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Integrating Multiphysics Models for Enhanced Water and Wastewater Treatment Performance: A Comprehensive Review

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Abstract

Multiphysics modeling is essential for improving both the comprehension and optimization of water and wastewater treatment processes. This review examines the core principles of multiphysics modeling, focusing on computational methodologies, practical applications, and the interconnections between physical, chemical and biological processes within treatment systems. Additionally, it discusses various validation techniques, computational constraints, and recent innovations in numerical modeling aimed at enhancing treatment efficiency and system performance.

Keywords: Multiphysics Modeling, Computational Fluid Dynamics (CFD), Hybrid Modeling Approaches, Energy Efficiency in Treatment Systems, High-Performance Computing (HPC), Environmental Sustainability.

Introduction

A comprehensive understanding and optimization of water and wastewater treatment processes rely heavily on multiphysics modeling(1-3). This review explores the fundamental principles of multiphysics modeling, emphasizing computational approaches, practical applications, and the intricate interactions among physical, chemical, and biological processes in treatment systems. Furthermore, it addresses different validation methodologies, computational limitations, and recent advancements in numerical modeling techniques designed to improve treatment efficiency and overall system performance(4). These models effectively simulate flow patterns and turbulence dynamics but do not account for simultaneous chemical or biological interactions. Chemical kinetics models, which define reaction mechanisms such as coagulation, oxidation, and chlorination, are useful for predicting reaction rates and chemical dosing efficiency. However, they often overlook the impact of hydrodynamic forces and mass transfer processes on reaction kinetics. Similarly, mass transport models describe pollutant diffusion in treatment systems and assess pollutant removal efficiency based on concentration gradients and reaction kinetics. Yet, they fail to incorporate the influence of physical mixing and fluid dynamics, which are critical factors in real-world treatment scenarios. Biological process models employ similar approaches to simulate microbial activity in processes such as activated sludge treatment and biofilm reactors. The widely recognized activated sludge model (ASM) family provides reliable predictions of microbial growth and substrate utilization. However, these models do not fully account for the interactions between fluid dynamics and mass transfer, which are essential for accurately representing real treatment conditions. Despite their valuable contributions, single-physics models inherently analyze each process in isolation, leading to inconsistencies when applied to complex treatment systems where multiple physical and chemical phenomena occur simultaneously. The absence of integrated modeling limits the ability of these models to optimize treatment processes effectively, often necessitating extensive experimental calibration(5). Moreover, wastewater treatment plants frequently operate under dynamic conditions, including fluctuating pollutant loads and temperature variations. Single-physics models struggle to adapt to such variability, reducing their practical applicability and predictive accuracy.

To overcome these limitations, multiphysics modeling has emerged as a sophisticated computational approach that integrates multiple physical processes within a unified simulation framework. By incorporating hydrodynamic effects, chemical reaction kinetics, and biological transformations into a coupled system, multiphysics models provide a more comprehensive and realistic representation of treatment processes.(6) Multiphysics models offer a more detailed and precise representation of treatment processes by simultaneously incorporating hydrodynamic interactions, chemical reaction kinetics, and biological transformations within an integrated system. These models have been extensively applied in various treatment simulations, including mass transfer in membrane filtration, fluid flow behavior in aeration systems, reaction kinetics in coagulation, and microbial activity in biofilm reactors. By accurately capturing the interdependencies among these mechanisms, multiphysics simulations contribute to improving overall system efficiency, optimizing energy consumption, and enhancing operational reliability. Despite their numerous advantages, the widespread implementation of multiphysics modeling faces several obstacles. challenges include the high computational demands associated with these models, the necessity for experimental validation to ensure accuracy, and the inherent complexity of simulating diverse physical and biochemical processes simultaneously(2, 7). Nevertheless, recent advancements in high-performance computing, data-driven modeling, and machine learning-driven optimization have substantially increased the practicality of multiphysics simulations in water and wastewater treatment applications.This review presents a systematic evaluation of multiphysics modeling in the context of water and wastewater treatment, focusing on computational methodologies, practical applications, and the technical challenges associated with their implementation.

Multiphysics Modeling

Water and wastewater treatment processes involve intricate interactions among physical, chemical, and biological mechanisms, necessitating the use of computational modeling for effective process optimization. Multiphysics modeling integrates these diverse phenomena within a unified computational framework, offering a more precise and comprehensive representation of treatment processes. This section presents an overview of the key multiphysics modeling approaches applied in water and wastewater treatment, including computational fluid dynamics (CFD), mass transfer modeling, reaction kinetics modeling, biological process modeling, electrochemical modeling, and heat transfer simulation. Each of these techniques plays a crucial role in elucidating the interdependencies among physical processes, ultimately contributing to improved system performance and operational efficiency(8). Table 1 provides an overview of different flow regimes and CFD modeling methods commonly used in water and wastewater treatment systems.

Computational Fluid Dynamics (CFD)

Computational Fluid Dynamics (CFD) modeling is a highly effective approach for simulating fluid flow, turbulence, and mixing dynamics within various treatment units, including sedimentation tanks, aeration basins, and membrane filtration systems. By employing the Navier-Stokes equations in conjunction with turbulence models such as k-ε and k-ω, CFD facilitates a detailed analysis of hydrodynamic behavior, aiding in the optimization of system configurations. These simulations offer valuable insights into key parameters such as shear stress, velocity distribution, and residence time, all of which play a crucial role in determining overall treatment efficiency and operational performance(9-11) .CFD modeling in wastewater treatment requires solving a series of partial differential equations (PDEs) that govern fluid dynamics, turbulence, species transport, and reaction kinetics. These equations provide a mathematical framework for simulating flow behavior and pollutant interactions within treatment systems. The key governing equations include:

- Continuity equation: Ensures mass conservation within the fluid system by accounting for the inflow and outflow of mass.
- Navier-Stokes equations: Describe the conservation of momentum, allowing for the simulation of velocity fields and flow dynamics under different hydraulic conditions.
- Species transport equations: Model the dispersion, diffusion, and advection of dissolved pollutants and chemical reactants throughout the treatment process.
- Turbulence models: Represent the chaotic nature of fluid flow, utilizing models such as k-ε and k-ω to improve accuracy in predicting turbulence intensity and mixing behavior.

- Energy equation: Essential in heat transfer applications, particularly in processes where temperature variations affect reaction kinetics and biological activity.

By incorporating these equations, CFD modeling enables a more detailed and predictive analysis of wastewater treatment processes, facilitating system optimization and efficiency improvements.

Table 1. Flow Regimes and CFD Modelling Approaches in Water and Wastewater Treatment Systems

Flow Regime	Treatment Process	CFD Modelling Approach	Advantages	Limitations	Ref.
Turbulent Flow	Open channel flow, pipe flow mixing chambers	- k-ε turbulence model - k-ω turbulence model - Reynolds Stress Model (RSM) - Large Eddy Simulation (LES)	- Provides high accuracy for turbulent flows - Suitable for large-scale systems	- High computational cost - Requires turbulence model validation	(12)
Laminar Flow	Sedimentation tanks	Laminar flow model	-Computationally efficient - Suitable for low-Reynolds-number flows	- Not applicable to high-Reynolds -number systems	(13)
Multiphase Flow	Coagulation flocculation flotation filtration disinfection	- Eulerian multiphase model - Lagrangian particle tracking model	- Can capture phase interactions - Suitable for modeling particulate transport	- Requires detailed calibration - Computationally demanding	(14)
Rotating Flow	Mixing chambers, flocculation	- Sliding mesh model - Multiple Reference Frames (MRF)	- Effective for modeling rotating impellers and mixers - Captures flow recirculation accurately	- Requires additional computational resources - May not be suitable for highly unsteady flows	(15)
Reactive Flow	Chemical dosing ozonation chlorination	- Species transport model - Reaction kinetics model	- Captures chemical interactions - Optimizes dosage and mixing efficiency	- Sensitive to reaction rate constants - Requires experimental validation	(16)

Applications of CFD in Wastewater Treatment Systems

Computational Fluid Dynamics (CFD) has emerged as a crucial tool for enhancing the design and operational efficiency of wastewater treatment systems by offering detailed analyses of flow behavior, mass transport, and reaction kinetics. Through the simulation of fluid dynamics and pollutant dispersion, CFD facilitates the identification of inefficiencies, enabling engineers to refine treatment processes and optimize energy consumption. Its applications extend across multiple treatment stages, including sedimentation, aeration, membrane filtration, and chemical mixing, allowing for precise regulation of system parameters to maximize performance and reliability(17). CFD has become a fundamental tool in optimizing water and wastewater treatment processes by offering a comprehensive analysis of flow dynamics, mass transfer, and reaction kinetics. With continuous advancements in CFD techniques, treatment efficiency has significantly improved, operational costs have been minimized, and environmental sustainability has been enhanced. The ongoing evolution of CFD modeling allows for more accurate simulations, enabling better process control and resource optimization in modern treatment facilities.

Sedimentation Modeling in Clarifiers

The efficiency of sedimentation in primary and secondary clarifiers is primarily influenced by flow distribution, particle settling behavior, and hydraulic retention time. CFD simulations offer a robust approach for analyzing and optimizing these parameters by replicating fluid flow and particle interactions under realistic operating conditions.

A fundamental principle governing particle settling in clarifiers is Stokes' Law, which defines the terminal settling velocity (vsv_s) of a particle in a fluid as:

$$v_5 = \frac{(\rho_1 - \rho_2)ga^2}{18\mu}$$

where:

ρ_p and ρ_f are the densities of the particle and fluid, respectively

g represents gravitational acceleration

d is the particle diameter

μ is the fluid viscosity

This equation demonstrates how settling velocity is affected by particle size, fluid viscosity, and density differences. However, real-world sedimentation is far more intricate due to turbulence, secondary currents, and interactions among suspended particles, which cannot be accurately predicted by simple theoretical models alone. Consequently, advanced CFD modeling is essential for capturing these complexities, providing more accurate predictions of clarifier performance, and enabling system optimization to improve solids removal efficiency(18-20).

Effect of Inlet Velocity on Sedimentation Efficiency

The inlet velocity is a critical factor in sedimentation efficiency within clarifiers, as it directly affects flow patterns, turbulence intensity, and particle settling dynamics. Excessively high inlet velocities can generate significant turbulence, disrupting the settling process and causing sludge re-suspension, which reduces clarifier efficiency. Conversely, low inlet velocities may lead to poor mixing and inadequate solids removal, compromising overall treatment performance. Optimizing inlet velocity is essential for achieving uniform flow distribution, minimizing short-circuiting, and enhancing clarifier performance. Properly designed inlet configurations ensure stable hydraulic conditions that promote effective particle settling. Computational Fluid Dynamics (CFD) simulations play a key role in assessing these effects, allowing for the precise evaluation of different inlet designs and operating conditions. By leveraging CFD, engineers can develop optimized clarifier designs that improve sedimentation efficiency, reduce sludge carryover, and enhance the overall reliability of wastewater treatment processes.

(18, 21). The Reynolds number (Re) is a fundamental dimensionless parameter used to characterize flow behavior in clarifiers, significantly impacting sedimentation efficiency. It is defined by the following equation:

$$\mathrm{Re} = \frac{\rho u L}{\mu}$$

where:

Re: Reynolds number (dimensionless)

ρ: Fluid density (kg/m³)

U: Inlet velocity (m/s)

L: Characteristic length of the sedimentation system (m)

μ: Dynamic viscosity of the fluid (Pa·s)

The Reynolds number helps determine whether the flow within the clarifier is laminar or turbulent, which directly influences the settling behavior of suspended particles:

- For Re < 2000: The flow remains laminar, promoting efficient sedimentation due to minimal turbulence, allowing particles to settle under gravity with minimal disturbance.
- For Re > 4000: The flow becomes turbulent, increasing mixing intensity and reducing sedimentation efficiency by disturbing settled particles and increasing re-suspension.

Between these two thresholds, in the transitional flow regime (2000 < Re < 4000), flow behavior is partially laminar and partially turbulent, leading to variable sedimentation performance. Optimizing the inlet velocity and system design is essential to maintaining flow conditions that enhance settling efficiency, which can be effectively analyzed using Computational Fluid Dynamics (CFD) simulations.

Turbulence Modeling in CFD

Turbulence significantly impacts the performance of sedimentation in clarifiers by influencing flow stability, energy dissipation, and particle transport. Accurate modeling of turbulence is essential for predicting flow behavior, optimizing clarifier design, and minimizing sludge re-suspension. Various turbulence models, such as the k-ε and Large Eddy Simulation (LES) approaches, are commonly employed in CFD simulations to capture the complex interactions between fluid flow and suspended solids. These models help improve flow uniformity, enhance settling efficiency, and provide into optimizing hydraulic conditions within treatment systems(22, 23). Turbulence models, such as the k-ε model and Large Eddy Simulation (LES), are extensively used in Computational Fluid Dynamics (CFD) to predict flow instabilities in clarifiers. These models enable the accurate simulation of turbulent behavior, which is essential for optimizing sedimentation efficiency, minimizing sludge re-suspension, and improving overall clarifier design. The standard k-ε model, one of the most commonly applied Reynolds-Averaged Navier-Stokes (RANS) turbulence models, is governed by the following equations:

$$\frac{\partial k}{\partial t} + u_j \frac{\partial k}{\partial x_i} = P_k - \varepsilon + \frac{\delta}{\partial x_i}\left((\vartheta + \frac{vt}{\delta k}\right)\frac{\delta k}{\delta x_j}$$

$$\partial \varepsilon / \delta t + U\mathrm{J} \frac{\delta \varepsilon}{\delta xj} = C1\varepsilon\left({}^{\varepsilon}/_{K}\, PK\right) - C_{2\varepsilon}(\varepsilon 2/K) + \frac{\delta}{\delta x_i}\left[\left(v + \frac{v_T}{\delta xj}\right)\delta\varepsilon/\delta xj\right]$$

where:

k: Turbulent kinetic energy (m²/s²)

ε: Turbulent dissipation rate (m²/s³)

Pk: Turbulent energy production term

ν: Kinematic viscosity (m²/s)

νt: Eddy viscosity (m²/s)

$C_1\varepsilon$, $C_2\varepsilon$, σk, σε: Model constants

These equations describe the generation and dissipation of turbulent energy, providing a mathematical framework for modeling turbulence in clarifiers. The k-ε model is widely used due to its balance between computational efficiency and accuracy, making it ideal for large-scale sedimentation studies.

Alternatively, Large Eddy Simulation (LES) resolves larger turbulent structures directly while modeling smaller-scale eddies, offering higher accuracy but requiring greater computational resources. LES is particularly useful for capturing unsteady turbulent phenomena in clarifiers where detailed turbulence resolution is required. By incorporating these turbulence models, CFD simulations help predict the effects of turbulence on sedimentation, enabling the design of more efficient clarifiers with improved sludge settling, reduced short-circuiting, and enhanced hydraulic performance.

Multiphase Modeling for Sludge Settling

Multiphase modeling plays a crucial role in accurately simulating sludge settling dynamics in clarifiers, where solid particles interact with the surrounding liquid phase. Given the complexity of these interactions, Computational Fluid Dynamics (CFD) utilizes two primary approaches for multiphase flow simulations:

- Eulerian-Eulerian approach: Treats both the sludge (solid phase) and the liquid phase as interpenetrating continua, making it suitable for large-scale clarifier simulations where particle-fluid interactions need to be resolved over extended timeframes.
- Eulerian-Lagrangian approach: Tracks individual sludge particles within the fluid flow, providing a more detailed representation of settling behavior, particle aggregation, and sludge blanket formation.

By implementing these approaches, CFD simulations can predict sludge distribution patterns, settling efficiency, and clarifier performance under varying hydraulic conditions. These models enhance the understanding of sludge transport mechanisms, allowing for improved operational control, optimized clarifier configurations, and enhanced treatment efficiency in wastewater systems. Furthermore, advanced multiphase modeling techniques can account for flocculation dynamics, hindered settling, and sludge rheology, which are critical factors affecting sedimentation performance. Incorporating these models into CFD frameworks enables engineers to identify inefficiencies, minimize sludge re-suspension, and enhance clarifier design, ultimately leading to more stable and effective wastewater treatment operations(24-26). The motion of sludge particles within clarifiers can be effectively simulated using the Eulerian-Lagrangian approach, which tracks individual particles within the fluid phase. The force balance equation governing the movement of a settling particle is expressed as:

$$m_p \frac{du_p}{dt} = F_9 + F_d + F_b$$

where:

m_p: Particle mass

U_p: Particle velocity

F_g: Gravitational force

F_d: Drag force

F_b: Buoyancy force

Among these forces, the drag force (F_d) is a key factor influencing particle settling behavior and can be approximated using Stokes' law:

$$F_d = 3\pi\mu d_P (U - U_P)$$

where:

d_p: Particle diameter

U: Fluid velocity

U_p: Particle velocity

μ: Fluid viscosity

These equations are widely employed in Computational Fluid Dynamics (CFD) simulations to predict sludge blanket formation, settling dynamics, and clarifier performance under varying flow conditions. By integrating these forces into multiphase CFD models, engineers can optimize clarifier configurations to enhance solid-liquid separation, minimize sludge re-suspension, and improve hydraulic efficiency. In addition to CFD-based approaches, other modeling techniques also play a critical role in optimizing wastewater treatment processes. These include biological models (ASM family), reaction kinetics models for chemical dosing optimization, and mass transport models for pollutant dispersion analysis. Combining CFD with these complementary modeling approaches enables a comprehensive and predictive framework for wastewater treatment process design and optimization.

Other Types of Multiphysics Models

Mass transport models are widely used to simulate the movement of contaminants, dissolved gases, and chemical species in water and wastewater treatment systems. These models typically rely on the advection-diffusion equation, which describes the transport of solutes in flowing water by considering both convective transport (advection) and molecular diffusion.

Mass transport modeling plays a crucial role in various treatment processes, particularly in:

-Membrane filtration, where solute transport and fouling behavior affect filtration efficiency.
-Chemical dosing systems, where precise reactant distribution ensures effective disinfection, coagulation, or oxidation.
-Biofilm reactors, where nutrient transport influences microbial activity and pollutant removal efficiency.

By integrating mass transport models with CFD simulations, engineers can accurately predict pollutant dispersion, reaction dynamics, and solute concentration gradients. This enables the optimization of treatment processes, ensuring better contaminant removal, improved resource utilization, and enhanced system efficiency in water and wastewater treatment applications(27). Reaction kinetics modeling is a fundamental approach for describing the chemical transformation of contaminants in water and wastewater treatment processes, including oxidation, coagulation, and disinfection. These models rely on ordinary differential equations (ODEs) and reaction rate laws to predict the efficiency of chemical reactions under different operating conditions. In water treatment applications, reaction kinetics models are widely used to:

- Optimize chemical dosing in processes such as coagulation-flocculation, ensuring efficient removal of suspended solids and organic matter.
- Predict disinfectant effectiveness in chlorination and ozonation, helping to maintain microbial safety while minimizing harmful disinfection byproducts.
- Enhance advanced oxidation processes (AOPs) by modeling the degradation pathways of emerging contaminants and optimizing radical generation.

To improve accuracy, reaction kinetics models are often coupled with Computational Fluid Dynamics (CFD) simulations, which provide insights into chemical mixing efficiency, reaction rate distribution, and hydrodynamic influences on reaction kinetics. This integrated approach enables more effective treatment system design, reduces chemical waste and operational costs, and enhances overall treatment performance and regulatory complianc(28, 29). Biological models play a crucial role in simulating microbial activity in wastewater treatment processes, such as activated sludge systems, anaerobic digestion, and constructed wetlands. The Activated Sludge Model (ASM) family, which includes ASM_1, ASM_2, and ASM_3, offers a mathematical framework for representing microbial growth, substrate consumption, and nutrient removal dynamics. To enhance predictive accuracy and operational efficiency, these models are often integrated with Computational Fluid Dynamics (CFD) and mass transport simulations. This coupling allows for a more comprehensive analysis of oxygen distribution, aeration efficiency, and biomass retention, leading to optimized treatment performance and improved resource utilization in wastewater treatment facilities(30, 31). Electrochemical models play a vital role in advanced wastewater treatment

technologies, including electrocoagulation, electrooxidation, and capacitive deionization (CDI). These models integrate electrode kinetics, ion transport mechanisms, and electric field interactions to predict contaminant removal efficiencies and optimize treatment performance. A widely used approach in electrochemical modeling is the Poisson-Nernst-Planck (PNP) equations, which describe the behavior of charged species within electrochemical systems. These equations enable precise simulation of mass transport, charge distribution, and electrostatic interactions, facilitating a deeper understanding of electrochemical separation processes. By incorporating PNP-based modeling with computational fluid dynamics (CFD), researchers can improve process design, enhance ion removal efficiency, and optimize operational conditions for sustainable wastewater treatment applications (32, 33). Heat transfer modeling plays a critical role in wastewater treatment processes where temperature variations significantly impact system performance. Key applications include anaerobic digestion, thermal hydrolysis, and membrane distillation, where precise temperature control is essential for maintaining efficiency and stability. These models are based on Fourier's law of heat conduction and convective heat transfer equations, which enable the evaluation of temperature gradients, energy consumption, and overall thermal efficiency within treatment units. By integrating heat transfer modeling with Computational Fluid Dynamics (CFD) and biochemical process simulations, researchers can optimize thermal management strategies, reduce energy costs, and enhance the operational performance of heat-sensitive treatment technologies(34). In real-world applications, these modeling techniques are often combined to improve predictive accuracy and optimize treatment system performance. By integrating Computational Fluid Dynamics (CFD) with mass transport models, researchers can analyze pollutant dispersion and sedimentation dynamics in treatment units such as clarifiers and filtration systems. Similarly, the combination of reaction kinetics and CFD simulations is widely used to optimize chemical dosing strategies and enhance mixing efficiency in coagulation, disinfection, and oxidation processes.
Furthermore, biological models and heat transfer simulations are frequently applied to study microbial activity under varying temperature conditions, ensuring the stability and efficiency of processes such as activated sludge treatment, anaerobic digestion, and biofilm reactors. This multiphysics approach enables a more comprehensive representation of treatment processes, allowing for improved design, better operational control, and enhanced energy efficiency in wastewater treatment facilities(35). Despite the significant advantages of multiphysics modeling, several challenges and limitations persist, including high computational costs, model complexity, and the need for extensive experimental validation. The integration of multiple physical, chemical, and biological processes increases the computational demand, making large-scale simulations resource-intensive. Additionally, ensuring model accuracy requires rigorous validation against experimental data, which can be time-consuming and labor-intensive. To overcome these challenges, researchers have adopted high-performance computing (HPC) to enable large-scale simulations and enhance computational efficiency. Additionally, machine learning algorithms are increasingly being incorporated to reduce computational overhead, improve predictive accuracy, and facilitate real-time process optimization. Furthermore, advanced experimental validation techniques, such as tracer studies and real-time sensor data acquisition, are being used to refine model accuracy and ensure alignment with empirical observations. These advancements contribute to making multiphysics modeling more reliable, scalable, and applicable to real-world wastewater treatment systems(36, 37). Table 2 presents a collection of case studies that highlight the application of multiphysics modeling techniques in wastewater treatment. The table provides an overview of the target treatment processes, modeling approaches, specific applications, and key results obtained from these studies. These case studies illustrate how computational simulations enhance process understanding, optimize operational efficiency, and support the development of advanced treatment technologies. Furthermore, they demonstrate the role of multiphysics modeling in bridging the gap between theoretical analysis and real-world industrial implementation, contributing to more sustainable and efficient wastewater treatment solutions.

Table 2. Multiphysics Modeling in Wastewater Treatment

Case Study	**Target Treatment Process**	**Modeling Approach**	**Applications**	**Results**	**Ref.**

Digital Modeling for Optimization of Wastewater Treatment Management	Optimization of Wastewater Treatment Plant Operations	Digital Twin Models + CFD + Kinetic Modeling	Optimization of cost and energy consumption in urban and industrial wastewater treatment plants	Improved treatment efficiency and reduced operational costs	(38)
Simulation-Driven Strategies for Enhancing Treatment Processes	Enhancement of Chemical and Industrial Treatment Performance	Combination of Multiphysics Models and Numerical Simulation	Optimization of chemical consumption and reduction of environmental impact	Higher treatment efficiency and lower chemical consumption	(7)
Multiphysics Modeling of Biofilm Growth in Constructed Wetlands	Enhancing Pollutant Removal In Natural Treatment Systems	CFD + Biological Models (COMSOL)	Analysis of hydrodynamic behavior and pollutant removal efficiency in wetlands	Accurate simulation of flow distribution and pollutant removal rates	(3)
Technological Innovations in the Application of Constructed Wetlands	Evaluation of New Materials in Wetland-Based Treatment	Hydrodynamic and Biological Modeling	Development of novel technologies to improve treatment performance	Assessment of effective innovations in natural wastewater treatment	(39)
Multiphysics Modeling of Photocatalytic Oxidation Processes	Enhancement of Refractory Pollutant Removal Efficiency	Multiphysics Modeling for Photocatalytic Oxidation	Management of persistent pollutants and energy optimization in treatment	Higher pollutant removal efficiency and energy optimization	(40)

Comparative Analysis of Multiphysics Models in Wastewater Treatment Processes

During the primary treatment stage, where suspended solids and larger contaminants are separated from the wastewater stream, Computational Fluid Dynamics (CFD) models are widely employed to analyze sedimentation dynamics, flow distribution, and particle settling behavior. By simulating hydrodynamic conditions within clarifiers and grit chambers, CFD assists in optimizing flow patterns, minimizing short-circuiting, and improving solid-liquid separation efficiency. However, mass transport models also play a crucial role at this stage by describing the advection and diffusion of smaller suspended particles that remain in the water column. These models enable accurate predictions of contaminant dispersion, which are essential for designing efficient sedimentation tanks and enhancing pollutant removal performance(41).In the secondary treatment phase, which focuses on biological degradation of organic matter and nutrient removal, Activated Sludge Models (ASM) are extensively utilized to simulate microbial activity and substrate transformation. The ASM family, including ASM_1, ASM_2, and ASM_3, provides mathematical frameworks to model key biochemical reactions, such as carbon oxidation, nitrification-denitrification, and biological phosphorus removal. These models are instrumental in optimizing aeration strategies, sludge age, and biomass retention, ultimately maximizing treatment efficiency while minimizing energy consumption.Meanwhile, CFD modeling complements ASM models by simulating oxygen transfer in aeration basins, ensuring uniform mixing, and preventing dead zones, where microbial activity may be inhibited. In this context, CFD and ASM models are often coupled to create hybrid simulations that integrate fluid dynamics with biological kinetics, allowing for more comprehensive process optimization in wastewater treatment systems.In advanced treatment processes, where chemical oxidation, disinfection, or adsorption mechanisms are employed to remove persistent contaminants, reaction kinetics models play a pivotal role(31, 42). These models describe the chemical transformation of pollutants in processes such as ozonation, chlorination, coagulation-flocculation, and advanced oxidation processes (AOPs). By integrating kinetic rate equations with CFD simulations, researchers can optimize chemical dosing, reaction times, and mixing conditions, ensuring efficient pollutant degradation while minimizing excess chemical consumption. At this stage, mass transport models also play a crucial role, particularly in membrane filtration systems, where they assist in predicting solute transport across membranes, fouling dynamics, and variations in permeate flux. These models help in understanding the interactions between contaminants and filtration membranes, enabling strategies to reduce fouling, enhance membrane lifespan, and improve treatment efficiency. By combining reaction kinetics with mass transport models, researchers can gain a deeper understanding of how pollutants interact with chemical reagents and how these reactions influence overall system performance. This integrated approach facilitates process optimization, enhances resource efficiency, and improves the effectiveness of advanced wastewater treatment technologies. In wastewater treatment systems utilizing electrochemical processes such as electrocoagulation, electrooxidation, and capacitive deionization (CDI), electrochemical models play a vital role in analyzing charge transport, electrode kinetics, and ion migration dynamics. These models employ Poisson-Nernst-Planck (PNP) equations to describe the movement of charged species under applied electric fields, enabling researchers to optimize electrode configurations, current densities, and overall energy efficiency in electrochemical treatment units. Unlike biological and kinetic models, which primarily focus on reaction pathways and microbial transformations, electrochemical models are particularly beneficial in industrial wastewater treatment, where high-strength pollutants demand targeted electrochemical degradation mechanisms. These models facilitate a deeper understanding of redox reactions, electrode surface interactions, and electrochemical efficiency, helping to enhance treatment effectiveness(43). Additionally, Computational Fluid Dynamics (CFD) complements electrochemical modeling by simulating fluid flow and mass transport around electrodes. This integration ensures optimal contact between contaminants and reactive surfaces, improving pollutant removal efficiency and electrochemical process stability in wastewater treatment applications. Heat transfer modeling plays a crucial role in wastewater treatment processes where temperature variations directly affect system performance, such as anaerobic digestion, thermal hydrolysis, and membrane distillation. These models are used to predict temperature gradients, assess energy consumption, and evaluate thermal conductivity within reactors, ensuring process stability and minimizing heat loss(44). By integrating heat transfer models with biological and kinetic simulations, researchers can analyze the impact of temperature fluctuations on microbial activity and reaction kinetics. This combined approach enhances process control, optimizes energy utilization, and improves the overall efficiency of heat-sensitive treatment technologies. Furthermore, incorporating Computational Fluid Dynamics (CFD) allows for a more detailed analysis of convective and conductive heat transfer mechanisms, ensuring better thermal management strategies in advanced wastewater treatment applications. Although each of these models serves a specific purpose, they are rarely employed in isolation. The increasing complexity of wastewater treatment processes necessitates hybrid modeling approaches that integrate multiple physics-based simulations to achieve more accurate and comprehensive predictions. For instance, CFD is frequently coupled with Activated Sludge Models (ASM) to simulate oxygen transfer dynamics in aeration tanks, while reaction kinetics and mass transport models are often used together to optimize chemical dosing and improve coagulation and filtration efficiency. Similarly, electrochemical models are increasingly integrated with CFD to refine electrode positioning and optimize current distribution in electrooxidation and electrocoagulation systems(45).

The adoption of multiphysics modeling has significantly advanced the field of water and wastewater treatment by offering a more profound understanding of the intricate interactions between fluid dynamics, microbial processes, chemical reactions, and electrochemical phenomena. These models contribute to virtually every stage of treatment, from contaminant transport and reaction kinetics to energy optimization and effluent quality enhancement. However, despite their advantages, several challenges remain, including high computational costs, the need for extensive data calibration, and the necessity for experimental validation to ensure model accuracy and reliability in large-scale applications. Future advancements in high-performance computing (HPC) and the integration of machine learning-assisted simulations may help overcome these limitations, making multiphysics modeling an even more effective tool for designing sustainable, energy-efficient, and highly optimized wastewater treatment systems.

Impact of Climate Change on Multiphysics Modeling in Water and Wastewater Treatment

Climate change is exerting a growing influence on the performance and reliability of water and wastewater treatment systems, presenting new challenges that necessitate a reassessment of existing multiphysics modeling approaches. Factors such as rising temperatures, shifts in precipitation patterns, extreme weather events, and prolonged droughts are significantly altering hydraulic conditions, pollutant loads, and overall treatment efficiency. As these environmental fluctuations become more pronounced, current computational models must be adapted to enhance predictive accuracy and operational flexibility under dynamic conditions.Traditional multiphysics models, which have largely been developed based on historical data and steady-state assumptions, may no longer be sufficient for capturing the variability and unpredictability introduced by climate change. Moving forward, these models must evolve to integrate real-time data, uncertainty-driven parameters, and adaptive algorithms, ensuring greater resilience and responsiveness in wastewater treatment planning and operation. By incorporating climate-adaptive modifications, computational simulations can more effectively predict system performance under extreme conditions, supporting the development of more robust and sustainable treatment strategies(46, 47). One of the most profound impacts of climate change on wastewater treatment systems is the rise in water temperature, which directly affects biochemical and chemical processes within treatment facilities. Biological models, such as ASM_1, ASM_2, and ASM_3, which are widely used to simulate microbial activity in activated sludge systems, exhibit a strong dependency on temperature variations. Warmer temperatures generally accelerate microbial reactions, leading to enhanced organic matter degradation and improved nutrient removal. However, excessive temperature increases can disrupt microbial community stability, negatively affecting nitrification efficiency and raising the risk of process failure. Similarly, reaction kinetics models, which simulate oxidation, disinfection, and coagulation processes, must be recalibrated to reflect temperature-dependent reaction rates. Standard kinetic models frequently rely on the Arrhenius equation to adjust for temperature variations, but non-linear effects induced by fluctuating environmental conditions require more advanced and adaptable modeling techniques to maintain predictive accuracy. Additionally, mass transport models must account for the reduced solubility of oxygen in warmer water, which directly impacts aeration efficiency and dissolved oxygen availability. This reduction can create inefficiencies in biological treatment processes, particularly in activated sludge systems and aerobic digesters, where oxygen transfer is critical for microbial metabolism. To address these challenges, updated multiphysics models incorporating real-time temperature adjustments and adaptive process control strategies are essential for ensuring stable and efficient wastewater treatment performance under changing climatic conditions(48, 49). Changes in precipitation patterns introduce additional complexities to wastewater treatment operations, necessitating adaptive strategies to maintain system efficiency. Intensified rainfall and flash floods can lead to hydraulic overloading of treatment plants, significantly reducing hydraulic retention times and compromising pollutant removal efficiency. To address these challenges, Computational Fluid Dynamics (CFD) models, which are widely used to simulate fluid flow and sedimentation dynamics, require enhancements to handle sudden variations in flow rates and turbulence levels. These models must be capable of adapting to transient hydraulic conditions to provide accurate predictions of clarifier performance and aeration basin stability under extreme stormwater inflow scenarios. Furthermore, increased stormwater runoff introduces elevated levels of heavy metals, nutrients, and organic pollutants, which necessitate refinements in reaction kinetics and mass transport models to effectively account for fluctuating pollutant concentrations and their impact on treatment efficiency. Conversely, in drought-prone regions, reduced water availability leads to more concentrated wastewater streams, altering the chemical and biological equilibrium of treatment processes. Under such conditions, multiphysics models must be modified to accurately simulate treatment performance under high contaminant loads and limited dilution capacity. Advanced modeling techniques integrating real-time data assimilation and adaptive process controls are essential for ensuring stable operation and regulatory compliance in wastewater treatment systems exposed to extreme climatic variability(50-52). The necessity for adaptive multiphysics models has become increasingly evident due to the uncertainties introduced by climate change. Traditional CFD, biological, and chemical reaction models can be significantly enhanced by incorporating real-time monitoring systems and machine learning algorithms, allowing for more responsive and predictive wastewater treatment strategies.AI-driven analytics offer a powerful tool for process optimization, enabling the identification of patterns in aeration efficiency, chemical dosing, and microbial activity in response to climate-induced fluctuations. By leveraging machine learning techniques, treatment plants can anticipate operational challenges, optimize resource utilization, and adjust system parameters in real time to maintain efficiency. Additionally, hybrid modeling approaches that integrate fluid dynamics, reaction kinetics, and biological transformations can facilitate dynamic adjustments to hydraulic and biochemical conditions. These models improve treatment system resilience against extreme environmental variations, ensuring stable pollutant removal performance, reduced operational costs, and enhanced sustainability in the face of changing climate conditions(38). To further strengthen the robustness of multiphysics models in the face of climate change-related uncertainties, more advanced calibration methods are necessary. Traditional models typically rely on static parameter assumptions, which limit their adaptability to rapidly changing environmental conditions. Future modeling approaches should integrate real-time sensor data, enabling dynamic adjustments to system parameters and enhancing the accuracy of treatment performance predictions.The incorporation of high-performance computing (HPC) and reduced-order modeling (ROM) techniques can significantly reduce computational costs, allowing for large-scale simulations that effectively account for climate-driven variability in wastewater treatment processes. By optimizing computational efficiency, these approaches make multiphysics modeling more feasible for real-time applications and large-scale industrial implementations. Moreover, linking climate forecasting data with wastewater treatment process simulations can facilitate proactive decision-making, ensuring that treatment facilities are better prepared for extreme weather events such as intense rainfall, prolonged droughts, and sudden temperature shifts. By integrating climate-responsive predictive modeling, treatment plants can develop adaptive operational strategies, improving resilience, efficiency, and sustainability in the face of evolving environmental challenges (38, 53). Despite significant advancements in multiphysics modeling, several challenges persist. Current models often struggle to accurately account for sudden changes in wastewater composition, fluctuating energy demands, and variations in pollutant removal efficiency under unpredictable climatic conditions. The complex interactions between fluid dynamics, biochemical reactions, and contaminant transport require further refinement to enhance model accuracy, adaptability, and reliability.To improve the applicability of these models, long-term validation using real-world data from wastewater treatment plants operating in diverse climatic conditions is essential. Such validation efforts ensure that computational models can effectively simulate system behavior across different environmental scenarios, thereby increasing their practical utility in wastewater management.Beyond operational improvements, multiphysics modeling plays a crucial role in promoting sustainability in wastewater treatment. CFD and biological models contribute to optimizing aeration strategies, leading to substantial energy savings in activated sludge systems. Additionally, advanced reaction kinetics modeling enables precise chemical dosing in disinfection and coagulation processes, which helps minimize excessive chemical consumption and reduce the formation of harmful disinfection byproducts.By improving energy efficiency and optimizing resource utilization, these models significantly aid in reducing greenhouse gas emissions, aligning wastewater treatment practices with global environmental sustainability goals. As high-performance computing (HPC), machine learning integration, and real-time monitoring continue to evolve, multiphysics modeling will become an even more powerful tool for designing resilient, cost-effective, and environmentally sustainable wastewater treatment systems (3, 38).

The Role of Hybrid Multiphysics Modeling in Wastewater Treatment Optimization

The comparison of multiphysics modeling techniques underscores the necessity of hybrid modeling approaches in wastewater treatment. While each modeling technique provides valuable insights into specific treatment processes, no single model can comprehensively represent the complex interplay between fluid dynamics, biochemical reactions, and mass transport mechanisms. By integrating Computational Fluid Dynamics (CFD) with Activated Sludge Models (ASM), reaction kinetics models, and electrochemical simulations, researchers can develop more precise and predictive simulations, ultimately leading to greater treatment efficiency, reduced operational costs, and improved environmental sustainability.Looking ahead, advancements in high-performance computing (HPC) and real-time sensor integration will significantly enhance the accuracy, computational efficiency, and scalability of multiphysics models in wastewater treatment. These technological developments will play a pivotal role in the design and implementation of next-generation treatment systems, ensuring they are both energy-efficient and resilient to the increasing challenges posed by climate change(7, 54). Table 3. Comparison of multiphysics models in wastewater treatment is shown.

Table3. Comparison of Multiphysics Models in Wastewater Treatment

Model	Application in Wastewater Treatment	Advantages	Limitations	Best Integration with Other Models
Computational Fluid Dynamics (CFD)	Analysis of hydrodynamics, mass transport, and optimization of sedimentation and aeration units.	Provides accurate flow and turbulence analysis; optimizes system design.	Computationally intensive; does not model biochemical reactions.	ASM for biological process modeling; Mass Transport Models for pollutant distribution.
Activated Sludge Model (ASM)	Simulation of microbial growth, organic matter degradation, and nutrient removal in biological treatment.	Accurately models biological processes and nutrient removal mechanisms.	Does not account for hydrodynamic effects; requires calibration with empirical data.	CFD for oxygen transfer simulation; Reaction Kinetics Models for degradation studies.
Mass Transport Models	Simulation of contaminant and chemical species movement in filtration and biofilm reactors.	Enables tracking of pollutant dispersion and solute transport in various systems.	Lacks chemical reaction modeling; less accurate under transient conditions.	CFD for flow behavior analysis; Reaction Kinetics Models for chemical transformations.
Reaction Kinetics Models	Modeling oxidation, disinfection, and coagulation processes to optimize chemical treatment.	Improves chemical dosing efficiency and optimizes reaction rates.	Does not include spatial variations; requires CFD integration for real-world accuracy.	CFD for chemical dispersion analysis; Mass Transport Models for solute tracking.
Electrochemical Models	Analysis of charge transport, electrode kinetics, and ion migration in electrochemical treatment methods.	Optimizes electrode positioning and enhances energy efficiency in electrochemical processes.	Complex computational models requiring detailed electrochemical data.	CFD for electrode-fluid interaction; Mass Transport Models for ion movement.

Advancements and Future Directions in Multiphysics Modeling for Water Treatment

The integration of multiphysics modeling in water treatment is fundamental for enhancing process efficiency, reducing operational costs, and ensuring the delivery of high-quality treated water. By combining Computational Fluid Dynamics (CFD), mass transport models, reaction kinetics, and electrochemical simulations, researchers can develop more precise and predictive treatment strategies. These approaches facilitate:

- Optimization of filtration and disinfection processes, improving overall system performance.

- Increased efficiency in chemical treatment, ensuring effective contaminant removal while minimizing reagent consumption.
- Enhanced management of emerging contaminants, enabling better control over pollutants resistant to conventional treatment methods.

Looking ahead, emerging innovations in high-performance computing (HPC), machine learning-driven simulations, and real-time sensor integration will further refine multiphysics models, making them more adaptive, efficient, and sustainable for future water treatment applications. These advancements will play a key role in developing next-generation treatment systems, ensuring they are both energy-efficient and resilient to evolving environmental and operational challenges(55, 56). Table 4 shows a comparison of multiphysics models in water treatment.

Table4. Comparison of Multiphysics Models in Water Treatment

Model	Application in Water Treatment	Advantages	Limitations	Best Integration with Other Models
Computational Fluid Dynamics (CFD)	Optimization of flow patterns in filters, coagulation basins, and disinfection systems	Accurate analysis of flow and mixing; optimization of physical treatment processes	High computational cost; does not model chemical reactions	Mass Transport Models for chemical dispersion analysis; Reaction Kinetics Models for disinfection and oxidation
Mass Transport Models	Modeling the movement of contaminants and chemical species in water treatment processes	Precise prediction of chemical distribution and pollutant transport; widely applied in filtration	Does not account for hydrodynamic effects; less accurate in transient conditions	CFD for hydrodynamic analysis; Reaction Kinetics Models for understanding disinfection efficiency
Reaction Kinetics Models	Analysis of chemical reactions such as chlorination, ozonation, and coagulation	Optimizes chemical dosing and predicts disinfection process efficiency	Lacks spatial resolution; requires CFD for chemical dispersion modeling	CFD for mixing efficiency analysis; Mass Transport Models for chemical transport assessment
Electrochemical Models	Modeling electrochemical processes like electrodialysis and desalination	Enhances process efficiency for ion removal and heavy metal elimination	Complex computational modeling; requires detailed electrochemical data	CFD for electrode-fluid interaction analysis; Mass Transport Models for ion migration studies

CONCLUSION

Multiphysics modeling has emerged as a powerful tool for optimizing water and wastewater treatment processes. The integration of CFD, mass transport, reaction kinetics, biological, and electrochemical models has significantly improved the understanding of physical, chemical, and biological phenomena in treatment systems. These models enhance treatment efficiency, reduce energy consumption, and optimize the use of chemical reagents. This study highlights the crucial role of CFD and mass transport models in improving sedimentation, filtration, and disinfection processes. Reaction kinetics models contribute to the optimization of chemical dosing and enhance the effectiveness of coagulation and oxidation processes, while biological models, particularly ASM, are essential for simulating microbial activity in biological treatment and anaerobic digestion. The combination of multiphysics modeling with machine learning and high-performance computing (HPC) can further enhance simulation accuracy and speed, ultimately supporting better operational decision-making in treatment facilities. Despite these advancements, challenges such as high computational costs, the need for extensive experimental data for model calibration, and the complexity of integrating multiple models remain. Future research should focus on developing hybrid models that simultaneously incorporate physical, chemical, and biological characteristics within a unified simulation framework. The direct integration of real-time data from remote sensing and smart sensors will further enhance efficiency and enable better prediction of operational changes. Overall, multiphysics modeling holds great promise for advancing water and wastewater treatment, contributing to improved water quality, reduced environmental impacts, and increased energy efficiency. Continued investment in the development of more precise and computationally efficient models will play a crucial role in strengthening the sustainability of treatment systems and improving water resource management.

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