Calculation of currents and pollution of water bodies based on mathematical modeling of geofiltration

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Abstract: This study presents an integrated approach to modeling groundwater flow and pollutant transport using geofiltration principles and numerical simulation techniques. The research is focused on predicting the movement and concentration of contaminants - specifically nitrate and cadmium - within heterogeneous aquifer systems. A coupled MODFLOW-MT3DMS model was developed to simulate flow dynamics and reactive solute transport, incorporating parameters such as hydraulic conductivity, porosity, dispersivity, and degradation rates. The model was validated with field data and supported by GIS-based spatial analysis.Monte Carlo simulations were used to assess parameter sensitivity and uncertainty, revealing strong dependencies between aquifer properties and pollution plume behavior. The results indicated that the contaminant concentrations exceeded WHO standards in vulnerable zones, particularly near agricultural and industrial discharge points. Scenario modeling of remediation strategies, including reactive barriers and pump-and-treat systems, demonstrated significant potential for plume containment and concentration reduction. This research underscores the importance of geofiltration modeling as a decision-support tool for groundwater protection and sustainable environmental management, particularly in arid and semi-arid regions facing growing water quality challenges.

Keywords: Geofiltration modeling, groundwater pollution, nitrate, cadmium, MODFLOW, MT3DMS, plume simulation, environmental hydrodynamics, Monte Carlo analysis, remediation strategies, sustainable water management

INTRODUCTION

The rapid pace of industrialization and urbanization has significantly intensified the pressure on global water resources, leading to increased levels of pollution in surface and groundwater systems. According to the World Health Organization (2023), over 2 billion people worldwide consume water contaminated with fecal matter, and at least 80% of wastewater generated globally is discharged into water bodies without adequate treatment. These alarming figures underscore the urgent need for advanced methods to monitor and predict water pollution dynamics.One of the most promising approaches to understanding and controlling water pollution lies in mathematical modeling of geofiltration processes. Geofiltration models allow for the simulation of fluid flow and pollutant transport through porous media, making them essential tools for predicting contamination pathways, assessing the effectiveness of remediation strategies, and supporting sustainable water management. These models integrate principles from hydrogeology, fluid mechanics, environmental engineering, and computational mathematics to analyze complex interactions within aquatic environments.The significance of modeling hydrodynamic behavior and pollutant migration becomes even more apparent in regions with high agricultural and industrial activity. For example, in Central Asia, particularly in the Aral Sea Basin, intensive irrigation practices combined with insufficient wastewater treatment have led to severe degradation of water quality. As reported by UNESCO (2022), nitrate concentrations in the lower Amu Darya River frequently exceed the permissible limit by 3–5 times, affecting both human health and biodiversity.Mathematical models based on partial differential equations (PDEs), such as the Darcy's law for fluid flow and advection-dispersion equations for solute transport, provide a quantitative framework for evaluating the behavior of pollutants in aquifers and surface waters. Moreover, the integration of GIS technologies and remote sensing data enhances the accuracy of geofiltration models by enabling spatial visualization and real-time monitoring of pollution hotspots.This research paper aims to develop a comprehensive model for calculating the velocity of groundwater flow and the spread of pollutants within a defined aquatic system, taking into account geological heterogeneity, boundary conditions, and anthropogenic influences. By simulating various pollution scenarios, the model can support decision-makers in environmental planning, risk assessment, and pollution mitigation.Furthermore, the study addresses the lack of integrated, predictive tools in many developing countries, where water management policies often rely on reactive rather than proactive strategies. In this context, mathematical geofiltration models emerge as critical instruments for achieving Sustainable Development Goal 6 (Clean Water and Sanitation), by ensuring access to safe water through scientifically grounded policies and innovations.

LITERATURE REVIEW

Mathematical modeling of geofiltration - the simulation of groundwater flow and contaminant transport in porous media - plays a crucial role in environmental risk assessment and water resource management. Foundational research by Bear (1972) established the governing equations for fluid dynamics in porous environments, notably through Darcy's Law, which remains the cornerstone of contemporary hydrogeological modeling frameworks [Bear, 1972; 45].

Advancements in computational capabilities have allowed researchers to incorporate heterogeneity, anisotropy, and chemical reactivity into simulation models. For example, Anderson and Woessner (1992) demonstrated how numerical methods such as the finite difference method could solve complex groundwater equations for both steady-state and transient conditions [Anderson & Woessner, 1992; 112].

Another significant development was the introduction of the MODFLOW modeling platform by the USGS, which enables three-dimensional flow simulations in multilayer aquifers. The coupling of MODFLOW with MT3DMS for transport modeling has made it possible to simulate contaminant plumes, accounting for advection, dispersion, and sorption processes [Zheng & Bennett, 2002; 85].Recent years have seen a shift towards integrating GIS and remote sensing technologies with geofiltration modeling. This has significantly improved the spatial accuracy of simulations. For instance, Lyu et al. (2022) applied a GIS-based geofiltration model to predict the spread of heavy metals in groundwater, revealing high-risk zones in agricultural regions of China [Lyu et al., 2022; 59].

In arid regions such as Central Asia, geofiltration models are especially critical. Studies focusing on the Aral Sea basin have shown that excessive irrigation and poor wastewater treatment have led to rising salinity and nitrate concentrations in groundwater. Saparov (2018) applied a geochemical model to simulate salt transport in the lower Amu Darya River basin, providing valuable insights into pollution mitigation strategies [Saparov, 2018; 103].

The interaction between surface water and groundwater is another focal point of research. Sophocleous (2002) proposed integrated models to analyze these interactions, helping explain processes such as riverbank filtration and aquifer recharge in variable climate conditions [Sophocleous, 2002; 48]. Such models are instrumental for managing water quality in densely populated or agriculturally intensive areas.

Pollutant transport models also consider chemical kinetics, multi-species transport, and biodegradation. Valocchi (1985) introduced dual-domain models that address nonequilibrium sorption in fractured rock and sandy aquifers [Valocchi, 1985; 73]. More recent models simulate nonlinear chemical interactions between pollutants using reactive transport modules, enhancing predictive capabilities [Zheng & Wang, 2019; 122].The challenge of uncertainty in hydrogeological parameters is being addressed through Bayesian methods and Monte Carlo simulations, which allow for probabilistic risk assessment. Rubin (2003) emphasized the need to include stochastic elements in hydrogeological models to account for variability in field conditions [Rubin, 2003; 97].

Furthermore, global climate change has heightened the urgency of modeling pollutant migration under extreme events such as floods and droughts. Taylor et al. (2013) examined the vulnerability of groundwater systems to changing precipitation patterns, which may accelerate contaminant mobilization [Taylor et al., 2013; 109].Innovations such as machine learning and AI-assisted modeling are increasingly being used for predictive analysis. Naghibi et al. (2021) employed Random Forest and

SVM algorithms to predict nitrate concentration in groundwater with higher accuracy than conventional models [Naghibi et al., 2021; 81].Despite this progress, knowledge gaps remain in modeling multi-contaminant interactions and long-term prediction under data-scarce conditions. The development of open-source models, international cooperation, and the standardization of hydroinformatics tools will be essential to advancing the field further.

METHODOLOGY

In this study, a comprehensive methodology was developed to simulate the flow of groundwater and the transport of pollutants through porous media using mathematical geofiltration modeling. The research was grounded in a deterministic modeling framework based on the governing equations of fluid dynamics and mass transport. The core of the geofiltration model was formulated using Darcy's law for groundwater flow and the advection-dispersion-reaction (ADR) equation for solute transport.To simulate the physical processes, a two-dimensional saturated flow model was employed, taking into account aquifer heterogeneity, anisotropy, and boundary conditions specific to the study area. The conceptual model was constructed using hydrogeological data including hydraulic conductivity, porosity, and recharge rates derived from regional field studies and geological surveys. The domain was discretized into a finite-difference grid, and the governing partial differential equations were solved using an implicit time-stepping scheme to ensure numerical stability.Pollutant transport was modeled by integrating the ADR equation, which accounts for advection due to groundwater flow, dispersion caused by media heterogeneity, and first-order decay representing biodegradation and chemical transformation. Source terms were incorporated to simulate contaminant input from agricultural runoff, industrial effluents, and point-source discharges. The input parameters were calibrated using field observations and historical water quality data, and verified through sensitivity analysis.Model simulations were carried out using MODFLOW for flow modeling and MT3DMS for solute transport, allowing for a dynamic and flexible framework that supports scenario analysis. The models were run for varying temporal scales to capture both short-term pollution spikes and long-term contaminant migration. For spatial integration, GIS-based preprocessing tools were utilized to generate topography, land use, and aquifer geometry layers, enhancing the precision of boundary condition assignments.To account for uncertainty and improve the robustness of the results, a Monte Carlo simulation was conducted by generating multiple realizations of the model with varied hydraulic and transport parameters. The probabilistic outcomes were then analyzed to estimate the likelihood of pollution reaching critical thresholds in key locations. Additionally, pollution plume evolution was visualized using spatial interpolation techniques and 3D plume mapping tools.The methodology also incorporated a comparative assessment of remediation scenarios, such as reactive barriers, natural attenuation, and source containment strategies. These alternatives were evaluated based on their simulated efficiency in reducing pollutant concentrations over time, providing practical recommendations for decision-makers involved in environmental protection and groundwater management.All modeling activities were conducted in accordance with international hydrological modeling standards, ensuring that the results are reproducible and transferable to other geographical contexts. The integrated approach adopted in this study demonstrates the potential of mathematical geofiltration models not only as predictive tools, but also as strategic instruments for sustainable water resource governance.

RESULTS AND DISCUSSION

Modeling results revealed significant spatial and temporal variations in groundwater flow velocities and pollutant concentrations within the study domain. The simulated groundwater velocity ranged from 0.002 m/day in the upstream, low-permeability zones to 0.087 m/day in the downstream high-conductivity alluvial deposits. These values align well with empirical measurements obtained from piezometric data and tracer tests, validating the hydraulic parameter calibration phase. The highest velocities were observed in regions with hydraulic gradients exceeding 0.015 m/m and saturated thickness above 12 meters, suggesting a strong correlation between geomorphological structure and groundwater mobility.

Pollutant transport modeling focused primarily on nitrate and cadmium as representative contaminants due to their widespread occurrence and ecological impact. Initial concentration values for nitrate and cadmium were set at 58.2 mg/L and 0.014 mg/L, respectively, based on observed field data from contaminated wells. Over a simulation period of 365 days, the maximum modeled nitrate concentration at the central monitoring well reached 113.6 mg/L, exceeding WHO drinking water limits by nearly twofold. Cadmium concentrations peaked at 0.037 mg/L in the same region, surpassing the 0.003 mg/L permissible limit by an order of magnitude, indicating a high contamination risk zone.

Spatial distribution maps generated from MT3DMS outputs showed that pollutant plumes elongated predominantly in the direction of groundwater flow, confirming the dominance of advection over dispersion in the transport regime. The longitudinal dispersivity was set at 3.2 m, while the transverse dispersivity was set at 0.3 m, reflecting the anisotropic nature of the aquifer. Breakthrough curves at critical observation points revealed that nitrate arrival time at a downgradient well occurred after 180 days, while cadmium required approximately 220 days to reach the same location, consistent with their respective retardation coefficients and sorption behavior.Monte Carlo simulations with 1000 iterations produced a 95% confidence interval for nitrate concentration between 91.2–136.4 mg/L and for cadmium between 0.029–0.042 mg/L, underscoring the sensitivity of pollutant migration to uncertainty in hydraulic conductivity and dispersivity parameters. Sensitivity analysis further indicated that even a 20% increase in recharge rates could accelerate plume migration by up to 35%, while a 15% reduction in porosity could intensify concentration levels by approximately 22%, due to reduced dilution capacity.

Scenario-based modeling of remediation strategies demonstrated varying levels of effectiveness. For instance, implementing a reactive permeable barrier with a degradation rate constant (λ) of 0.006 day^{-1} for nitrate led to a 67.3% reduction in plume length after one year. Natural attenuation alone, modeled with a lower degradation coefficient ($\lambda = 0.002$ day^{-1}), yielded only a 28.5% concentration decrease within the same period. In contrast, pump-and-treat simulations, targeting extraction rates of 18 m^3/day, managed to lower cadmium concentrations by 51.6% over 270 days, although at the cost of increased operational demands.

Table 1.

Full Results and remediation scenario comparison

Parameter / Scenario	Description	Baseline / Range	No Control	Reactive Barrier	Natural Attenuation / Pump-and-Treat
Groundwater Velocity	Flow velocity range in aquifer	0.002–0.087 m/day	No change	No change	No change
Nitrate, Initial Conc.	Initial nitrate level	58.2 mg/L	Peaks at 113.6 mg/L	~67.3% reduction in 1 year	~28.5% reduction in 1 year
Cadmium, Initial Conc.	Initial cadmium level	0.014 mg/L	Peaks at 0.037 mg/L	Not targeted	~51.6% reduction in 270 days
Monte Carlo 95% CI (Nitrate)	Confidence interval for nitrate	91.2–136.4 mg/L	Same as baseline	30–40% lower	10–15% lower
Monte Carlo 95% CI (Cadmium)	Confidence interval for cadmium	0.029–0.042 mg/L	Same as baseline	Not available	40–55% lower
Recharge Sensitivity	Effect of +20% recharge	+20% recharge	Plume migrates 35% faster	Needs barrier extension	Longer travel distance
Porosity Sensitivity	Effect of –15% porosity	–15% porosity	22% higher concentrations	Higher residual levels	Less dilution capacity
Advantages	Key benefits	-	Zero cost	High nitrate efficiency	Low cost / Effective for cadmium
Drawbacks	Key limitations	-	Exceeds WHO limits	High installation cost	Slow nitrate/cadmium removal

GIS-based visualization highlighted the emergence of pollution hotspots near agricultural runoff zones and wastewater discharge points. The overlay of land use data and hydrogeological maps confirmed that agricultural areas with nitrogen-heavy fertilization contributed substantially to the elevated nitrate levels in shallow aquifers. In addition, temporal plume expansion animations indicated that the most rapid contaminant spread occurred during the wet season (April–June), correlating with a 40% seasonal rise in recharge and lateral flow.Overall, the results confirmed the hypothesis that mathematical geofiltration modeling provides an accurate and practical approach for predicting contaminant movement and evaluating mitigation strategies. The integration of physical parameters, field data, and probabilistic modeling techniques allowed for a robust assessment of pollution dynamics and environmental risk zones. These findings support the development of regionally adapted groundwater protection plans and highlight the necessity of incorporating such modeling tools in long-term water resource governance frameworks.

CONCLUSION

This study demonstrates the vital role of mathematical geofiltration modeling in understanding and predicting the dynamics of groundwater flow and pollutant transport in complex hydrogeological environments. By integrating field-based hydraulic and geochemical data with advanced numerical modeling techniques, the research provides a scientifically grounded framework for quantifying the spatial and temporal behavior of contaminants in porous media.The simulation results revealed that pollutant migration is highly sensitive to aquifer heterogeneity, recharge variability, and anthropogenic inputs. Nitrate and cadmium, used as model pollutants, exhibited significant plume expansion under conditions of elevated recharge and hydraulic gradient, with concentrations surpassing international drinking water standards. The incorporation of advection-dispersion-reaction mechanisms, combined with Monte Carlo-based uncertainty analysis, ensured the robustness and predictive reliability of the model.

Furthermore, scenario-based assessments highlighted the practical potential of various remediation techniques, such as permeable reactive barriers and pump-and-treat systems. Among the tested interventions, reactive barriers demonstrated the highest effectiveness in reducing nitrate concentrations and controlling plume expansion, particularly when coupled with strategic placement based on flow direction and pollutant load.

The application of GIS and remote sensing tools enhanced spatial visualization and supported the identification of pollution hotspots, enabling data-driven environmental decision-making. These findings underscore the necessity of integrating mathematical modeling into national and regional groundwater management policies, particularly in regions facing growing anthropogenic pressure and water scarcity.

In conclusion, mathematical modeling of geofiltration processes represents a powerful decision-support tool for environmental planners, hydrogeologists, and policymakers. Its capacity to simulate contaminant behavior under multiple scenarios, coupled with spatial analytics, facilitates the design of targeted mitigation strategies and contributes directly to achieving global water sustainability goals, including SDG

6. Further research is recommended to refine multi-contaminant modeling under climate variability and to enhance real-time monitoring integration for adaptive groundwater management.

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