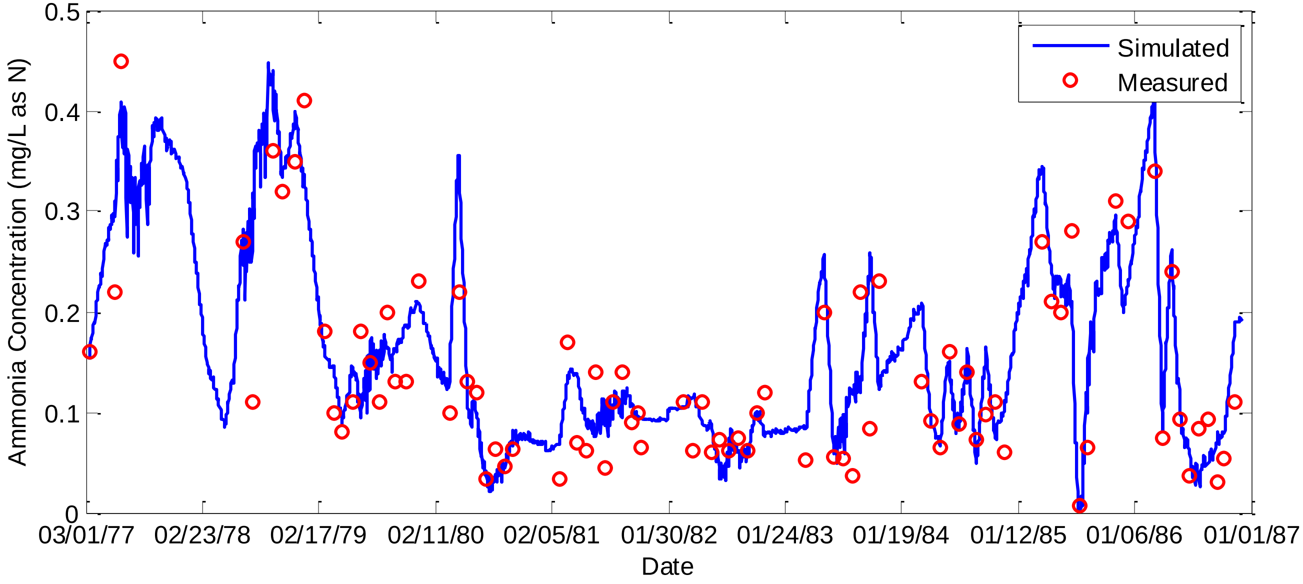
LMB: Largemouth bass

AMEL: American eel

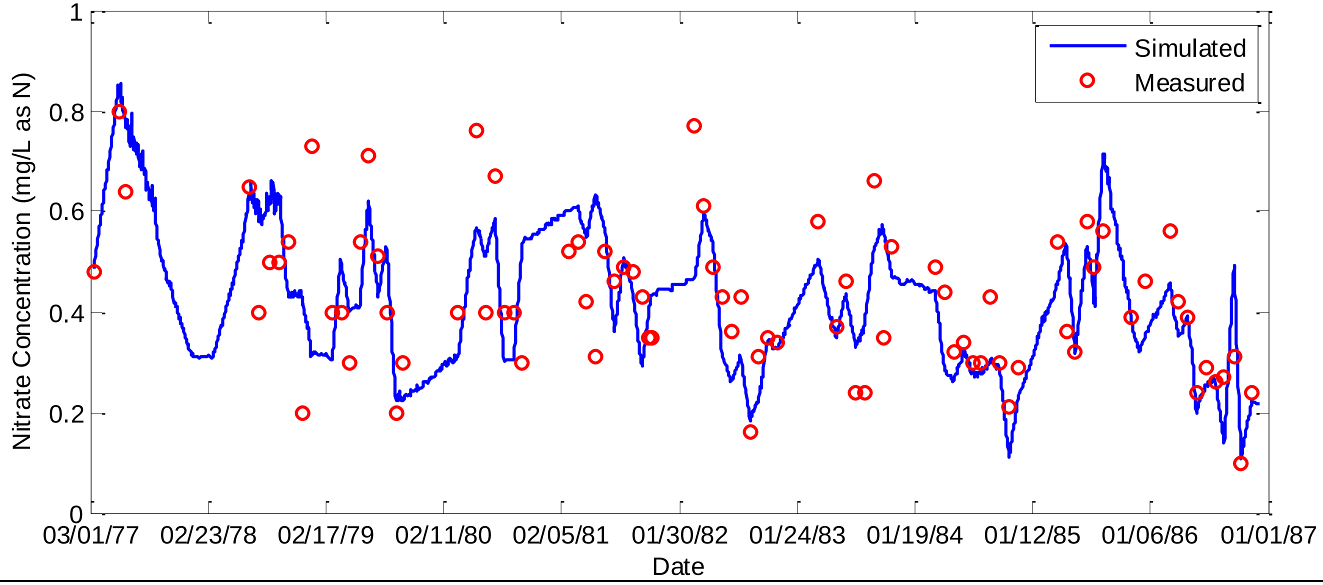
Number of fish classified by weight

Fish	Fish weight (g)						Total
	<200	200-400	400-600	600-800	800-1000	>1000	
AMEL	8	8	7	5	0	0	28
LMB	16	58	60	47	16	7	204
Total	24	66	67	52	16	7	232

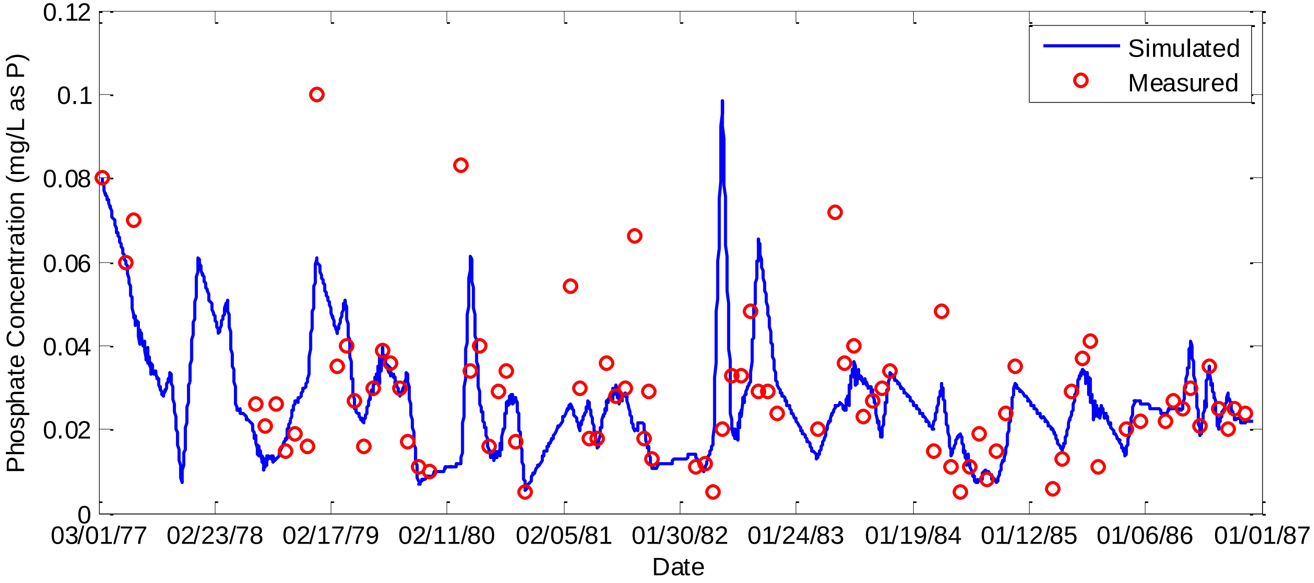
Simulation Results



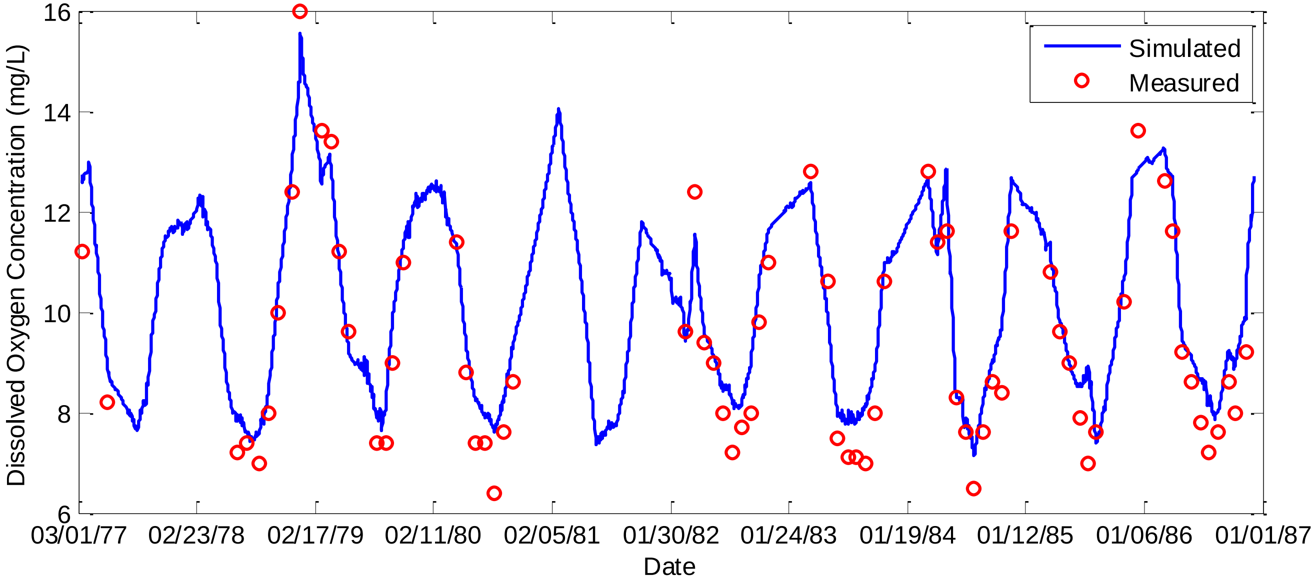
Ammonia



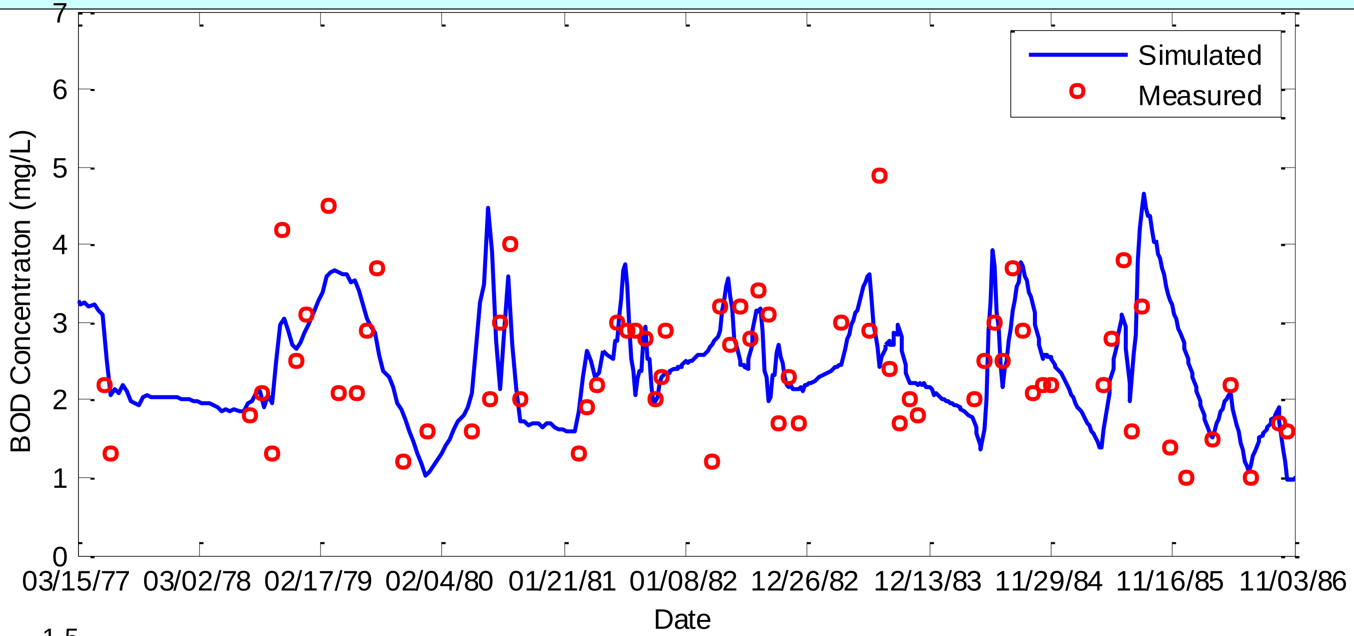
Nitrate



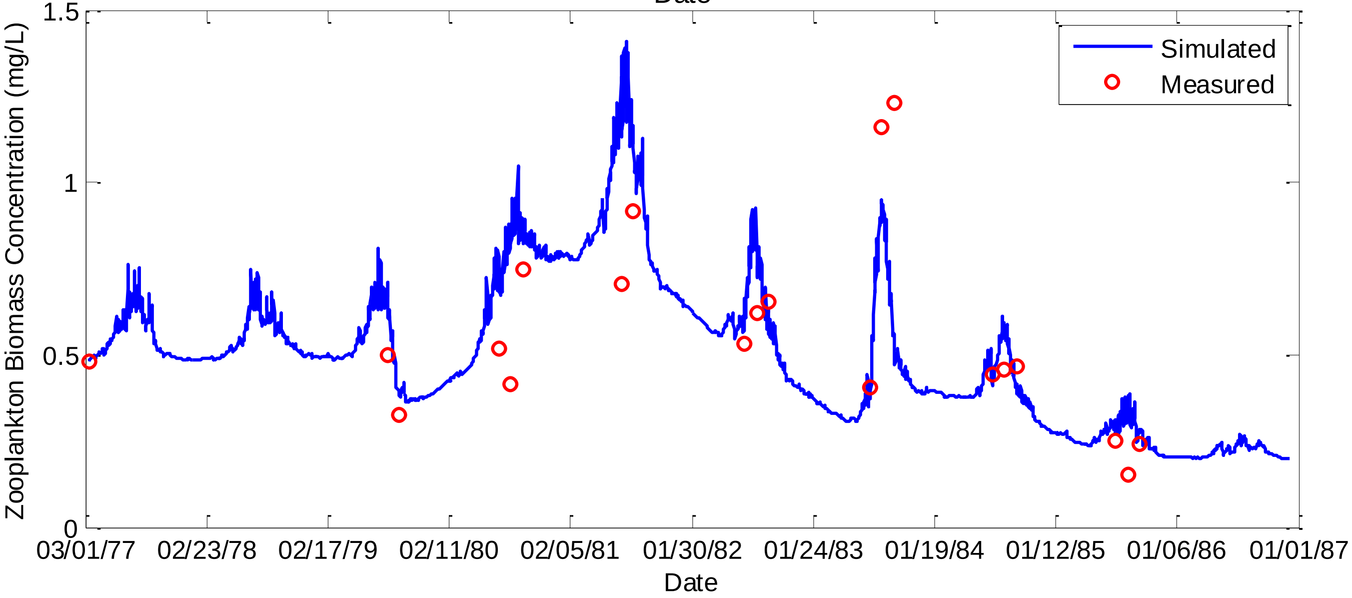
Phosphate



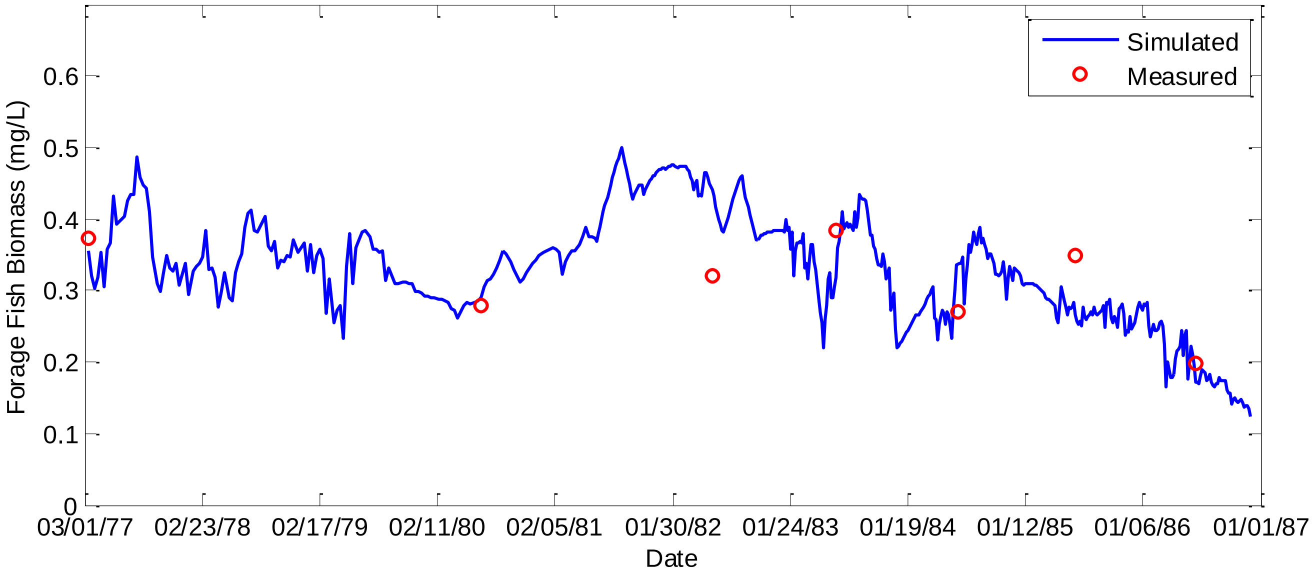
DO



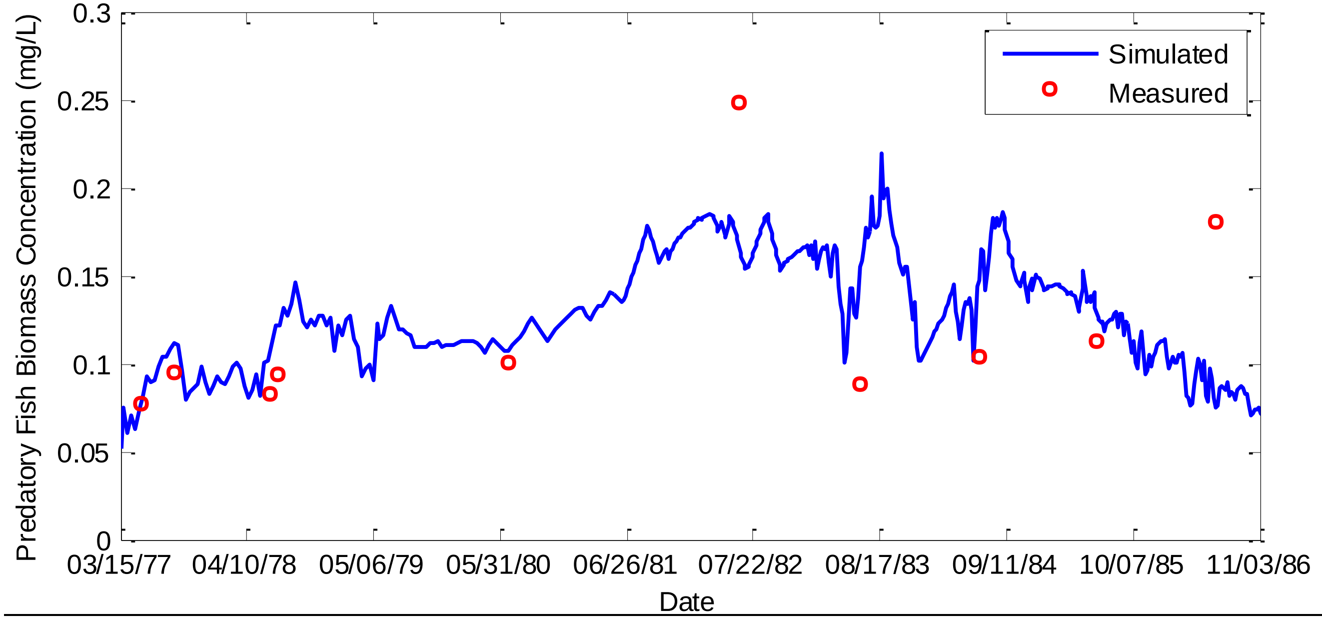
BOD



Zooplankton

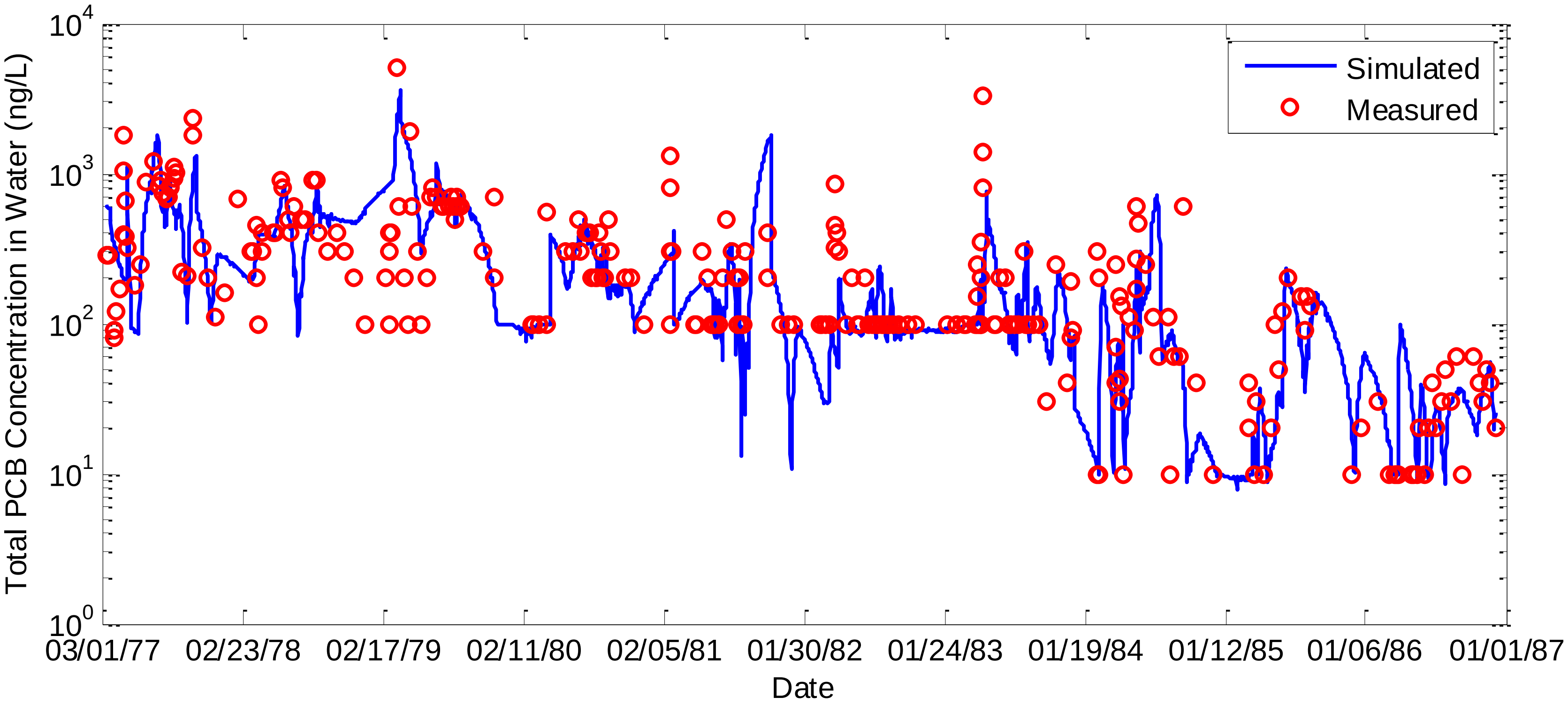


Forage Fish

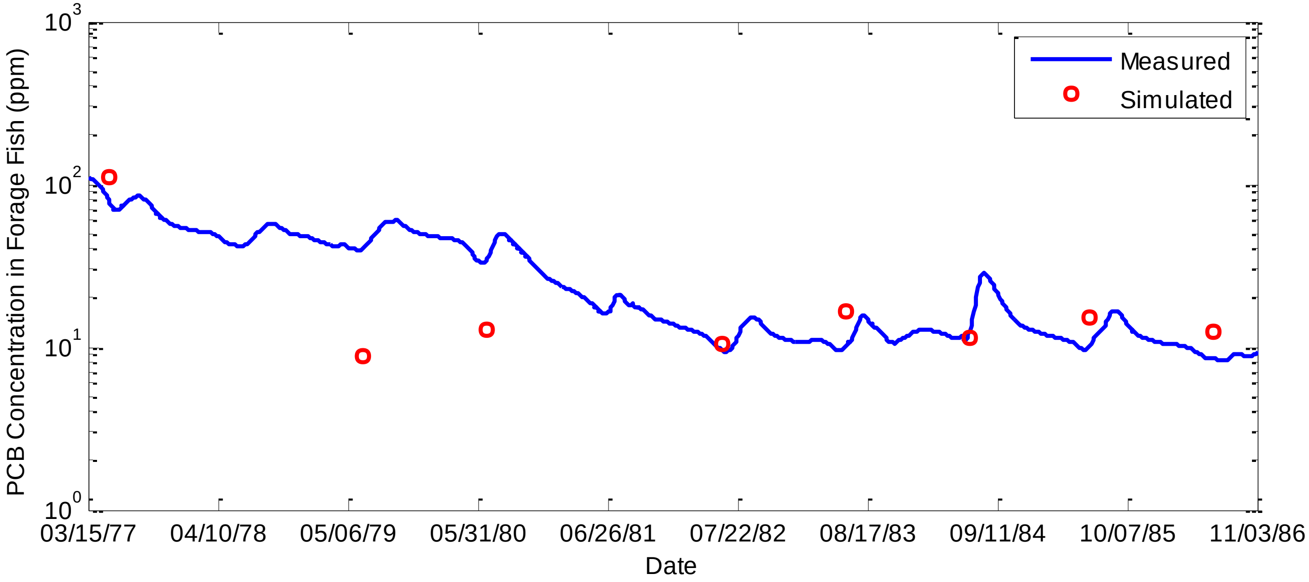


Predatory Fish

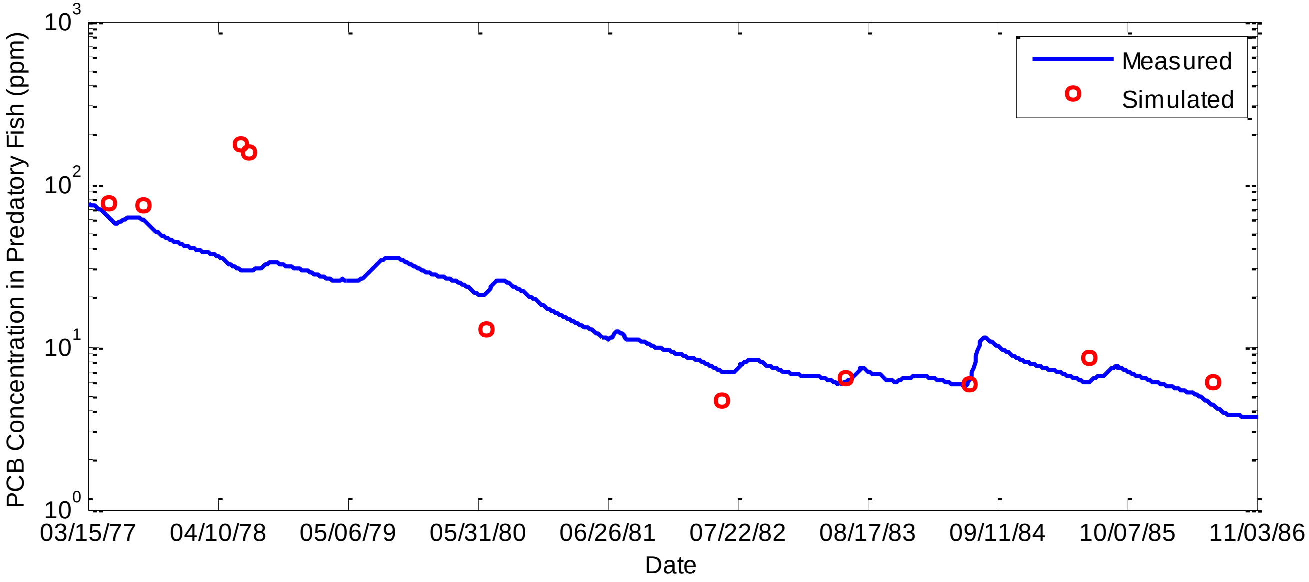
Total PCB Concentration in Water at Stillwater



PCB Concentration in Fish



Forage Fish



Predatory Fish

Conclusions

- A water temperature model has been implemented in the existing CCHE1D model package, which calculates the water temperature by considering four major heat fluxes: short-wave radiation, long-wave radiation, latent heat flux, and sensible heat flux.
- An integrated water quality and aquatic ecosystem model has been developed to simulate eight water quality constituents and four trophic levels: phytoplankton, zooplankton, forage fish, and predatory fish.
- A contaminant transport and aquatic ecotoxicology model has been implemented to simulate the transport of contaminants in water column and sediment bed.
- In bioaccumulation model, the concentrations of toxic chemicals in organisms are influenced by the direct uptake from water, depuration, respiration, and dietary.
- The model computes the toxicity effects of contaminants through modification factors for the growth, grazing, reproduction, and mortality of organisms in the aquatic food web.
- The model has been applied in the simulation of the fate and transport of polychlorinated biphenyls (PCBs) in the Upper Hudson River, New York.

Publications Related

P. Inthasaro (2010). “A one-dimensional aquatic ecology and ecotoxicology model in river systems.” PhD Dissertation, The University of Mississippi, USA.

P. Inthasaro and W. Wu (2014). “One-Dimensional Model of Water Quality and Aquatic Ecosystem/Ecotoxicology in Rivers.” Advances in Water Resources Engineering, C.T. Yang and L.K. Wang (eds), The Humana Press, Inc., Totowa, NJ, USA, in press.