Environmental Applications of Mathematical Modeling in Aquatic Systems

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Abstract: - Managing aquatic systems needs a good prediction of water movement or the degradation of organic compounds. These phenomena are simulated using mathematical models that represent the structure and function of the systems, serving as tools for hypothesis testing and forecasting. This work reviews the mathematical models used to describe aquatic systems such as rivers, lakes, reservoirs, groundwater systems, aquifers, and watersheds.

Key-Words: - Rivers, lakes, reservoirs, groundwater systems, aquifers, watersheds, environmental systems, fluid flow simulation, Integrated Catchment Model, Soil and Water Assessment Tool, water systems, surface water, groundwater.

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1 Introduction

Controlling complex environmental issues through evidence-based policy creation and development of solutions for managing natural resources is crucial and needs mathematical modelling, which allows the development of mathematical representations of biological, chemical, and physical phenomena derived from empirical data, while simultaneously providing ordered and measured parameters, [1], [2].

Mathematical models are needed about matters like climate change, land use, soil erosion, water quality, and air pollution, [3], [4] and may take into account the impact of multiple parameters, interactions, and uncertainties, which is essential for comprehending intricate environmental systems, [5]. Simulation models are used in hydrology to assess flow, runoff, and surface water quality at the basin level, [6]. When it comes to air pollution, models are useful for chemical transformation and pollutant transport prediction under various climatic and local conditions, [7]. Environmental modeling is continuously expanding and changing to increase forecast accuracy and satisfy contemporary demands, [8], [9]. According to an increasing number of scholars, [10], [11], [12], [13], environmental models should be used for more than merely forecasting.

An important application of mathematical modeling is in water systems, which helps to efficiently manage and protect water resources. In order to better scientific research and environmental decision-making, this method enables the simulation of water movement, quality, and availability, [3], [14]. The foundation for models of aquatic systems is the conservation of mass principle. The continuity equation, when linked with the rules of hydraulics, chemical kinetics, and thermodynamics, yields differential equations that describe the flow and dispersion of substances in the environment, [15]. The main concerns of surface water simulations, like those of rivers and lakes, are flow (advection), dispersion, and chemical/biological changes in pollutants (reaction). The Advection-Dispersion-Reaction equation, which combines the three aforementioned processes into a single mathematical form, is usually the basis for models for these systems and is widely employed in surface water pollution modeling, [15], [16].

Groundwater flow models are used to describe the allocation of pressure and hydraulic potential in the aquifer, whereas the movement of dissolved pollutants through groundwater flow is described by transport models that use dispersion equations, [17]. Hydrological models for watersheds connect hydrological processes to human interventions in land use and agriculture and have been designed to predict runoff, erosion, and the movement of nutrients and pollutants using large-scale climatic and soil data, [18].

Solid understanding of physical processes, accurate data, and accurate estimation of uncertainty are all necessary for modeling water systems. The reliability and adaptability of hydrological and hydrogeological models are enhanced by the combination of geoinformatics tools (GIS), remote sensing methods, and processing power, [19], [20]. Some relevant study can be found in [21].

2 Water Systems Modeling Applications

The general methodological foundation that underpins the development, calibration, and application of mathematical models in aquatic systems should be described prior to the implementations. The framework assures that simulation results for water resource management are accurate, reproducible, and relevant.

The modelling approach begins with system conceptualization [15], [22] and continues with model parameterization. In the first step, the physical, chemical, and biological characteristics of the aquatic environment are defined, such as system boundaries, dominant processes, and key variables (flow dynamics, nutrient loading, and ecological interactions), and in the second step, numerical values are assigned to model parameters using field measurements, laboratory experiments, or values reported in the scientific literature, such as dispersion coefficients, reaction rate constants, [23], [24], [25].

The model is then calibrated by modifying parameters within physically feasible boundaries to reduce disparities between simulated and observed data. Statistical measures like RMSE (Eq.1), NSE (Eq.2), and R^2 (Eq.3) are often used to assess model performance, [26]. Following calibration, model validation is performed using independent datasets to measure predictive performance under various hydrological and climatic circumstances. After validation, models are used in scenario analysis to assess management plans, land-use changes, climate variability, and pollution control measures, [27].

$$RMSE = \sqrt{\frac{1}{n}\sum(C_{obs} - C_{sim})^2} \quad (1)$$

where:
RMSE is the root mean square error,
n is the number of observations,
C_{obs} is the observed value, and
C_{sim} is the simulated value.

RMSE represents the average magnitude of the differences between observed and simulated values, with lower values indicating better model performance.

$$NSE = 1 - \frac{\left[\sum_{i=1}^{n}(C_{obs,i} - C_{sim})\right]^2}{\sum_{i=1}^{n}(C_{obs,i} - \bar{C}_{obs})^2} \quad (2)$$

where:
NSE determines the Nash–Sutcliffe efficiency coefficient,
$C_{obs,i}$ is the observed value,
$C_{sim,i}$ is the simulated value,
$\bar{C}_{obs}$ is the mean of observed values,
n is the number of observations.

NSE demonstrates if the simulated values match well enough the observed data relative to the mean of observations. Perfect agreement means an NSE value of 1, while values less than zero indicate poor model performance.

$$R^2 = \frac{\left[\sum_{i=1}^{n}(C_{obs,i} - \bar{C}_{obs})(C_{sim,i} - \bar{C}_{sim})\right]^2}{\sum_{i=1}^{n}(C_{obs,i} - \bar{C}_{obs})^2 \sum_{i=1}^{n}(C_{sim,i} - \bar{C}_{sim})^2} \quad (3)$$

where R^2 is the coefficient of determination, and $\bar{C}_{sim}$ is the respective mean values, and n is the number of data points. R^2 measures the strength of the linear relationship between observed and simulated values, with values closer to 1 indicating a stronger correlation.

2.1 Surface Waters: Rivers, Lakes, and Reservoirs

Mathematical modeling in surface waters, such as rivers, lakes, and reservoirs, is one of the most developed areas of environmental simulation research. Complex physicochemical and biological processes that affect surface waters are influenced by human activity, changes in land use, and weather patterns. Aquatic ecosystem management is deeply involved in the use of mathematical models to comprehend the temporal and spatial fluctuation of water quality and quantity, [15].

Most surface water quality models are based on conservation-of-mass principles and are formulated as partial differential equations describing transport and transformation processes. These equations are solved numerically due to the complexity of natural systems and boundary conditions.

A mechanistic environmental simulation model called Integrated Catchment Model (INCA) was used in the River Thames, United Kingdom, for the estimation of nitrate ions (NO_3^-) movement and transformation (Figure 1), [16]. The model was based on an equation to predict the transport of dissolved solutes in groundwater caused by physical and biological processes called Advection-Dispersion-Reaction equation:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial^2 x} - kC \quad (4)$$

where:
C determines the pollutant concentration (mg/L),
u the flow velocity (m/s),
D the dispersion coefficient (m²/s),
k the degradation/reaction constant (1/s),
x the distance along the river (m) and
t the time (s).

The natural flow of water delivers nitrates along the river (Advection), causes nitrate spread due to flow inhomogeneity (Dispersion), and refers to chemical and biological processes, such as denitrification, that reduce nitrate concentration (Reaction).

The numerical solution of the advection–dispersion–reaction equation is typically achieved using finite difference or finite volume discretization schemes, combined with implicit time-stepping methods to ensure numerical stability during long-term simulations.

Nitrate intake from agricultural areas through runoff was modeled using the INCA (Integrated Catchment Model), which also predicted how the nitrate would behave in the river over the course of the year. The results highlighted the contribution of hydrological conditions and agricultural practices on water pollution by illustrating a strong capacity to forecast seasonal variations in nitrate concentration, [16].

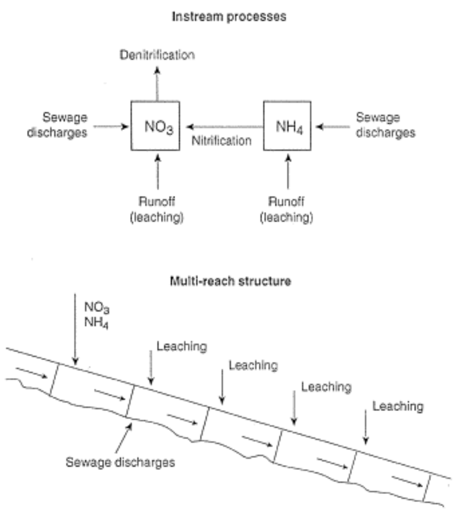

Fig. 1: Processes in the river system
Source: [16]

When simulating water quality in lake ecosystems, thermal stratification, biogeochemical interactions, and other physical processes such as vertical and horizontal flows should all be taken into account. These complex processes are illustrated by Two-dimensional or multi-level dynamic models, such as CE-QUAL-W2 and DYRESM-CAEDYM (Table 1).

The first model is a two-dimensional simulation tool commonly used in lakes and reservoirs that has proven to be successful in controlling eutrophication and is particularly helpful in situations with vertical stratification. It employs extensive stratification and elongated geometries to investigate temperature, water quality, and hydraulic flow and takes into account physicochemical processes, deposition, seepage, and surface inputs while simulating the movement of nutrients (including nitrates and phosphates), dissolved organic matter, dissolved oxygen, and pH, [28].

Its hydrodynamics are governed by the continuity and momentum equations under hydrostatic and Boussinesq approximations:

$$\frac{\partial A}{\partial t} + \frac{\partial (Au)}{\partial x} + \frac{\partial (Aw)}{\partial z} = 0 \quad (5)$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + w\frac{\partial u}{\partial z} = -\frac{1}{\rho}\frac{\partial P}{\partial x} + v\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial z^2}\right) \quad (6)$$

In Eq.5 and 6:
A determines the cross-sectional area,

u, w the longitudinal and vertical velocities,

ρ the water density,

P the pressure,

v the turbulent viscosity.

Water quality transport is described by advection–diffusion–reaction equations as presented in Eq.4.

In contrast, the second model is a three-dimensional thermal stratification simulation system that represents biogeochemical processes. It incorporates the Computational Aquatic Ecosystem Dynamics Model (CAEDYM), which is used to simulate the upstream CO_2 flux dynamics.

The reservoir's thermal and hydraulic behavior is studied by the Dynamic Reservoir Simulation Model (DYRESM) (Figure 2), whereas CAEDYM examines the transit and response of nutrients, contaminants, and biotic factors such as phytoplankton. This combined model helps us dominate the effects of climate change and human action on water quality, [29].

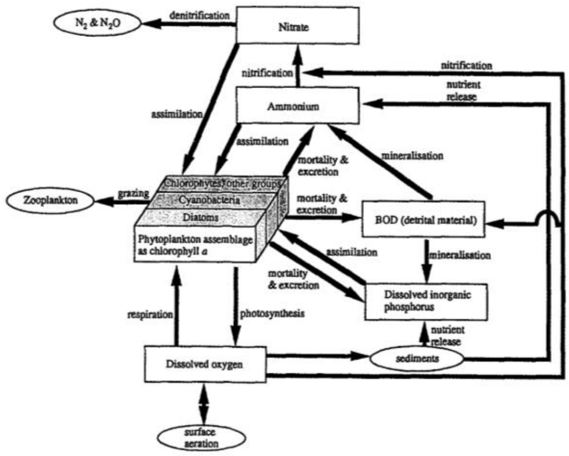

Fig. 2: Variables and processes of the Dynamic Reservoir Simulation Model - Computational Aquatic Ecosystem Dynamics Model
Source: [29]

Table 1. An overview of the simulated environmental conditions, functionality, and application to water bodies for the DYRESM-CAEDYM and CE-QUAL-W2 models

Characteristics	CE-QUAL-W2	DYRESM-CAEDYM
Dimension	2D (length + depth)	1D/3D (by height, with possibility of ecological analysis)
Main focus	Flow, temperature, physicochemical water quality	Thermal stratification, nutrients, pollutants, ecological processes
Environmental focus	Eutrophication, water quality in lakes/reservoirs	Impacts of climate change and anthropogenic interventions
Application geometry	Elongated and narrow applications	General use in reservoirs and lake ecosystems
Suitability	Physicochemical (temperature, DO, pH, nitrates, phosphates)	Combination of physical, chemical, and biological processes (e.g., phytoplankton)

Source: [28]

DYRESM-CAEDYM is a one-dimensional, vertically stratified model for lakes and reservoirs. DYRESM simulates thermal and hydrodynamic processes using the 1D Navier–Stokes equations under the Boussinesq approximation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho w)}{\partial z} = 0 \quad (7)$$

$$\frac{\partial w}{\partial t} = -\frac{1}{\rho}\frac{\partial P}{\partial z} + v\frac{\partial^2 w}{\partial z^2} \quad (8)$$

$$\frac{dC_i}{\partial t} = f(C_1, C_2, ..., C_n; T, light, mixing)$$
(9)

In Eq.7, 8 and 9:

ρ the water density,
w the vertical velocity,
P the pressure,
v the turbulent viscosity,
C_i the concentration of the i-th water quality constituent,
T the temperature,
$light$ the irradiance affecting reactions,
$mixing$ the vertical or lateral mixing effects,

Reservoir modeling employs both mass balance and dynamic hydrochemical models. It exhibits significant differences from natural lakes because of deliberate control over water levels and outflows. Their mathematical modeling includes operational efficiency and water quality, aiming to improve reducing pollution, storage volume, and better decision-making during drought or flood events.

Quality 2000 (River and Stream Water Quality Model: QUAL2K) is a one-dimensional static water quality model used in reservoir modelling. It was created by the United States Environmental Protection Agency (EPA) and was based on the previous version of QUAL2E. It has been employed in a variety of applications, most notably the assessment of agricultural contamination and water system management, by maintaining non-uniform flow and steady hydraulic conditions throughout the simulation. By intending to replicate quality characteristics in rivers and streams, the model can examine many quality indicators, including nitrate (NO_3^-), ammonia (NH_4^+), phosphate (PO_4^{3-}), dissolved oxygen (DO), biochemical oxygen demand (BOD), phytoplankton, temperature, and pH, [30].

Another study on the Polyphytos reservoir [31] looked into the impact of agricultural activity on nitrogen delivery. They specifically examined the enrichment of water with nitrates, phosphates, and organic substances.

There is another dynamic and adaptable simulation model (Figure 3) that may be used not only for rivers and lakes, but also for reservoirs and estuaries called the Water Quality Analysis Simulation Program (WASP).

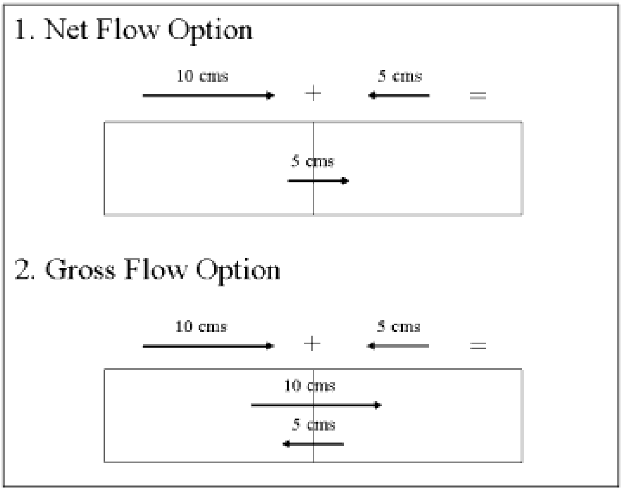

Fig. 3: Descriptive flow options during the simulation with the Water Quality Analysis Simulation Program
Source: [25]

The latter enables the monitoring of quality measures in environments with changing conditions over time and offers two-dimensional or three-dimensional simulation capabilities [32].
Its flexible structure allows for integration of geographical data through GIS and adaptation to climate and land use changes, and is an excellent tool for spatially dispersed environmental simulation and management, including processes such as the behavior of toxic pollutants, heavy metals, and organic compounds, oxygen reactions (photosynthesis, aeration etc.), nutrient transport and thermal processes [33], [34].

2.2 Groundwater and Aquifers

The use of mathematical models to better understand groundwater and aquifers is an important technique in hydrogeology and water resource management.

Modeling allows for the analysis of water movement in the soil's saturation and aeration zones, as well as the monitoring of contaminant transport. Underground hydrological systems have high reaction latency, complicated physical features due to geological formation heterogeneity, and frequently have little direct data, making the modeling process particularly complex, [17], [35], [36], [37], [38], [39], [40], [41].

Groundwater flow and solute transport models are governed by partial differential equations derived from Darcy's law and the continuity equation, which serves as the foundation for the bulk of hydrogeological models. Due to geological heterogeneity and data uncertainty, calibration and statistical evaluation play a critical role in assessing model reliability. The general form of the equation describing unstable (non-permanent) flow in three dimensions is provided below.

$$s_s \frac{ah}{at} = \nabla.(K\nabla h) + W \tag{10}$$

In Eq.10:
h is the hydraulic head (m),
s_s the specific storage (1/m),
K is the hydraulic conductivity tensor (m/s),
W is the source/sink rate (e.g., pumping or enrichment) (1/s) and
t is the time (s).

The bulk of hydrogeological models are built on the basic equation of groundwater flow, which is the result of combining Darcy's law and the continuity equation and may be numerically solved using methods such as the finite difference method and the finite element method.

One of the most well-known and utilized groundwater modeling software is the MODular finite-difference groundwater FLOW model, also known as MODFLOW, [42]. It solves a three-dimensional water flow problem in a porous aquifer by using the finite difference approach, [43].
The Transient Groundwater Flow Equation is provided below.

$$S_s\, \partial h/\partial t = \nabla \cdot (K\, \nabla h) + W \tag{11}$$

In Eq.11:
h the hydraulic head (m),
S_s the specific storage (1/m),
K the hydraulic conductivity tensor (m/s),
W the source/sink term (1/s)

It helps evaluate the aquifer's behavior under various pumping scenarios, the prediction of pollutant distribution in the subsurface, and the assessment of the risk of salinization.

MODFLOW is used in many areas of Greece and the Mediterranean where uncontrolled wastewater disposal or intensive fertilizer use can seriously pollute groundwater reserves, [44], [45]. Its main assumptions are based on the depiction of the groundwater system as a grid of cells. Each cell has homogeneous hydrogeological parameters such as hydraulic conductivity, storage capacity, and layer thickness; the flow within follows Darcy's law, and that groundwater movement is continuous and consistent, [46].

Moreover, MODFLOW is especially effective in stressed water supplies owing to over-pumping or pollution. It was used in a study on the Ganges plain in India, where heavy pumping of groundwater for irrigation resulted in a reduction in the level of more than 10 meters within three decades, leading to agricultural sustainability [47], and in California, where it demonstrated the importance of implementing policies to control pumping and artificial enrichment due to the potential for salinization in coastal aquifers caused by over pumping, [48].

Overall, MODFLOW remains the international standard for hydrogeological modeling, providing a comprehensive quantitative assessment of groundwater movement and its impact on human activity, despite the need for significant data and simplified assumptions about aquifer systems.

In the Thessaly Aquifer, a three-dimensional mathematical model that simulates nitrate flow and transport was created and combines MODFLOW for hydrodynamic simulation and MT3DMS for pollutant diffusion to monitor nitrate ion (NO_3^-) concentrations over time and place, [49]. It was utilized to provide management recommendations for lowering nitrogen fertilizer usage and replenishing aquifers with clean water.

Numerical simulation of groundwater flow is a valuable planning tool for long-term groundwater resource management because it can account for the uncertainty resulting from a lack of accurate geological or hydrological data by employing stochastic factors. Stochastic techniques allow for probabilistic predictions about the distribution of pollutants in the aquifer make them suitable for situations with limited accessible information, [50], [51].

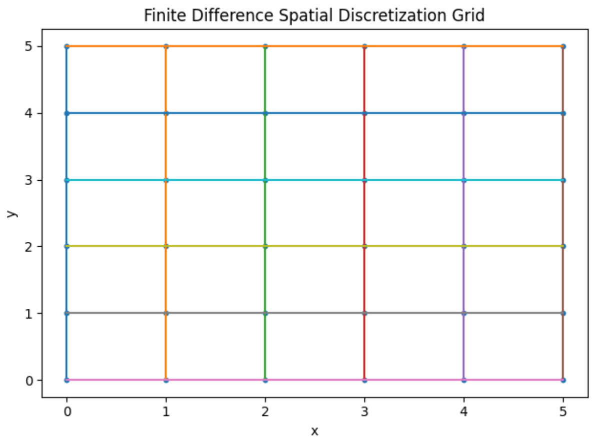

Fig. 4: Example of spatial discretization using the finite difference method for hydrological modeling
Source: [35]

MODFLOW and QUAL2K are FDM-based models. In those models, the computational domain is divided into a structured grid, and spatial derivatives are approximated using difference quotients. Figure 4 illustrates a typical two-dimensional finite difference grid used to approximate hydraulic head or concentration gradients.

2.3 At the Watershed Level

The Soil and Water Assessment Tool (SWAT) is one of the most used models for simulating long-term hydrological balance at the watershed scale. The USDA-ARS developed it to better understand the link between land use, agricultural practices, and water quality, [52]. It works by simulating processes including runoff, infiltration, erosion, sediment, and nutrient movement, and interactions with agricultural activities.

In this tool, processes such as evaporation and transpiration are simulated using empirical relationships with watersheds being divided into homogenous hydrological units (Hydrological Response Units, or HRUs) with consistent soil composition, land use, and climatic variables. The quality of the input data, such as soil maps, topography, and meteorological data, determines the accuracy of the final results, [53].

At the watershed level, models require rigorous calibration and rely on semi-distributed water balance equations to ensure that simulated runoff, sediment, and nutrient fluxes realistically represent observed conditions. Scenario-based simulations and statistical performance measures are essential for evaluating the impacts of agricultural practices and climate variability (Figure 5).

SWAT Water Balance Equation on a Watershed Scale is described below:

$$SW_t = SW_0 + \Sigma\,(R - Q - ET - P - Q_R) \quad (12)$$

In Eq.12:
SW_t is the soil water content at time t,
SW_0 the initial soil water content,
R the precipitation,
Q the surface runoff,
ET the evapotranspiration,
P the percolation,
Q_R the return flow

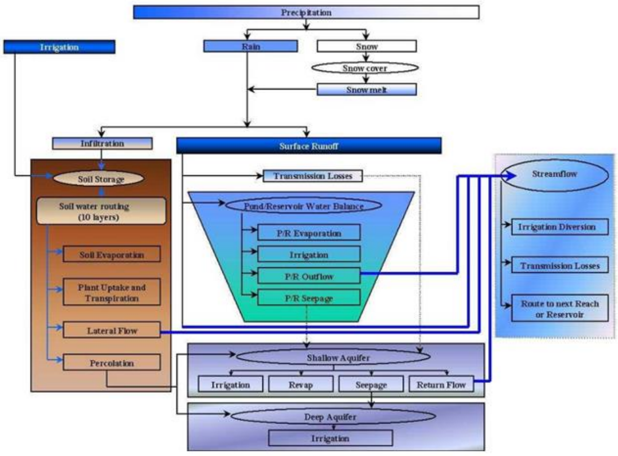

Fig. 5: Pathways in Soil and Water Assessment Tool
Source: [47]

Soil and Water Assessment Tool has been used in a study in the Upper Mississippi River basin that includes assessing agricultural pollution. Significant nitrogen and phosphorus losses were found in surface waters as a result of intense fertilizer use, which contributed to the Gulf of Mexico's "dead zone", [54]. This method was also utilized to promote sustainable agriculture, effective in irrigation management and erosion reduction in Mediterranean basins, such as Spain and Italy, [55].
To summarize, although there are limits in the necessity for rigorous calibration and the assumption of homogeneity, SWAT analysis is a useful tool for understanding the interplay of agriculture, water, and pollution, allowing for the testing of various management strategies while also preserving water resources and supporting watershed management plans.

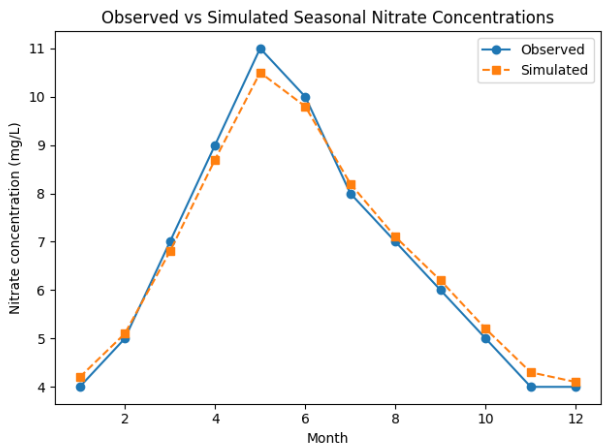

Fig. 6: Observed versus simulated seasonal nitrate (NO_3^-) concentrations, illustrating model performance under transient conditions
Source: [56]

To illustrate practical model application, Figure 6 presents a representative comparison between observed and simulated seasonal nitrate concentrations in a river system. The simulation captures the temporal variability of nitrate loading, with concentration peaks occurring during periods of increased runoff and fertilizer application.

The close agreement between simulated and observed values demonstrates the model's ability to reproduce seasonal nutrient dynamics and highlights the importance of accurately representing hydrological forcing and reaction kinetics.

4 Conclusion

Different approaches for modelling natural and environmental systems were outlined. The key characteristics of these methods were discussed along with their value on long-term resource management, as it is useful in simulating pollutant flow, transport, and transformation in a variety of hydrological, chemical, and biological environments. In watershed-scale level, it integrates land use, climate, and human activity to predict runoff, erosion, and nutrient transfer, and helps in making informed decisions by combining precise data, process understanding, and uncertainty analysis. This analysis assists in pollution reduction, water use optimization, and planning for climate change or intensive agriculture situations.

5 Future work

Although mathematical modelling has shown significant developments, it is advisable to further strengthen some of its critical aspects. Initially, upgrading the quality and accessibility of data, utilizing more reliable, geographically adapted, and long-term datasets, is important and contributes to reducing uncertainty levels and improving the accuracy of model results. It is also considered important to expand the application of mathematical models to contemporary and emerging environmental issues, such as the spread of microplastics, the valuation of ecosystem services, and the assessment of climate resilience at the local level.

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