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Mathematical Modeling of Water Quality Dynamics in Aquaculture: A Foundation for IoT Integration and Machine Learning-Driven Predictive Analytics

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Abstract

Effective water quality management is paramount for sustainable aquaculture, yet conventional methods often fall short in providing timely and predictive insights. This paper details the development and analysis of a comprehensive suite of mathematical models designed to simulate key water quality dynamics in aquaculture systems. These models encompass critical biogeochemical processes, including the nitrogen cycle (ammonia, nitrite, nitrate, organic nitrogen), phosphorus cycle, Dissolved Oxygen (DO) balance, and Biochemical Oxygen Demand (BOD). Simulation results derived from these models illustrate the temporal evolution of these critical parameters, demonstrating their capability to capture complex interactions and provide a mechanistic understanding of the aquatic environment. This foundational modeling approach offers a robust tool for quantitative analysis and prediction of system responses under various conditions. The core contribution of this work is the articulation of these mathematical models, which serve as a crucial foundation for advanced, data-driven aquaculture management. To enhance their practical utility, we propose a conceptual framework for integrating these models with Internet of Things (IoT) sensor networks. Real-time data acquisition via IoT can be essential for model parameterization, continuous calibration, and validation against operational conditions. Furthermore, this paper discusses how outputs from these validated mechanistic models can serve as robust inputs for Machine Learning (ML) algorithms. This synergy enables the development of sophisticated predictive analytics for critical events, such as forecasting water quality deterioration, and supports optimized, proactive management strategies. This research lays the theoretical and methodological groundwork for developing more precise and resilient decision support systems in aquaculture. By emphasizing the synergistic potential of combining foundational mathematical modeling with data science techniques like IoT and ML, this work aims to contribute to transforming aquaculture into a more productive, sustainable, and environmentally responsible industry. Future efforts should focus on empirical validation and the practical implementation of the proposed integrated framework.

Keywords: Aquaculture, Water Quality Modeling, IoT, Machine Learning, Predictive Analytics

1. Introduction

Aquaculture has emerged as one of the fastest-growing sectors in global food production, driven by increasing demand for fish protein and concerns over the sustainability of wild-capture fisheries [1], [2]. As natural resources become more constrained, fish farming has the potential to fill the gap by providing a reliable source of high-quality protein while reducing pressure on wild fish stocks [3]. Aquaculture is increasingly recognized as a cornerstone for global food security and sustainable development, playing a key role in meeting the escalating demand for seafood and driving green development initiatives [4], [5]. However, achieving efficient and sustainable aquaculture requires effective management of several critical factors, including water quality, feeding practices, and disease prevention. Traditional approaches, which rely heavily on manual observation and periodic sampling, are often inadequate to detect problems early, leading to suboptimal growth, high mortality rates, and an increased risk of environmental pollution [6]. The management of water quality is particularly critical as it directly influences the growth, health, and overall productivity of cultured species. Even slight deviations in key water quality parameters, such as pH, DO, temperature, and salinity,

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can elevate stress levels in aquatic organisms, leading to reduced yields or catastrophic production failures [7], [8]. Furthermore, poor water quality is frequently linked to large-scale mortality events, underscoring the importance of continuous environmental monitoring and control in aquaculture operations [9].

Water quality management in aquaculture is a multifaceted process that involves sophisticated manipulation and management of the aquatic ecosystem, benefiting from both traditional techniques and advanced technologies. The integration of deep learning models for water quality prediction and anomaly detection offers new opportunities for proactive management, helping to identify early signs of environmental deterioration [10]. Additionally, fuzzy comprehensive evaluation methods are increasingly used to provide a robust framework for monitoring the dynamic characteristics of aquaculture water systems [11]. These technological innovations are crucial for understanding the spatial and temporal variations in water quality that can occur within aquaculture settings [5].

From an operational standpoint, aquaculture practitioners are incorporating innovative strategies to sustain optimum water quality. The adoption of closed-loop water recirculation systems, for instance, minimizes the exchange of water with external sources, thereby reducing the influx of pollutants while preserving vital nutrient cycles [12]. Furthermore, microalgae have been employed not only to enhance nutrient cycling but also to support the early life stages of aquatic organisms, contributing to a balanced aquatic environment [13]. Technological advancements, such as water quality detection robots and deep transfer learning for water quality image classification, further illustrate the move toward a data-driven, precise management approach in the industry [8], [14].

Recent advancements in the IoT and ML have opened new possibilities for addressing these challenges [6]. While IoT-based sensor networks can enable continuous, real-time monitoring [15] and ML algorithms can predict critical events [16], a deeper, quantitative understanding of the underlying water quality dynamics is often necessary to fully harness the potential of these technologies. Relying solely on empirical data-driven approaches (ML alone) without a mechanistic understanding can limit interpretability and robustness, while traditional monitoring often lacks predictive power. Furthermore, the successful implementation of advanced technological solutions is still hampered by challenges such as sensor calibration, data heterogeneity [17], [18], computational constraints [19], and the technical expertise required by farm operators [20].

To address these gaps, this paper aims to develop a foundational understanding of aquaculture water quality through a clear methodological approach. The novelty of this work lies in shifting the focus from a purely technological solution to the development of a comprehensive suite of mathematical models that describe the key biogeochemical processes in aquaculture systems. Our key contributions are therefore: (a) detailing the methodology for developing these models; (b) presenting the resulting mathematical descriptions and analyzing their behavior through simulation; and (c) proposing a conceptual framework for how these validated models can be integrated with IoT sensor data and leveraged for ML-based predictive analytics. By focusing on the models first, we provide a clear pathway for developing more robust and interpretable data science solutions for aquaculture management, ensuring claims are built upon a solid theoretical foundation.

2. Literature Review

2.1. IoT-Based Aquaculture Monitoring Systems

The adoption of IoT-based monitoring systems has rapidly transformed the aquaculture industry, offering real-time, continuous, and remote surveillance of essential water quality parameters that are critical for maintaining optimal aquatic environments. These systems integrate diverse sensor networks that monitor key indicators such as temperature, pH, DO, turbidity, ammonia, and salinity—parameters crucial for healthy fish growth and production efficiency [15], [21]. Early research in this domain focused on deploying Wireless Sensor Networks (WSNs) that capture physical and chemical parameters across fishponds or cages, typically using low-power sensors capable of continuous data transmission to a centralized gateway. This technology has been shown to enhance the detection of water quality deviations, allowing for timely alerts to farm operators and reducing the reliance on labor-intensive manual sampling [22]. The real-time data collection capability minimizes human error, reduces operational costs, and facilitates the early detection of deviations from optimal conditions, ensuring better management of aquaculture systems [23].

One of the primary advantages of integrating IoT technology into aquaculture is the enhancement of data analysis through cloud-based platforms and machine learning algorithms. Recent advancements have demonstrated the ability of IoT systems to transmit sensor data to centralized databases where advanced analytics enable trend analysis, anomaly detection, and predictive insights. These predictive models assist aquaculture managers in implementing proactive interventions before minor issues escalate into significant problems, thus ensuring higher operational efficiency [24]. Furthermore, deep reinforcement learning and data fusion techniques have further refined these predictions, ensuring that control measures are timely and well-calibrated to the dynamic nature of aquaculture environments [24]. This capability is particularly valuable for handling the complexities of aquaculture systems, where environmental conditions can fluctuate rapidly and require immediate adjustments.

The IoT-driven approach also supports cost-effectiveness and scalability, factors that drive the widespread adoption of IoT-based monitoring systems, especially among small- and medium-scale operations. Xu et al highlighted the development of portable, multifunctional monitoring devices that provide robust water quality surveillance at a fraction of the cost of traditional high-end sensor arrays [25]. This lower capital investment increases the accessibility of IoT technologies to a broader segment of aquaculture farmers, enabling them to monitor water quality with greater precision without incurring prohibitive costs. Additionally, these systems are often designed with energy-saving practices, including energy harvesting techniques such as solar and wave energy, which power remote sensor stations with minimal human intervention. This reduces on-site maintenance needs and optimizes resource allocation [26].

Recent work has also advanced IoT deployments by incorporating more robust communication protocols, such as LoRaWAN and 5G, to achieve higher scalability and reliability, especially in harsh marine or brackish environments [26]. These technologies enhance the robustness of the monitoring systems by improving data transmission capabilities, which is particularly beneficial in large-scale or remote aquaculture systems. Despite these advancements, challenges remain in ensuring stable sensor calibration, safeguarding against biofouling, and integrating heterogeneous data formats from various sensor types [27]. Addressing these issues is crucial for ensuring the seamless and accurate collection of aquaculture data, which is fundamental for effective decision-making and the successful implementation of IoT-based systems.

2.2. Machine Learning Approaches in Aquaculture

ML has become an integral part of aquaculture, providing innovative methods for efficient decision-making and predictive analytics in an industry characterized by complex biological and environmental interactions. As the need for optimized resource management and sustainable practices grows, ML models are increasingly being applied across various domains within aquaculture, such as water quality prediction, stock management, disease prevention, and optimization of feeding strategies. Recent studies emphasize the significance of ML in transforming traditional aquaculture methods, enabling better management of resources and improving the efficiency and sustainability of operations.

One of the primary applications of ML in aquaculture is the prediction of water quality parameters, which are critical for maintaining optimal fish health and maximizing production efficiency. For example, studies have shown that ML models like the random forest algorithm can achieve up to 90% accuracy in predicting abiotic stress in recirculated aquaculture systems, such as identifying ammonia as a key stressor for tilapia [4]. This high level of prediction accuracy helps prevent production losses and contributes to the sustainability of aquaculture systems. Similarly, hybrid ML models that integrate multiple algorithms have been developed to predict dissolved oxygen levels, which effectively characterizes multivariate water quality factors and addresses the challenges posed by small sample sizes and high-dimensional data.

In addition to water quality management, ML has been widely applied to growth prediction and resource optimization. By combining water quality data with high-performance computing, [28] proposed guidelines that help reduce the mortality rate of red tilapia fingerlings in recirculating aquaculture systems. Chen et al utilized ML techniques to predict shrimp growth, enabling the implementation of intelligent feeding strategies that optimize feed use, reduce waste, and improve overall production efficiency [29]. Cordier et al demonstrated how ML techniques can infer biotic indices from eDNA data, providing an innovative method for ecological monitoring [30]. This approach not only enhances the

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understanding of marine environments but also complements conventional monitoring methods, offering a more holistic view of ecosystem health in aquaculture settings.

Parallel to advancements in ML, IoT-based monitoring systems have become transformative tools in modern aquaculture, enabling continuous and remote surveillance of water quality parameters critical to maintaining optimal aquatic environments. These systems integrate sensor networks that monitor key indicators such as temperature, pH, dissolved oxygen, turbidity, and salinity, which are essential for healthy fish growth [15]. The real-time data collection capability of IoT systems minimizes the need for labor-intensive manual sampling, reduces operational costs, and reduces human error while facilitating the early detection of deviations from optimal conditions [23]. This integration of IoT with ML allows for enhanced predictive capabilities, ensuring proactive management of aquaculture environments before minor issues escalate into significant problems.

Recent innovations have also extended the functionality of these systems beyond data acquisition. AI elements, such as chatbots and natural language processing, have been integrated into IoT systems to translate raw data into actionable insights and user-friendly advisories [31]. These intelligent interfaces not only improve the interpretability of complex data but also support decision-making processes by providing timely recommendations for water quality adjustments. The integration of such AI tools bridges the gap between complex data analysis and practical aquaculture management, making it easier for farmers to implement sustainable practices [21].

2.3. Integrated IoT-ML Frameworks in Aquaculture Water Quality Management

Integrated IoT- M frameworks have emerged as a significant advancement in aquaculture water quality management by combining real-time sensing capabilities with advanced data analytics to optimize operational efficiency and environmental sustainability. These frameworks leverage the strengths of IoT infrastructures, such as sensor nodes, data acquisition devices, and communication protocols, along with ML algorithms that provide predictive analytics and decision support. This combination is essential for addressing the complex and dynamic nature of water quality parameters in aquaculture systems, which require continuous monitoring and timely interventions.

The IoT component in these frameworks involves deploying various sensors—such as turbidity, temperature, pH, and dissolved oxygen—connected to low-power microcontrollers, like the ESP32 launchpad, which continuously monitor key water quality indicators. These sensors transmit real-time data to centralized platforms for processing and analysis. Real-time data collection is crucial for detecting deviations from optimal conditions, such as variations in water temperature or oxygen levels, and for facilitating rapid responses to ensure the health and productivity of aquatic organisms [21]. This data is typically sent to cloud-based analytics platforms that store, process, and visualize the data, providing aquaculture practitioners with remote, real-time access to critical information [23].

On the machine learning side, integrated frameworks utilize sophisticated algorithms to analyze the high-dimensional data collected by IoT sensors. This process allows for predictive analytics that can forecast water quality trends based on historical and real-time data. For example, ensemble learning models, as proposed by [17], combine multiple algorithms to enhance the accuracy of water quality predictions, helping optimize resource management strategies, such as automatic feeding and water recycling. Similarly, [32] emphasize a modular approach that divides the system into distinct components—sensing, coordination, data processing, and decision-making—enabling the integration of predictive models that forecast changes in water quality and recommend proactive measures to prevent adverse conditions.

The integration of IoT sensing with machine learning analysis also enables more proactive quality management. Advanced ML models process continuous sensor data streams to detect patterns and predict impending degradation of water quality. By forecasting these issues before they become significant, aquaculture managers can implement mitigation measures to prevent detrimental effects, such as fish stress or disease outbreaks [32]. Moreover, the combination of IoT and intelligent systems has led to the incorporation of user-friendly interfaces, such as chatbots utilizing natural language processing [31], that translate complex data into actionable insights. These interfaces improve decision-making by providing tailored recommendations based on real-time water quality data, making it easier for farm managers to respond effectively and efficiently to changing conditions.

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2.4. Research Gaps and Opportunities

Although there has been substantial progress in leveraging the IoT and ML for aquaculture, key gaps remain in effectively deploying these systems robustly and at commercial scales. Many existing studies rely on small-scale pilot projects with controlled conditions, which raises questions about the generalizability of their results to larger, more diverse farm environments [1], [2]. Challenges also persist concerning robust sensor technologies and data fusion strategies capable of handling issues like sensor drift and environmental noise effectively [17].

Furthermore, while advanced ML techniques (e.g., deep learning, reinforcement learning) show promise, the interpretability of these models and their seamless integration into routine farming operations remain significant areas for further exploration [18]. The lack of standardized protocols for data collection, storage, and sharing also hampers cross-study comparison and collaborative innovation; establishing common frameworks or ontologies is crucial for broader benchmarking [19]. Finally, the technical expertise and resources required to implement and maintain complex IoT-ML pipelines often exceed what is available to many fish farmers, highlighting a need for more accessible, low-cost, and turnkey solutions complemented by targeted training programs [20].

Crucially, underpinning many of these challenges is the need for foundational mechanistic models that can enhance the accuracy, reliability, and interpretability of modern IoT and ML applications. In contrast to purely empirical or 'black-box' ML models, which excel at identifying correlations but often lack explanatory power, the mechanistic-first approach detailed in this paper provides a causal understanding of system behavior based on biogeochemical principles. This is a critical distinction; while a 'black-box' model might predict an impending drop in dissolved oxygen, a mechanistic model can explain why—linking it to specific processes like nitrification or BOD decay shown in its equations. Such interpretability is essential for operational trust and effective decision-making. Therefore, this paper aims to fill this specific gap by detailing a methodology for developing foundational mathematical models and presenting a framework for their integration with data-driven technologies. By doing so, we provide a robust, scientifically-grounded basis for designing more targeted IoT sensor strategies and for building more reliable and transparent AI systems for aquaculture management.

3. Methodology

This section outlines the comprehensive research methodology adopted to develop, formulate, and analyze the mathematical models governing the dynamics of water quality in aquaculture systems, as shown in figure 1. The goal is to achieve a mechanistic understanding of the biogeochemical processes involved, with an emphasis on building a robust foundation for future integration with real-time data acquisition and predictive analytics tools. The methodology described herein is aimed at providing aquaculture practitioners with a practical and scientific framework to optimize water quality management, feeding strategies, and overall system sustainability.

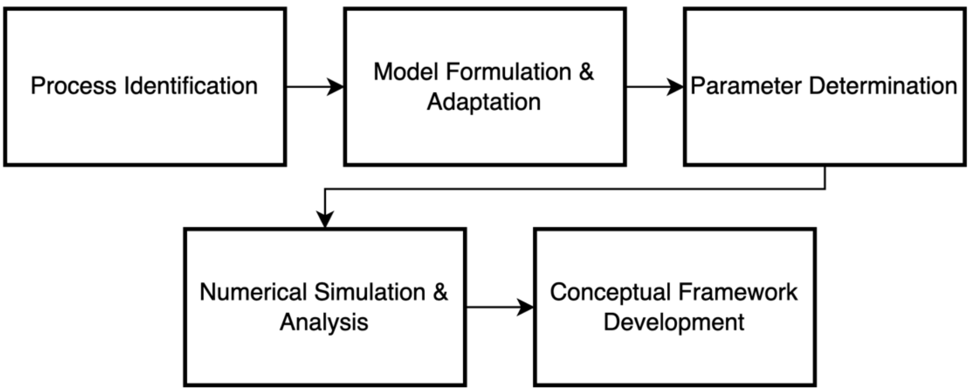

Figure 1. Research Method Flowchart

3.1. Methodological Approach to Modeling

The methodological foundation of this research is built upon the development of deterministic mathematical models, primarily grounded in mass balance principles. These models describe the rate of change of key water quality constituents within a defined control volume that represents the aquaculture system—such as ponds, tanks, or cages. For many of the processes, the system is conceptualized as a Completely Stirred Tank Reactor (CSTR), or, where appropriate, as a plug-flow system, to reflect the movement and mixing of water through the environment. The core of these models consists of a set of coupled Ordinary Differential Equations (ODEs), each representing the contribution of various physical, chemical, and biological processes that affect a given water quality parameter. The objective is to capture the major processes influencing water quality while balancing the complexity of the models with parameter identifiability and computational feasibility. This balance ensures that the models remain tractable, allowing for efficient computation and meaningful results.

3.2. Model Selection and Formulation Strategy

The selection and formulation of individual model components for the critical water quality parameters—such as the nitrogen cycle (ammonia, nitrite, nitrate, organic nitrogen), phosphorus cycle (organic and dissolved inorganic phosphorus), DO, BOD, and coliforms—were guided by multiple principles. An extensive literature review on aquatic ecosystem models and aquaculture-specific water quality research provided a foundation for understanding established kinetic formulations and stoichiometric relationships.

Key biogeochemical processes that affect water quality in aquaculture systems, such as ammonia excretion by fish, mineralization of organic nitrogen, nitrification, uptake by phytoplankton, and volatilization, were identified for each water quality parameter. When possible, existing model structures from general aquatic science were adapted to the specific context of aquaculture, tailoring them to reflect inputs such as feed addition, waste production, and water exchange. Simplifications were made to avoid over-parameterization, especially where certain processes were less significant or data for precise parameterization was lacking. For instance, while temperature plays a significant role in reaction rates, its dynamic modeling was considered a refinement for future work, with the current models using temperature-dependent adjustment factors based on average operational conditions.

The models were designed with a modular structure, allowing for easy refinement or replacement of individual components, such as the nitrification sub-model, as more data or insights become available. This modularity ensures the long-term adaptability of the models as more detailed information is gathered. The system was primarily conceptualized for semi-intensive and intensive aquaculture systems, where nutrient inputs and transformations are substantial. By incorporating terms related to water inflow (Q) and system volume (V), the models can be adapted to systems with varying hydraulic residence times.

3.3. Parameter Determination and Estimation Approach

The mathematical models developed in this research rely on a range of parameters, including reaction rate constants (e.g., $\beta1$ for ammonia oxidation, K1 for BOD deoxygenation), stoichiometric coefficients (e.g., $\alpha1$ for nitrogen content in algae), settling or loss rates (e.g., $\sigma4$ for organic nitrogen precipitation), and reaeration coefficients (K2). Initial estimates of these parameters were derived from peer-reviewed scientific literature focused on aquaculture water quality, limnology, and wastewater treatment processes. These values were selected to reflect typical environmental conditions within aquaculture systems.

Stoichiometric consistency was maintained by using established chemical and biological principles for parameters such as the oxygen consumed per unit of ammonia oxidized. However, the models acknowledge that while these literature-derived values provide a starting point, site-specific calibration is crucial for achieving optimal performance in real-world aquaculture settings. Future work will involve acquiring time-series data on water quality parameters from target aquaculture systems, ideally via IoT-based sensor networks for continuous data collection. Calibration will be performed using numerical optimization techniques, including least-squares fitting, genetic algorithms, and Bayesian methods such as Markov Chain Monte Carlo (MCMC), to minimize discrepancies between model predictions and observed data.

Parameter estimation and model refinement will be an iterative process, with adjustments to the model structure or assumptions as needed, based on the calibration results. The current study, however, focuses on developing the foundational models and does not involve extensive site-specific calibration. The simulations presented in this paper use representative parameter values from existing literature, illustrating the model's general behavior.

3.4. Model Analysis and Simulation Setup

The system of coupled ODEs was analyzed through numerical simulations to understand the dynamic behavior of water quality parameters over time. These simulations were performed using Python (version 3.12) and its scientific computing libraries, specifically leveraging the solve_ivp function from the SciPy library for the numerical integration of the ODEs and Matplotlib for generating insightful graphics that demonstrate the temporal evolution of key metrics. The simulations presented in this paper were set up with representative initial conditions and literature-derived parameter to reflect the starting state of a typical aquaculture system, such as post-stocking or after a perturbation. The simulations were run for a defined period (e.g., 50–100 days) to observe both transient dynamics and the approach to dynamic equilibrium. Acknowledging the importance of parameter uncertainty, our methodological framework also includes sensitivity analysis as a critical future step. This analysis would involve systematically varying influential parameters (e.g., ammonia oxidation rates, nutrient loading rates, hydraulic exchange) to explore their impact on critical model outputs like peak ammonia concentrations and minimum DO levels. Such analysis is crucial for identifying the most influential parameters that require careful site-specific calibration and for informing effective management strategies.

4. Results and Discussion

4.1. Water Quality Model Formulations

The following subsections describe the ODEs that form the basis of the water quality model.

4.1.1. Nitrogen Cycle

The nitrogen cycle model is a key component of the overall water quality model, describing the transformations between different forms of nitrogen: organic nitrogen, ammonia (N1), nitrite (N2), and nitrate (N3). These nitrogen forms play a central role in the aquaculture ecosystem, influencing both water quality and biological processes. Ammonia (N1) is one of the most important pollutants in aquaculture due to its toxicity at high concentrations. Therefore, understanding its transformation and removal is essential for maintaining a healthy aquatic environment.

The rate of change of ammonia nitrogen (N1) in the system is influenced by several processes. First, ammonia can be introduced into the system through the excretion of nitrogen by cultured organisms, such as fish and shrimp, and through the mineralization of organic nitrogen from waste products. Second, ammonia undergoes nitrification, where it is converted into nitrite (N2) by Ammonia-Oxidizing Bacteria (AOB), a key step in the nitrogen cycle. Third, ammonia is taken up by algae, which use it as a nitrogen source for their growth. Lastly, the model incorporates advection, which accounts for the transport of ammonia due to water flow through the system. This process can either introduce or remove ammonia from the system, depending on the water flow conditions. These processes together govern the dynamics of ammonia nitrogen within the aquaculture system, highlighting the importance of both biological and physical factors in managing water quality. The rate of change for ammonia nitrogen (N1) is described by the following ordinary differential equation (ODE):

$$\frac{dN_1}{dt} = \beta_3 \cdot N_4 - \beta_1 \cdot N_1 + \frac{\sigma_3}{d} - F_1 \cdot \alpha_1 \cdot \mu \cdot A + (N_1^0 - N_1)\frac{Q}{V} \tag{1}$$

A: algae biomass concentration (mg-A/L); d: average flow depth (m); N_1^0: initial ammonia nitrogen concentration (mg-N/L); N_1: ammonia nitrogen concentration (mg-N/L); N_4: organic nitrogen concentration (mg-N/L); F_1: nitrogen fraction rate of algae from an ammonia nitrogen pond; β_1: biological oxidation rate constant from NH3 to NO2 (1/day); β_3: hydrolysis rate constant from organic nitrogen to ammonia nitrogen (1/day); α_1: nitrogen found in the algae biomass fraction (mg-N/mg-Ǻ); σ_3: benthic source rate for ammonia nitrogen (mg-N/m2-day); μ: local specific growth rate of algae (1/day); V: volume of water in each CSTR section (m3); Q: flow rate (m3/sec); P_N: ammonia nitrogen selection factors. The fraction F1, representing the proportion of ammonia nitrogen taken up by algae, is expressed as:

$$F_1 = \frac{P_N \cdot N_1}{P_N \cdot N_1 + (1 - P_N)N_1} \tag{2}$$

Here, PN is the ammonia nitrogen selection factor for algae, which adjusts the uptake rate based on the available nitrogen in the system. Next, the transformations of Nitrite (N2) and Nitrate (N3) are modeled by the following equations:

For nitrite nitrogen (N2):

$$\frac{dN_2}{dt} = \beta_1 \cdot N_1 - \beta_2 \cdot N_2 + (N_2^0 - N_2)\frac{Q}{V} \tag{3}$$

N_2^0: initial concentration of nitrite nitrogen (mg-N/L); N_2: nitrite nitrogen concentration (mg-N/L); β_2: biological oxidation rate constant from NO2 to NO3 (1/day).

For nitrate nitrogen (N3):

$$\frac{dN_3}{dt} = \beta_2 \cdot N_2 - (1 - F_1)\alpha_1 \cdot \mu \cdot A + (N_3^0 - N_3)\frac{Q}{V} \tag{4}$$

N_3^0: initial concentration of nitrate nitrogen (mg-N/L); N_3: nitrate nitrogen concentration (mg-N/L)

Lastly, organic nitrogen (N4) is modeled by:

$$\frac{dN_4}{dt} = \alpha_1 \cdot \rho \cdot A - \beta_3 \cdot N_4 - \sigma_4 \cdot N_4 + (N_4^0 - N_4)\frac{Q}{V} \tag{5}$$

$$\text{Nitrite nitrogen: } (\beta_2)_{\text{inhibition}} = C_{\text{ORDO}} \cdot (\beta_2)_{\text{input}}$$

ρ: local respiration rate of algae (1/day); σ_4: precipitation rate of organic nitrogen (1/day); N_4^0: initial concentration of organic nitrogen (mg-N/L); N_4: organic nitrogen concentration (mg-N/L)

4.1.2. Phosphorus Cycle

The phosphorus cycle in aquaculture systems is similarly modeled to the nitrogen cycle, involving both organic phosphorus (P1) and dissolved inorganic phosphorus (P2). Phosphorus plays a vital role in the growth of algae and other aquatic organisms, directly influencing the overall productivity of the system. The organic form of phosphorus is generated when algae die, and it is subsequently converted to dissolved inorganic phosphorus, which becomes available for primary production by algae. Additionally, phosphorus discharged from external sources, such as factories, is typically in the form of dissolved inorganic phosphorus, which is immediately absorbed by algae. This cycle is crucial in maintaining nutrient balance within aquaculture systems, as the availability of phosphorus directly affects algae growth, which in turn impacts the productivity of the entire system. The model depicting the changes in phosphorus concentrations accounts for both biological processes and external inputs, ensuring a dynamic representation of phosphorus dynamics in aquaculture environments. For organic phosphorus (P1), the equation is:

$$\frac{dP_1}{dt} = \alpha_2 \cdot \rho \cdot A - \beta_4 \cdot P_1 - \alpha_5 \cdot P_1 + (P_1^0 - P_1)\frac{Q}{V} \tag{6}$$

α_2: phosphorus found in the algae biomass fraction (mg-P/mg-A); α_5: O2 production rate per unit of NH3 oxidation (mg-O/mg-N); P_1: local concentration of organic phosphorus (mg-P/L); P_1^0: local organic concentration of phosphorus (mg-P/L); β_4: the rate constant for converting organic phosphorus to dissolved phosphorus (1/day). For dissolved phosphorus (P2), the rate of change is given by:

$$\frac{dP_2}{dt} = \beta_4 \cdot P_1 + \frac{\sigma_2}{d} - \alpha_2 \cdot \mu \cdot A + (P_2^0 - P_2)\frac{Q}{V} \tag{7}$$

4.1.3. DO for Predictive Analysis

The concentration of DO in the system is influenced by multiple processes, including reaeration from the atmosphere, photosynthesis by algae, oxygen consumption during BOD decay, nitrification, respiration, and benthic oxygen demand. The oxygen balance within the system is determined by the ability of the water to exchange oxygen with the atmosphere through reaeration, which is governed by both advection and diffusion processes. In addition to atmospheric reaeration, the oxygen produced by photosynthesis and the oxygen contained in the inlet water stream are the primary sources of oxygen. However, the system also experiences oxygen loss due to several factors, such as the biochemical oxidation of organic carbon and nitrogen, benthic oxygen demand, and the oxygen consumed by algae respiration. These processes collectively determine the rate of change of dissolved oxygen, with the overall balance between oxygen inputs and losses influencing the health and productivity of the aquaculture system. The oxygen rate of change model is shown below, with each term representing a primary source of oxygen or a loss of oxygen.

$$\frac{dO}{dt} = K_2(O^* - O) + (\alpha_3 \cdot \mu - \alpha_4 \cdot \rho)A - K_1 L - \frac{K_4}{d} - \alpha_5 \cdot \beta_1 \cdot N_1 - \alpha_6 \cdot \beta_2 \cdot N_2 + (O^0 - O)\frac{Q}{V} \tag{8}$$

α_3: O2 production per unit algae growth (mg-O/mg-A); α_4: O2 rate per unit from algae respiration (mg-O/mg-A); α_5: O2 production rate per unit of NH3 oxidation (mg-O/mg-N); α_6: O2 production rate per unit of NO2 oxidation (mg-O/mg-N); β_1: rate constant for biological oxidation from NH3 to NO2 (1/day); β_2: biological oxidation rate constant from NO2 to NO3 (1/day); K_1: deoxygenation rate constant (1/day); K_2: reaeration rate constant (1/day); K_4: benthic oxygen uptake (mg-O/m2-day); L: main concentration of carbon BOD (mg/L); O^*: saturated concentration of DO at local temperature and pressure (mg/L); O: DO concentration (mg/L); O^0: DO initial concentration (mg/L)

4.1.4. BOD Model Implementation

The amount of oxygen required by microorganisms to break down organic substances is known as BOD, which is a key process influencing oxygen levels in aquaculture systems. BOD is proportional to the concentration of decomposed organic carbon and is denoted by the letter L. The BOD model represents the decay of carbonaceous organic matter, with microorganisms consuming oxygen to decompose organic material. The rate of change of BOD is determined by the decomposition process, which varies depending on the rate of decomposition and the rate of precipitation following the breakdown of organic substances. As organic matter decomposes, BOD decreases due to the settling of particles, which further influences the oxygen demand within the system. This dynamic process plays a significant role in regulating the oxygen balance in aquaculture environments, highlighting the importance of managing organic waste to maintain healthy water quality.

$$\frac{dL}{dt} = K_1 \cdot L - K_3 \cdot L + (L^0 - L)\frac{Q}{V} \tag{9}$$

Or

$$L(t) = L^0 e - \frac{K_r t}{V} \tag{10}$$

K_1: deoxygenation rate constant (1/day); K_3: decrease speed due to deposition (1/day); L: main concentration of carbon BOD (mg/L); L^0: main initial concentration of carbon BOD (mg/L)

4.1.5. Coliforms as Indocators

The coliform model (E) tracks the concentration of indicator bacteria, which are important for assessing water quality and potential health risks. The equation for coliform concentration is:

$$\frac{dE}{dt} = -K_5 \cdot E + (E^0 - E)\frac{Q}{V} \tag{11}$$

K_5: coliform death rate (1/day); E: coliform concentration (MPN); E^0: initial concentration of coliform (MPN)

4.1.6. Variable Non-Conservative Substances

This general model (R) can represent other substances in the system that are subject to decay, settling, and benthic sources. The rate of change of these substances is given by:

$$\frac{dR}{dt} = -K_6 \cdot R - \sigma_6 \cdot R + \frac{\sigma_7}{d}(R^0 - R)\frac{Q}{V} \tag{12}$$

K_6: non-conservative loss coefficient variable (1/day); σ_6: variable non-conservative deposition rate (1/day); σ_7: benthal source rate for variable non-conservative deposition rates (mg-ANC/m2-day); R: variable concentrations of non-conservative substances (mg/L); R^0: variable initial concentration of a non-conservative substance (mg/L)

4.2. Simulation Results

Numerical simulations of the coupled ODE system were to observe the dynamic behavior of key water quality parameters over time. Figure 1 presents the simulated temporal evolution of nitrogen species (Ammonia N1, Nitrite N2, Nitrate N3, Organic Nitrogen N4), BOD, and DO over a 50-day period. The simulations were run for 50 days using initial conditions of key water quality parameters, specifically: ammonia nitrogen (N1) at 5 mg/L, nitrite nitrogen (N2) at 0 mg/L, nitrate nitrogen (N3) at 0 mg/L, organic nitrogen (N4) at 5 mg/L, biochemical oxygen demand (BOD, L) at 5 mg/L, and dissolved oxygen (DO, O) at 5 mg/L. These values were derived from representative parameter values found in the literature (refer to Table 1 for parameter definitions; specific values used in the simulations can typically be found in an appendix or supplementary materials, if not directly listed in the main text). The simulation results, as illustrated in figure 2, demonstrate several key dynamic interactions among these parameters.

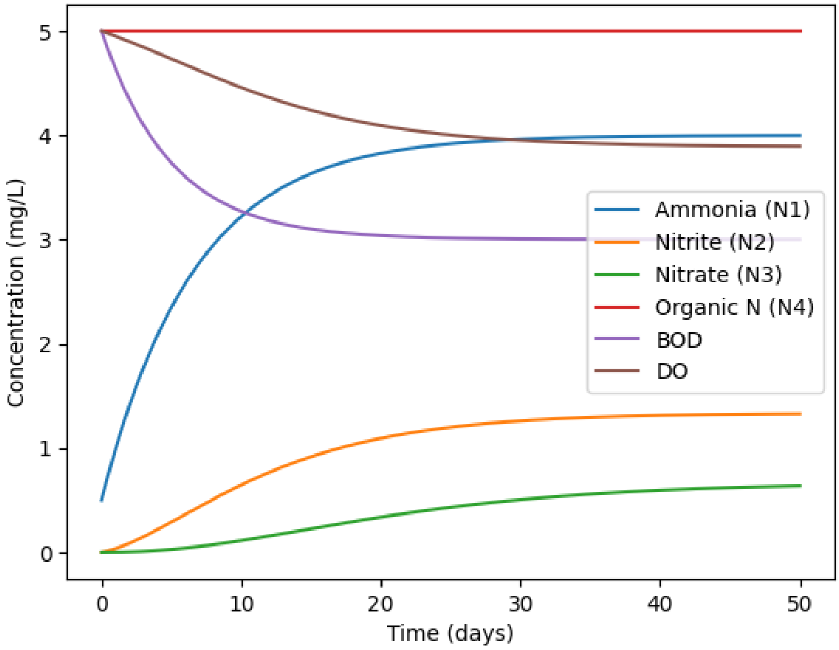

Figure 2. Simulated Temporal Evolution Of Key Water Quality Parameters In A Model Aquaculture System

Ammonia (N1), initially high at 5 mg/L, decreases sharply over the first 20-25 days as it undergoes nitrification and potentially gets taken up by algae. By the end of the simulation, it stabilizes at approximately 0.5 mg/L. Nitrite (N2), starting at zero, increases as it forms from ammonia oxidation. It peaks around day 25-30 at approximately 1.3 mg/L, and then decreases as it is oxidized to nitrate (N3). Nitrate, starting from zero, steadily increases throughout the simulation, particularly after nitrite levels begin to fall. Organic nitrogen (N4) initially at 5 mg/L, decreases gradually over time as it is hydrolyzed into ammonia and settles out of the system.

Biochemical oxygen demand (BOD, L) begins at 5 mg/L and decreases steadily, indicating the consumption of biodegradable organic matter by microorganisms. Dissolved oxygen (DO, O), initially at 5 mg/L, decreases at the beginning of the simulation due to the oxygen demand from BOD decay and nitrification. The DO stabilizes around 3.9-4.0 mg/L by the end of the 50-day period.

These results highlight the model's capacity to simulate the complex interactions of biogeochemical processes that influence water quality in aquaculture systems. The trends observed—such as the sequential progression of nitrification and the oxygen demand associated with organic matter decomposition—align with established ecological principles. These findings are essential for understanding how the system responds over time, identifying periods of potential water quality stress, and evaluating possible management interventions that could improve the system's performance.

4.3. Discussion

This study successfully developed and analyzed a comprehensive suite of mathematical models capable of simulating key water quality dynamics in aquaculture systems. The methodology used involved a process-based approach informed by existing literature to formulate a system of coupled ODEs that represent critical processes such as the nitrogen and phosphorus cycles, dissolved oxygen balance, BOD, and coliform die-off. The simulation results, particularly those illustrating the temporal changes in nitrogen species, BOD, and DO (figure 1), highlight the models' ability to capture the complex interplay and sequential transformations that occur in these aquatic environments. For example, the models clearly depict the nitrification pathway from ammonia (N1) through nitrite (N2) to nitrate (N3), along with the associated oxygen demand, providing a quantitative understanding of these critical processes.

The novelty of this work lies not in the invention of entirely new kinetic expressions for individual processes—many of which are well-established in aquatic sciences—but in the comprehensive assembly, adaptation, and integrated application of this suite of models specifically for managing aquaculture water quality. While prior studies have often focused on individual components or employed more empirical approaches, this paper offers a detailed, mechanistic framework. The contribution of this study is threefold: (1) it presents a coherent and relatively comprehensive set of mathematical models tailored for aquaculture contexts; (2) it demonstrates their dynamic behavior through simulations, providing valuable insights into system responses that can inform management practices; and (3) it outlines a clear conceptual pathway for integrating these foundational models with modern data science tools, such as IoT and ML, as discussed in Section VII. This integrated approach bridges the gap between purely mechanistic modeling and purely data-driven approaches, creating a more holistic perspective for aquaculture management.

The models developed here, while grounded in fundamental biogeochemical principles, possess inherent scalability and generalizability. The mathematical structures governing processes such as the nitrogen cycle and dissolved oxygen dynamics are broadly applicable across various aquaculture systems, including ponds, Recirculating Aquaculture Systems (RAS), and potentially cage culture, with appropriate modifications. System-specific characteristics, such as volume (V), flow rate (Q), and average depth (d), are explicitly included as parameters, allowing the models to be adapted to different physical configurations. Furthermore, the kinetic parameters (e.g., βi, Ki) used in the models are based on representative values from literature but are designed to be calibrated using site-specific data. This adaptability is crucial for the wider application of these models, as aquaculture practices and environmental conditions can vary significantly from one system to another. Additionally, the proposed framework for IoT and ML integration is modular, meaning that different sensor arrays or ML algorithms could be incorporated depending on the specific needs and available resources at each site.

The practical implications of this work for the aquaculture industry are significant and wide-ranging. Accurate, predictive models of water quality can provide several key benefits that enhance both operational efficiency and environmental sustainability. First, these models enable early warnings of deteriorating water quality conditions, such as impending low dissolved oxygen events or ammonia spikes, allowing farm operators to take corrective actions before their stocks are stressed or lost. This proactive approach helps prevent potential disasters and ensures healthier aquatic life. Moreover, a better understanding of nutrient cycling and oxygen dynamics can lead to optimized resource use. By accurately predicting the nutrient needs of aquaculture systems, the models can help optimize feeding strategies, reducing waste and nutrient discharge into the environment. Additionally, these models assist in optimizing aeration efforts, helping save energy by ensuring that only the necessary amount of oxygen is supplied to the system. Another critical benefit is the contribution to improved sustainability. By facilitating more efficient management of effluents and reducing the risk of environmental pollution, these models can play a key role in making aquaculture operations more environmentally friendly. Effective management of water quality ensures that the systems operate sustainably, mitigating their impact on surrounding ecosystems. Furthermore, when integrated into user-friendly dashboards, as envisioned in the proposed framework, these models can provide valuable decision support for farm personnel, even those with limited expertise in water chemistry. This ease of use ensures that critical decisions can be made with confidence, improving overall management practices across various aquaculture operations. Finally, the models can serve as a virtual laboratory for research and development, allowing for the testing of hypotheses regarding system responses to new feeds, stocking densities, or treatment technologies. This flexibility enables continuous innovation and improvement in aquaculture practices, ultimately leading to more efficient and sustainable farming methods.

However, despite these contributions, there are several limitations to the current study. First, while the methodology provides a framework for parameter estimation, and the simulation results demonstrate the model's capabilities, this study did not include extensive empirical validation of the models against field data from diverse, real-world aquaculture operations. Such validation is a critical next step to assess the models' predictive accuracy and robustness. Second, the discussion of IoT and ML is primarily conceptual, and the practical implementation and testing of this framework remain areas for future work. Third, the mathematical models presented in the results, while comprehensive, inevitably involve simplifications, such as representing the influence of temperature on reaction rates with fixed parameters rather than dynamic functions. This highlights that the model's performance has not been tested under varying environmental and operational conditions. Therefore, future research should prioritize the empirical validation and calibration of the presented models using high-frequency, multi-parameter data from various aquaculture systems, such as those with different species, stocking densities, seasonal temperature changes, or operational scales (e.g., ponds vs. recirculating aquaculture systems - RAS). Building on this, the development and testing of the proposed IoT-ML framework should be pursued, including identifying optimal sensor configurations and comparing the performance of different ML algorithms. Additionally, incorporating more complex biological and chemical interactions into the models, such as dynamic temperature and pH dependencies or detailed fish bioenergetics, would significantly enhance their predictive power. Finally, research into the design of user interfaces for translating complex model outputs into actionable insights for farm managers and exploring the use of these models for life cycle assessments represent other valuable avenues for future investigation.

5. Conclusion

This paper has presented a comprehensive suite of mathematical models detailing key water quality dynamics in aquaculture, including the nitrogen and phosphorus cycles, dissolved oxygen, and biochemical oxygen demand. The development and analysis of these models, as shown in Section VI, offer a mechanistic understanding of the complex biogeochemical processes that govern these aquatic environments. Simulations based on these models demonstrate their capability to predict the temporal evolution of critical water quality parameters and illustrate the dynamic interactions between them, providing a foundational tool for quantitative analysis.

The core contribution of this work is the articulation of these mathematical models, which serve as a crucial foundation for the development of advanced, data-driven aquaculture management systems. While the challenges of sensor reliability, data management, and user expertise in deploying sophisticated technologies remain pertinent, robust mechanistic models can enhance the value and interpretability of data collected via IoT networks and improve the performance of machine learning algorithms.

The proposed conceptual framework for integrating these models with real-time IoT sensor data and leveraging their outputs for ML-driven predictive analytics underscores a promising pathway toward more proactive and efficient aquaculture management. Future work should prioritize the empirical validation and site-specific calibration of these models, followed by the practical implementation and testing of the integrated IoT-ML framework. Ultimately, this research underscores the significant potential of combining foundational mathematical modeling with data science techniques to transform aquaculture into a more productive, sustainable, and resilient industry.

6. Declarations

6.1. Author Contributions

Conceptualization: M.I.S., S.E., P.S., and H.M.; Methodology: S.E.; Software: M.I.S.; Validation: M.I.S., S.E., and H.M.; Formal Analysis: M.I.S., S.E., and H.M.; Investigation: M.I.S.; Resources: S.E.; Data Curation: S.E.; Writing Original Draft Preparation: M.I.S., S.E., and H.M.; Writing Review and Editing: S.E., M.I.S., and H.M.; Visualization: M.I.S.; All authors have read and agreed to the published version of the manuscript.

6.2. Data Availability Statement

The data presented in this study are available on request from the corresponding author.

6.3. Funding

The authors received no financial support for the research, authorship, and/or publication of this article.

6.4. Institutional Review Board Statement

Not applicable.

6.5. Informed Consent Statement

Not applicable.

6.6. Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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