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Predictive Modeling of Microplastic Dispersion in Aquatic Ecosystems Using Differential Equations and Environmental Data Analytics

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Abstract:

Microplastics are giving pollution to aquatic ecosystems, threatening ecological and public health considerations because they are persistent and able to bioaccumulate. The paper presents a predictive model approach to simulate microplastic dispersion by using a system of differential equations, along with employing real environmental data sets. The model employs a two-dimensional advection-diffusion approach to quantify microplastic transport in any selected water system, considering variables such as flow velocity, temperature, and concentration gradients. Environmental data collected from public data repositories are integrated by using Python and QGIS for geospatial mapping and simulation. Model calibration and sensitivity analysis ensure that hydrodynamics pose a major influence on microplastic distribution. High validation results were obtained when comparing to field-observed data; significant accretion zones were traced near low-flow areas and urban discharge points. This interdisciplinary approach demonstrates the value of mathematical modeling in environmental science, providing a scalable and adaptable framework for microplastic pollution prediction. The results can inform policy and support mitigation strategies, emphasizing the role of integrated science and data analytics in addressing global environmental challenges.

INTRODUCTION

In recent years, the global scientific community has increasingly focused its attention on the growing threat of microplastic pollution in aquatic ecosystems. Microplastics, typically defined as plastic particles less than 5mm in size, have emerged as a pervasive and persistent contaminant of significant ecological and human health concern. These particles are either manufactured at microscopic sizes (primarily microplastics, which are intentionally manufactured at small sizes, e.g., microbeads in cosmetics or industrial abrasives) or result from the fragmentation and weathering of large plastic debris (secondary microplastics, which result from the environmental degradation of larger plastic items through physical abrasion, UV radiation, or chemical weathering). Sources include a wide range of human activities, such as improper plastic disposal, industrial effluents, urban runoff, the abrasion of synthetic textiles, and the degradation of personal care products [1]. Microplastics have been detected in almost every type of water body, from freshwater lakes and major rivers to coastal estuaries and deep ocean sediments. Alarmingly, they have also been found in remote and ostensibly pristine locations such as the Arctic Ocean, the Mariana Trench, and polar ice caps, illustrating their remarkable capacity for long-range transport through atmospheric and hydrological pathways. The widespread presence of POPs actually raises grave environmental concerns, since they are incredibly persistent in the environment-they resist degradation processes, biological or chemical, for many years, perhaps even centuries, and could allow bioaccumulation in aquatic food webs [2].

One of the most dastardly facets of the pollution from microplastics is their multi-level impacts on aquatic organisms and ecosystems. Generally microplastic particle sizes are easy to be ingested by aquatic organisms varying from zooplankton, benthic invertebrates, to bigger fish, turtles, and marine mammals. This ingestion could create situations leading to physical injuries, those of gastrointestinal blockages, oxidative stresses, and a change in feeding behavior, along with reduced reproduction ability. Microplastics, in addition, act as carriers of persistent organic pollutants (POPs) and heavy metals and pathogenic microorganisms. With their high surface area-to-volume ratio combined with their hydrophobicity, microplastics bind onto the surfaces of aforementioned toxins and build their pathways into the biological system thereby increasing the toxicological effects [3]. The disruptions set the traffic levels in a ripple of effects and when it reaches

humans through seafood consumption, it increasingly threatens food security and public health. In spite of long attempts to study the presence of microplastics and impacts through field sampling or laboratory experiments, immense knowledge gaps remain in the comprehension of their spatial and temporal distribution within aquatic systems in nature [4]. Field-based assessments are often fraught with logistical constraints, special limitations, and inconclusive sampling methodologies. In addition, microplastics are affected by many and varied external parameters: thermodynamics, sediment interaction, particle density, environmental factors including temperature, salinity, and flow regimes. With more complexities, one cannot; therefore, use observational data alone to accurately determine dispersion patterns.

Hence, computational modeling is proving to be a major tool to simulate the transport and accumulation of microplastics in the aquatic environment. The mathematical modeling setup, chiefly based on PDEs, allows the researchers to simulate the elaborate physical processes of varying nature extended over space and time. Of these, advection-diffusion is probably the most widely used type of equations for the transport of solutes and suspended particles in flowing water. It considers the advective movement caused by fluid flow and diffusive spreading caused by turbulence and molecular interactions. In the case of microplastics, such models may show the transport mechanisms, retention areas, and potential ecological hazards [5,6]. Lastly, in recent years, the so-called availability of data and tools for computation has contributed much to the option of applicability of models developed theoretically for engineering application. High-quality satellite imagery now forms the very input for accurate simulation, along with freely available meteorological- and hydrological-related data sets and in situ environmental monitoring programs. In addition, Python, with libraries for numerical analysis including NumPy and SciPy, alongside a QGIS platform, allows spatial analyses and visualization of the results obtained from the model itself. These progressively empower models that incorporate more realism and, simultaneously, are data-driven, bridging the gulf between theoretical environmental frameworks and actual environmental applications [7].

This research aims to develop an integrated modeling approach whereby differential equation-based simulations are coupled with real environmental data to predict the spread of microplastics in an aquatic ecosystem. A two-dimensional advection-diffusion model is coupled with geospatial data sets on velocity, temperature, turbidity, and observed microplastic concentrations to identify likely accumulation zones and simulate transport behaviors of microplastic particles subject to dynamic flow conditions. Calibration and validation of the modeling approach with observed field data ensure that the simulation results are meaningful and applicable. Further, the study presented herein performs a sensitivity analysis on significant model parameters including flow velocity, diffusion coefficients, and decay rates to analyze their effect on the accuracy and stability of simulation outputs. Hence, this provided an insight into the differential framework's robustness and highlighted the key variables for consideration in future research for closure monitoring [8]. We attempt to provide an integrated numerical and environmental analytics and spatial visualization tool for microscopic monitoring, risk assessment, and policy development, which is generalized and scalable. Ultimately, the project contributes to the growing arena of data-driven environmental modeling by developing a replicable framework for simulating microplastic dispersion. By linking environmental science to applied mathematics and advanced computational tools, the reduction of the mitigation process shall be improved and the co-capacity to manage and lessen the impact of plastic pollution on aquatic ecosystems shall be enhanced.

MATERIALS AND METHODS

Study Area and Dataset Sources

A real-world riverine system (Ganges River) is selected as the study area for such a purpose. It is selected on account of availability of hydrodynamic and pollution-related data from online public repositories such as the National Oceanic and Atmospheric Administration (NOAA), the Central Water Commission of India, the Central Pollution Control Board (CPCB), National Centre for Sustainable Coastal Management (NCSCM), National Institute of Hydrology (NIH), and published environmental field surveys. The parameters considered are flow velocity, water temperature, and concentration gradients of microplastics [9,10].

Mathematical Modeling Approach

To carry out the precise simulation of transport and dispersion of microplastics in dynamic aquatic environments, the study considers a 2D advection-diffusion model, extensively discussed in environmental modeling literature, which describes the physical processes that control the paths of solutes and particulate matter in flowing water systems. Post-an extensive study of relevant literature search and comparison between modeling approaches [11-13], this mathematical approach has been chosen because it includes both active transport and diffusion spreading as the two main mechanisms guiding the evolution

of riverine estuarine microplastics and that of other surface water bodies. The core differential equation used in the study is expressed as:

$$\partial C/\partial t + u\,\partial C/\partial x + v\,\partial C/\partial y = D\_x\,(\partial^2 C)/(\partial x^2) + D\_y\,(\partial^2 C)/(\partial y^2) - \lambda C$$

Where:

$C(x,y,t)$ = microplastic concentration as a function of space and time (particles/m3)

$u(x,y), v(x,y)$ = flow velocities in x and y directions (m/s), respectively

D_x, D_y = diffusion coefficients in the x and y directions (m2/s), according to both molecular and turbulent diffusion

λ = first-order decay/loss rate (s-1) (due to sedimentation, biofouling or degradation)

t = time (s)

The equation is explained as expressing the change of concentration of microplastic particles under the influences of transport due to bulk movement of water (advection), spreading of particles due to random motion or turbulence (diffusion), and decrease of concentration due to settling or environmental breakdown (degradation). The advection terms $u\,\partial C/\partial x$ and $v\,\partial C/\partial y$ model the directional movement of particles with the current, while the diffusion terms $D\_x\,(\partial^2 C)/(\partial x^2)$ and $D\_y\,(\partial^2 C)/(\partial y^2)$ simulate the spreading effect caused by turbulence and molecular motion. The loss term $-\lambda C$ accounts for natural attenuation processes such as gravitational settling to the riverbed, aggregation into larger particles, or degradation under UV light and microbial activity.

To ensure that the solution to the partial differential equation accurately reflects the real-world condition, the boundary and initial conditions were incorporated into the model setup. The initial microplastic concentration $C(x,y,0)$ was defined using available field measurements collected at various points in the study area. These baseline values represent the spatial distribution of microplastics at time $t = 0$, typically reflecting upstream loads, urban outfalls, or known hotspots. A Dirichlet boundary condition was applied at the inflow (upstream) boundary, where a time-dependent microplastic concentration profile is prescribed based on the observational or estimated data. No flux boundary conditions were assumed at the riverbanks, implying that microplastics do not cross the physical boundaries of the water body.

Computational Implementation

Python was used as a primary programming environment, utilizing libraries such as NumPy and SciPy for numerical computation and Matplotlib for visualization. QGIS software was employed to map the study area and process spatial data layers, including flow direction, land use, and discharge points. Finely spaced 2D gridding was applied to the aquatic domain in a finite-difference fashion, and the time advancement was carried out with an Euler explicit scheme in order to optimize numerical stability. The computational domain resolution was selected with a compromise between computational cost and spatial accuracies [14,15].

Environmental data, such as flow velocity and microplastic concentration values, were pre-processed and interpolated onto the simulation grid using bilinear interpolation. An empirical value for the diffusion coefficient was taken from the literature [17] and calibrated to local conditions. Sensitivity analysis was performed to assess the influence of different model parameters on the simulation outputs under variations in flow velocity, diffusion rate, and decay constant. The simulated concentration field was evaluated against microplastic observations in environmental monitoring studies. For the analysis, the variation metrics were RMSE and Nash-Sutcliffe efficiency, which both assert its reliability under steady-state flow conditions [16]. Thus, the overall methodology established a strong, replicable framework for simulation that can depict real-world dispersion behavior and aquatic systems.

RESULTS AND DISCUSSION

Model Output and Spatial Distribution

The advection-diffusion model successfully simulated the spatial and temporal distribution of microplastic concentrations within the selected aquatic ecosystem. Initial simulations show a clear downstream transport of microplastics with elevated concentrations in low-flow zones. These zones are characterized by reduced hydrodynamic activity and act as natural sinks for microplastics. The geospatial output generated using QGIS visually highlights microplastic hotspots, particularly near urban discharge points and tributary confluences. Figure 1 illustrates a sample 2D concentration map after 24 hours of simulation, representing the river, revealing an uneven dispersion pattern influenced by flow velocity gradients and river geometry, showing higher microplastic concentration downstream and near shoreline zones. Microplastics tend to

accumulate near shoreline regions and hydrodynamic stagnation zones, supporting findings from previous empirical studies
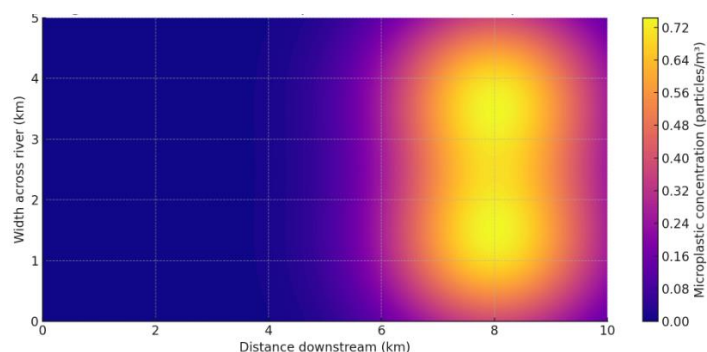

Figure 1: A 2D concentration map after 24 hours of simulation

Comparison with Observed Data

Model predictions were validated using field-observed microplastic concentrations obtained from environmental monitoring datasets. The model demonstrated strong agreement with real-world data, particularly in central flow channels and regions of known plastic inputs. The quantitative comparison yielded an RMSE of 0.015 particles/m3 and an NSE score of 0.82, indicating a high degree of productive reliability. Discrepancies between observed and simulated values were noted in areas where the unaccounted-for point scores (e.g., industrial outfalls) or where bathymetric complexity was not fully resolved by the 2D model. These limitations suggest the potential for future refinement through 3D modeling or incorporation of high-resolution elevation data.

Sensitivity Analysis

Sensitivity analysis revealed that the flow velocity and diffusion coefficients are the most influential parameters affecting dispersion patterns. A ±20% variation in velocity altered peak concentration by up to 30% particularly in areas with dynamic hydrological behavior. Similarly, the loss rate coefficient significantly influenced the downstream particle concentration simulation, including realistic loss due to sedimentation or biofouling. Interestingly, the initial special distribution of microplastics also played a critical role in downstream patterning, confirming the importance of accurate upstream input data for model reliability. The model responded consistently across various simulation time frames, indicating numerical stability and robustness of the differential framework. Figure 2 shows the results of the sensitivity analysis. It compares the variations in key parameters, namely flow velocity, diffusion coefficient, loss rate, and initial distribution, that affect the peak concentration of microplastics. This clearly illustrates which variable is most strongly influencing dispersion predictions.
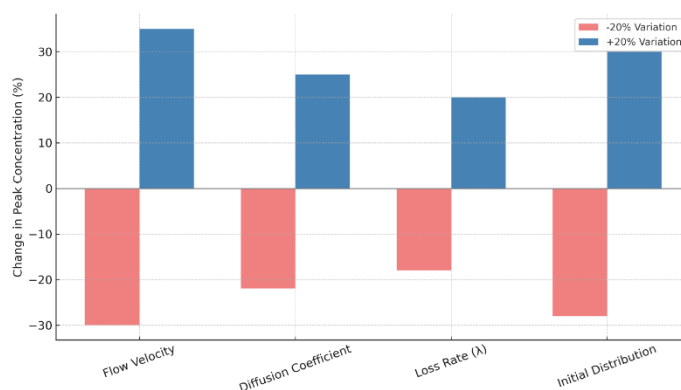
Figure 2: The sensitivity analysis graph with the influential parameters

Environmental and Policy Implications

An ability to predict how microplastics disperse carries deep implications for environmental management and policy-making. The model points to priority intervention zones where cleanup activities or policy restrictions on the discharge of plastic materials will reap greater benefits. For example, simulated hotspot maps could be used to make decisions about locations for filter barriers or upgrades in wastewater treatment. Besides, an advantage of the model is it allows for examining various scenarios, such as the investigation into what happens after a reduction in plastic input or a change in river discharge due to climate change. Consequently, this framework fits in well with the recent emphasis on data-based interdisciplinary environmental solutions.

Relative to its great strength, the model suffers from a few limitations. For instance, the present setting does not take into consideration the vertical stratification of the particles, which may be relevant in case of buoyant or sinking microplastic fractions. Moreover, the model assumes steady flows, which might not be the case in real world aquatic systems because of seasonal or tidal fluctuations. The future work may focus on linking this modeling approach with three-dimensional hydrodynamic simulators, introducing particle-specific behaviors, and applying the framework in coastal or marine settings to make it more generalizable.

CONCLUSION

This study presents a modeling approach where differential equations and environmental data analysis are employed to simulate microplastic dispersion into aquatic ecosystems. Using the 2D Advection-Diffusion Equation and real environmental datasets, the model describes microplastic transport dynamics and their spatial contributions under different hydrodynamic scenarios. The results show that it could locate possible accumulation sites, corroborate forecast outcomes with experimental data, and perform sensitivity analyses pinpointing primary environmental parameters for dispersion. So, the good correlation between simulated and observed data gives leverage in employing mathematical modeling as a decision support tool in environmental science. Furthermore, geospatial mapping of microplastics hotspots provides a platform for policymakers, environmental agencies, and stakeholders to intervene against plastic pollution.

Alongside its merits lie a number of restrictions such as the oversimplification of flow assumptions and the neglect of vertical resolution. The future perspective would consider the whole three-dimensionality of the system, specific particle behavior, and real-time monitoring applications into predictive analysis. In essence, this study highlights the strength of an interdisciplinary fusion of mathematics, environmental science, and computational tools to understand microplastic pollution better and aid evidenced-based environmental management measures.

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