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

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Abstract

This study presents a 1D water quality model that integrates hydrodynamics and biochemical processes capable of simulating both conventional indicators and emerging contaminants. 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.

Introduction

Water quality models are essential tools for managing aquatic systems, enabling the prediction of water quality responses to natural processes and anthropogenic pollution [1]. 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.

Model Equations

The 1D shallow water equations describe the water flow within a river reach. These equations encompass the mass and momentum conservation as following [2]:

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

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

Water Quality Model

A 1D water quality model with source/sink terms can be represented by a system of advection equations, incorporating reagent constituents and assuming a first-order decay reaction [3]. This equation can be written as follows:

$$\frac{\partial(A\O_i)}{\partial t}+\frac{\partial(Q\O_i)}{\partial x}=\pm A\mathrm{R_i}\pm f_i$$

To describe these kinetic processes, several formulations are adapted based on the Water Quality Analysis Simulation Program (WASP). WASP models the interactions between carbon, nitrogen, phosphorus, and phytoplankton [4]. CBOD undergoes oxidation, consuming DO. Phytoplankton assimilate carbon, nitrogen, and phosphorus to support growth. Upon death, phytoplankton release C-N-P constituents into the water column. Photosynthesis drives the oxidation of both organic and inorganic nutrient forms. Insoluble fractions, including IP, OP, ON, and carbonaceous particles, settle through the water column and integrate into the sediment. These processes form a dynamic benthic-nutrient structure, influencing nutrient cycling and ecosystem dynamics.

Emerging Contaminant Model

The 1D transport of emerging contaminants can also be described by a system of advection equations as follows:

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

The kinetic processes affecting the concentration of emerging contaminants in natural aquatic systems primarily include the biolysis, hydrolysis, photolysis, volatilization, bioconcentration, depuration, sorption and desorption [5, 6].

Sensitivity Analyses: The Ebro River

The study area spans from the Zaragoza gauging station to the Presa Pina gauging station, including a tributary segment of the Gallego River, which joins the main stem upstream.

In the first scenario, the simulation was conducted using the WASP model to reproduce water quality dynamics over a 9-day period under unsteady flow conditions. The unsteady flow was represented by time-varying discharge data obtained from historical records. The tributary segment was modeled as a source, contributing to the main stem during the simulation. The initial condition was set as the steady state computed in a prior model run. After the simulation, the measured and simulated water quality components recorded over the 9-day period at the Presa Pina gauging station were compared. Some results are shown in Figures 1 and 2.

In the second scenario, a hospital located along the Gallego River is assumed to pour a wastewater discharge containing antibiotics into the tributary over 4h. The simulation focuses on the dynamic change of antibiotics concentrations along the river, especially the resulting concentration peaks observed at the Presa Pina gauging station on the main river. Simultaneously, Zaragoza, on the upstream, is assumed to experience an elevated flow event characterized by a peak flow of 600 m³/s lasting 12 hours. This setting enables the investigation of the interplay between high-flow-induced dilution and enhanced transport capacity.

Conclusions

An integrated water quality model capable of simulating both conventional water quality indexes and emerging contaminants is introduced in this communication. The results indicate that the model can serve as a practical tool for understanding complex pollutant interactions and supporting water quality management under evolving environmental challenges.

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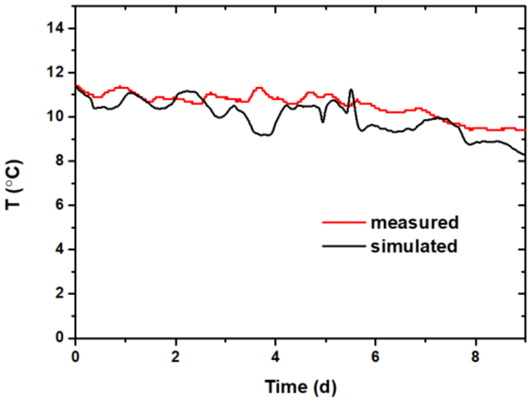

Fig.1. Temporal evolution of the water temperature at the Presa Pina monitoring station.

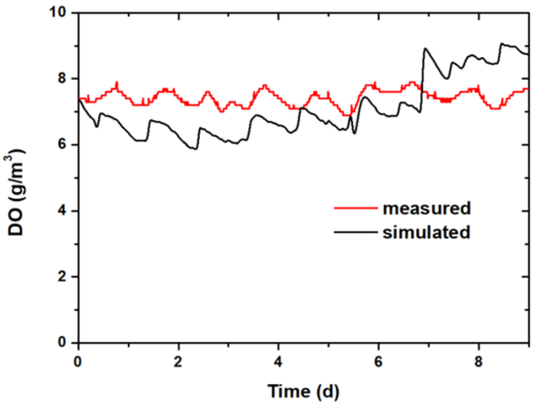

Fig.2. Temporal evolution of dissolved oxygen at the Presa Pina monitoring station.