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RESCUER

Modeling Water Quality in Dynamic River Systems: Simulating Nutrients and Emerging Contaminants Under Variable Flow Conditions

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Introduction

Water quality models are essential tools for managing aquatic systems, enabling the prediction of water quality responses to natural processes and anthropogenic pollution. This study presents a water quality model capable of simulating conventional indicators, including: water temperature, carbonaceous biochemical oxygen demand (CBOD), dissolved oxygen (DO), ammoniacal nitrogen (NH_3+NH_4^+), nitrate-nitrite nitrogen (NO_3^-+NO_2^-), organic nitrogen (ON), phosphates (IP), organic phosphorus (OP), phytoplanktons and coliforms.

In addition, the model addresses as well emerging contaminants such as pharmaceuticals and personal care products, per/polyfluoroalkyl substances, endocrine disrupting chemicals, pesticides, microplastics, and persistent organic pollutants, which pose new challenges to aquatic environment due to their potential toxicity and long-term stability.

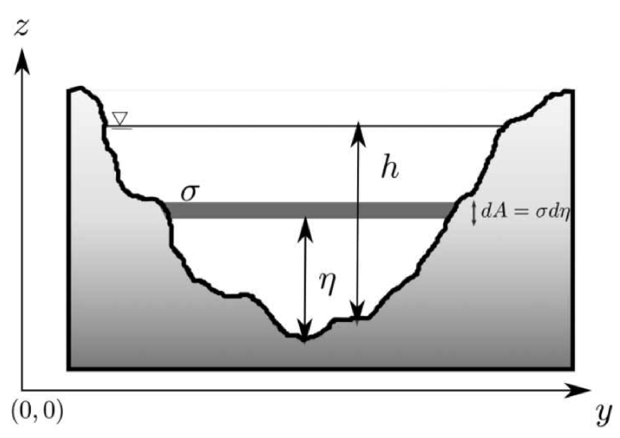
The primary objective of this study is to develop and validate both the conventional and extended models. Sensitivity analyses are conducted to ensure model robustness under varying environmental conditions.

1D Shallow Water Equations + Water Quality Model/Emerging Contaminant Model

(Hydrodynamics + Biochemical Processes)

Model Equations

Hydraulic Model



Mass Conservation Equation:

$$\frac{\partial(A)}{\partial t}+\frac{\partial(Q)}{\partial x}=q$$

Momentum Conservation Equation:

$$\frac{\partial Q}{\partial t}+\frac{\partial}{\partial x}\left(\frac{Q^2}{A}+gI_1\right)=g[I_2+A(S_0-S_f)]$$

A is the cross-section area, t is the time, Q is the discharge, x is the longitudinal distance, q is the lateral inflow per unit width, g is the acceleration due to gravity and S_0 is the bed slope, S_f is the friction slope, I_1 is the hydrostatic pressure force term and I_2 is the pressure force due to the longitudinal width variations.

Water Quality Model

A system of advection equations (incorporating reagent constituents and assuming a first-order decay reaction):

$$\frac{\partial(A\phi_i)}{\partial t}+\frac{\partial(Q\phi_i)}{\partial x}=\pm AR_i \pm f_i$$

φ_i is the cross-section average concentration of parameter i, f_i represents external sources/sinks (point and non-point sources/sinks) and R_i accounts for the kinetic processes affecting the concentration of i.

Variable	Symbol
Temperature	φ_0
carbonaceous biochemical oxygen demand (CBOD)	φ_1
dissolved oxygen (DO)	φ_2
ammoniacal nitrogen (NH_3+NH_4^+)	φ_3
nitrate-nitrite nitrogen (NO_3^-+ NO_2^-)	φ_4
organic nitrogen (ON)	φ_5
phosphates (IP)	φ_6
organic phosphorus (OP)	φ_7
Phytoplankton	φ_8
Coliform	φ_9

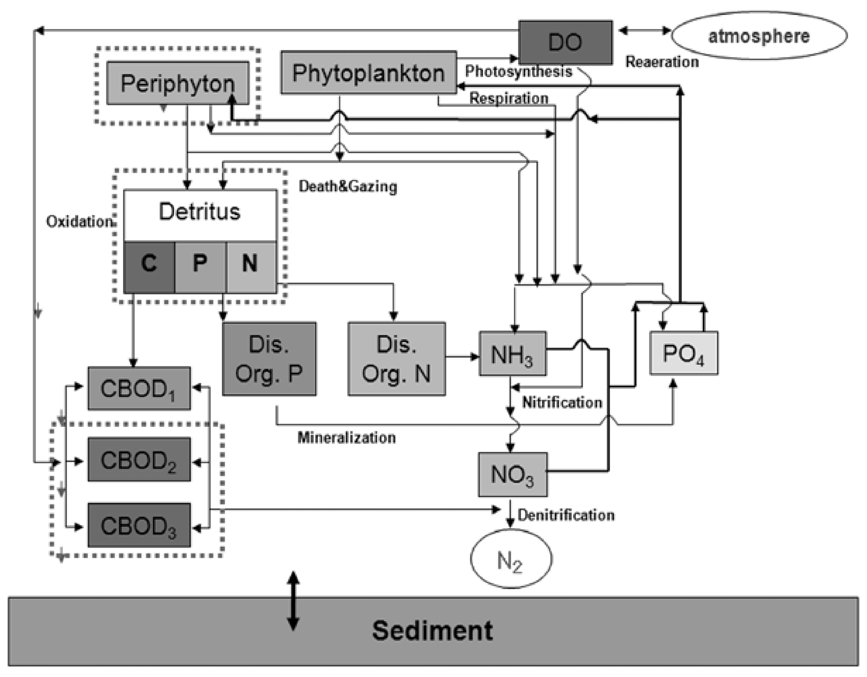


Figure: Interactions of Water Quality Variables of WASP Model. (Source: Zhenhao Yin & Dongil Seo, 2013)

Emerging Contaminant Model

The 1D Transport of Emerging Contaminants:

$$\frac{\partial(A\phi_{EM})}{\partial t}+\frac{\partial(Q\phi_{EM})}{\partial x}=\pm A\sum_{n=1}^{N}\Pr_n \pm f_{EM}$$

The Biochemical Processes Included:

- Biolysis
- Hydrolysis
- Photolysis
- Volatilization
- Sorption and Desorption
- Bioconcentration and Depuration

φ_{EM} is the cross-section average concentration of emerging contaminant, f_{EM} represents external sources/sinks (point and non-point sources/sinks) and Pr_n accounts for the kinetic processes affecting the concentration of emerging contaminant.

Sensitivity Analysis: THE EBRO RIVER

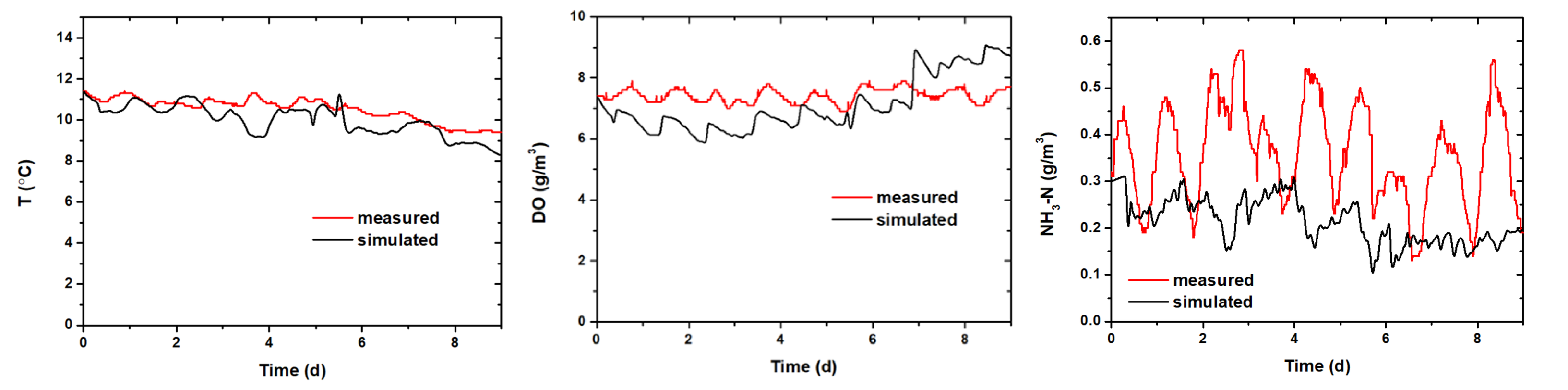
In the first scenario:

Time period:
- 2022.11.26-2022.12.4 (9 days)

Initial condition:
- Steady state (computed in a prior model run)

Boundary:
- Time-varying discharge and water quality data (T, DO, NH_3+NH_4^+) obtained from historical records in Zaragoza and Villanueva
- $Q_{zaragoza}$: 67-233 m^3/s, $Q_{Gállego}$: 2.0-2.99 m^3/s
- Uniform Outflow: bed slope=0.0013

River Length:
- Ebro (main river): 29.07 km
- Gállego (tributary): 11.06 km

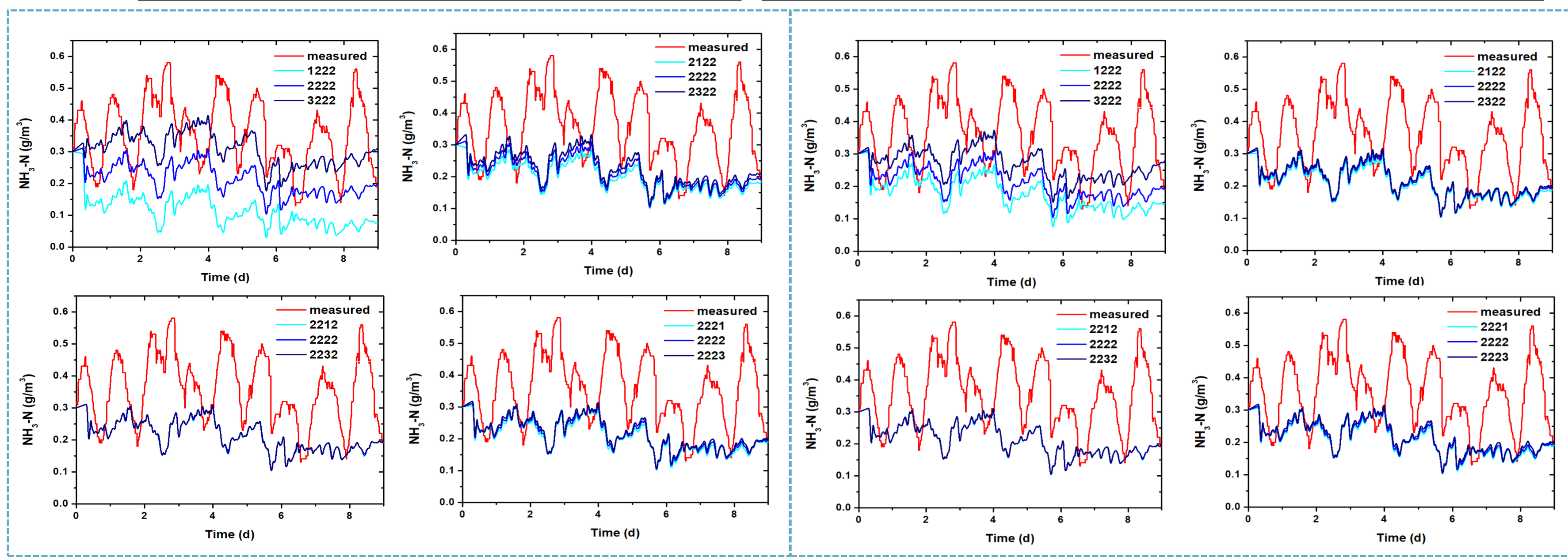


Reaction Rate Constant:

	1(Min)	2(Ave)	3(Max)
$K_{ON\_mineralization}$	0.02	0.21	0.4
$K_{Nitrification}$	1.0	0.505	0.01
$K_{Phytoplankton\_grow}$	3.0	2.0	1.0
$K_{Phytoplankton\_die}$	0.07	0.135	0.2

Temperature Coefficient:

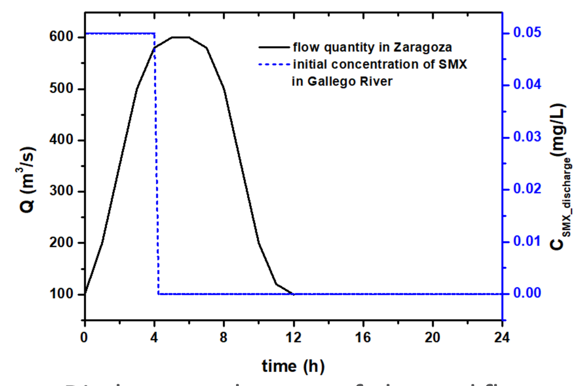
	1(Min)	2(Ave)	3(Max)
$tempCoeff_{\_ON\text{-}Mineralization}$	1.1	1.055	1.01
$tempCoeff_{\_Nitrfication}$	1.01		1.1
$tempCoeff_{\_phygrow}$	1.01		1.1
$tempCoeff_{\_phydie}$	1.1		1.01



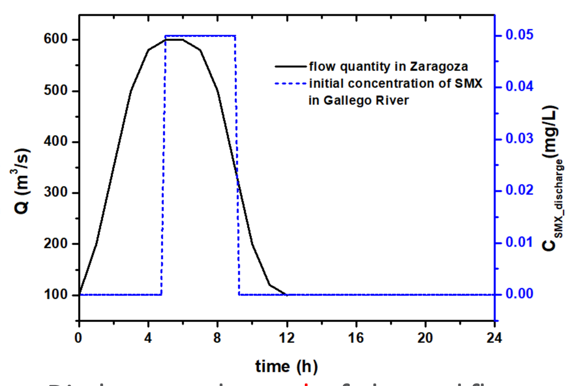
In the second scenario:

1. Assuming a hospital located along the Gallego River.
2. Pouring a wastewater containing antibiotics (sulfamethoxazole) into the tributary over 4 h.
3. Zaragoza is assumed to experience an elevated flow event characterized by a peak flow of 600 m^3/s lasting 12 hours.

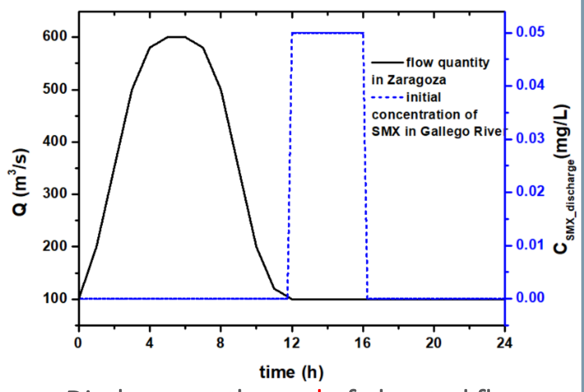
Changing three key variables:
- the timing of antibiotic discharge
- the inlet concentration of antibiotic in the discharge
- the flow quantity of the Gallego River



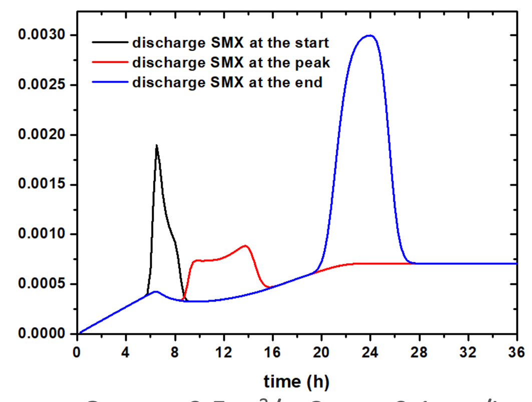
Discharge at the start of elevated flow



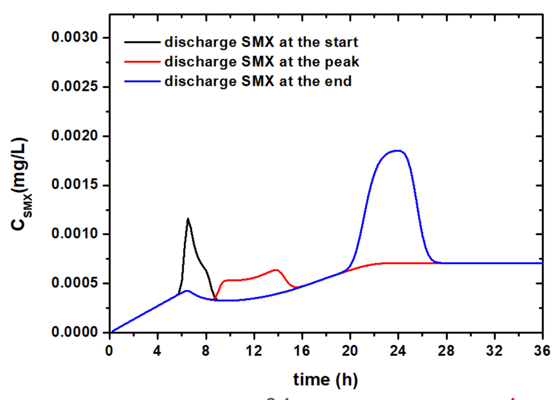
Discharge at the peak of elevated flow



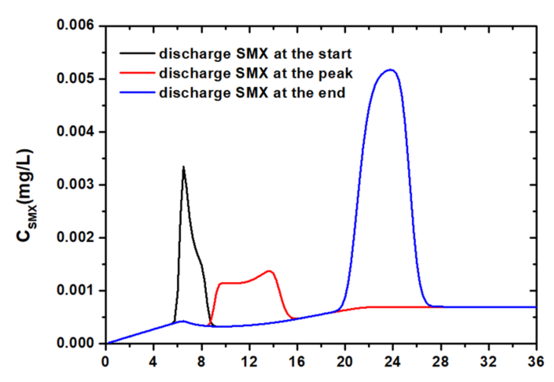
Discharge at the end of elevated flow



$Q_{Gallego}$= 2.5 m^3/s, C_{SMX0}= 0.1 mg/L



$Q_{Gallego}$= 2.5 m^3/s, C_{SMX0}= 0.05 mg/L



$Q_{Gallego}$= 5.0 m^3/s, C_{SMX0}= 0.1 mg/L

Conclusion and Future Works

- 1D Shallow Water Equations + Water Quality Model and Emerging Contaminant Model
- the sensitivity analysis highlights the model's potential in reproducing real water quality dynamics and capturing the behavior of emerging contaminants in dynamic extreme scenarios.
- the model can serve as a practical tool for understanding complex pollutant interactions and supporting water quality management under evolving environmental challenges.

Future work:
- Obtain WWTP data to reduce uncertainty in ammonia nitrogen simulation
- Collect more field data, especially on emerging contaminants, to validate the model
- Develop a 2D model for improved spatial simulation of water quality

References

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