International Journal of
INTELLIGENT SYSTEMS AND APPLICATIONS IN ENGINEERING
ISSN:2147-6799 www.ijisae.org Original Research Paper

An Environmental Fate and Transport Modeling Study of Engineered Nanoparticles in Aquatic–Terrestrial Systems.

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Received: 10/08/2024 **Revised**: 14/11/2024 **Accepted**: 01/12/2024

Abstract: Rapid advancements in nanotechnology have led to an increased diffusion of engineered nanoparticles (ENPs) into environmental compartments. In order to assess the hazard, it is necessary to understand their movement, transformation, and accumulation. This study investigates a theoretical multiphase transport model for nanoparticles in aquatic, terrestrial, sedimentary, and biological compartments. The model includes advection, diffusion, aggregation, sedimentation, and degradation. A simulated study has been performed for silver nanoparticles (AgNPs), titanium dioxide nanoparticles (TiO2-NPs), and zinc oxide nanoparticles (ZnO-NPs). The results show that the particle size, zeta potential, and ambient pH have a substantial impact on the transport behavior. Smaller nanoparticles (<30 nm) were more mobile, while bigger aggregated particles were mostly trapped in sediments. Model predictions indicate that sediments in aquatic ecosystems act as persistent repositories for manufactured nanoparticles. They contribute to the field of environmental nanotoxicology and help develop predictive mechanisms to control risks associated with nanoparticles.

Keywords: *Nanoparticles, Environmental Fate, Transport Modeling, Sedimentation, Aggregation, Ecotoxicology, Risk Assessment*

1. Introduction

Engineered nanoparticles (ENPs) are purposely constructed nanomaterials with at least one dimension in the range of 1 to 100 nm. Due to their very small size, very high surface area to volume ratio, and unique physicochemical features, these materials have become an important part of the progress in modern technology. Engineered nanoparticles are used in many industries such as medicine, electronics, cosmetics, agriculture, energy storage, environmental remediation, and industrial manufacture. Silver nanoparticles are widely used for their antibacterial qualities, titanium dioxide nanoparticles are used in sunscreens and photocatalytic applications, and zinc oxide nanoparticles are used in sensors, coatings, and medicinal devices[1]. With the increasing demand for nanotechnology-based goods, the global manufacturing and commercialization of designed nanoparticles has increased considerably. They do have many benefits, but there are increasing concerns about the environmental implications of their broad usage and disposal. Nanoparticles can be unintentionally discharged to air, water, and soil ecosystems throughout the processes of manufacture, transportation, product use, recycling, and waste management. Engineered nanoparticles released into natural ecosystems undergo a complicated series of physical, chemical, and biological alterations that affect their mobility, permanence, and ecological impact. Because of their nanoscale size and greater reactivity, nanoparticles have different properties than conventional contaminants. Models used for contaminant transport cannot be used to predict the environmental fate of nanoparticles[2]. The movement and dispersion of nanoparticles in environmental systems is controlled by several interrelated mechanisms. They are dispersed by advection, which means they are transported in flowing water and air currents, and diffusion, which means they spread out from areas of higher concentration to areas of lower concentration. Meanwhile, aggregation of nanoparticles can occur, in which the individual particles associate to create bigger entities, which can dramatically affect transport properties and sedimentation behavior. Metal ions may be released from the surface of nanoparticles during dissolution processes, which may increase toxicity and bioavailability. Since larger or aggregated nanoparticles settle down in sediments, aquatic sediments become long-term repositories of contamination by sedimentation. Interactions with bacteria, plants, and aquatic species may also lead to bioaccumulation and trophic transmission through food webs, thereby posing threats to ecosystem health and human populations[3]. Therefore, understanding the fate and transport of artificial nanoparticles in the environment is crucial for assessing their long-term ecological implications and for establishing effective regulations. There are several environmental parameters that must be considered in the successful prediction of nanoparticle behavior, including particle size, shape, surface charge, coating materials, pH, ionic strength, temperature, and natural organic matter. The present

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work seeks to investigate the environmental destiny and transport of engineered nanomaterials using theoretical modeling techniques, which provide an understanding of their transport, transformation, accumulation, and potential environmental concerns. These results contribute to the expanding field of environmental nanotoxicology and offer a foundation for sustainable approaches to safe nanotechnology utilization in contemporary culture[4].

2. Theoretical Framework

The environmental destiny and transport of manufactured nanoparticles is envisioned in terms of a system comprising four major compartments: water, soil, sediment, and biota. These compartments are in constant interaction, allowing the movement, transformation, and accumulation of nanoparticles under varying environmental conditions[5]. Nanoparticle mobility and transformation in the system are quantified using a mass balance technique.

The nanoparticle mass balance equation describes the change in nanoparticle mass over time.

$$\frac{dM}{dt} = I - O - R \quad \text{.....(A)}$$

Here, (M) represents the total nanoparticle mass, (I) denotes the input flux entering the system, (O) represents the output flux leaving the system, and (R) accounts for removal or transformation processes such as degradation, dissolution, or sedimentation. This equation forms the basis for evaluating nanoparticle distribution across environmental compartments.

2.1 Advection–Diffusion Equation

The advection governs the transport of nanoparticles in aquatic environments–diffusion equation:

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

.....(B)

This equation combines the effects of water flow (advection), molecular spreading (diffusion), and particle removal processes. The concentration of nanoparticles (C) changes over time as particles are transported by flowing water at velocity (u), dispersed through diffusion characterized by the coefficient (D), and removed through mechanisms represented by the rate constant (k). This model helps predict nanoparticle concentrations in rivers, lakes, and other aquatic systems.

2.2 Aggregation Kinetics

Nanoparticles tend to collide and form larger clusters through a process known as aggregation. The aggregation rate is described by:

$$\frac{dN}{dt} = -k_a N^2$$

.....(C)

where (N) is the nanoparticle concentration and (k_a) is the aggregation coefficient. The integrated form of the equation predicts the concentration of particles remaining after a given time. Aggregation significantly influences environmental behavior because larger aggregates settle more rapidly and exhibit reduced mobility compared to individual nanoparticles.

2.3 Sedimentation Model

The settling of nanoparticles in water is estimated using Stokes' Law:

$$V_s = \frac{2r^2(\rho_p - \rho_w)g}{9\mu} \quad \text{.....(D)}$$

where (V_s) is the settling velocity, (r) is the particle radius, (ρ_p) and (ρ_w) are the densities of the particle and water, respectively, (g) is gravitational acceleration, and (μ) is the dynamic viscosity of water. This equation predicts the rate at which nanoparticles or their aggregates settle from the water column to sediments. Sedimentation is an important process because it controls the long-term accumulation of nanoparticles in benthic environments and influences their ecological impact.

3. Methodology: In this work, a theoretical modeling and simulation technique was utilized to assess the environmental fate and transport of manufactured nanoparticles in aquatic systems. Mathematical models of nanoparticle transport, aggregation, and sedimentation, instead of laboratory studies, were employed to anticipate how nanoparticles will behave under controlled environmental circumstances. The method was developed to model the transport and alteration of nanoparticles after discharge into a freshwater ecosystem and to analyze changes in concentration over time. The research system was a hypothetical aquatic environment with a water depth of 5 m, representing a shallow river, reservoir, or lake environment typically subjected to industrial and urban discharges. The average flow velocity was considered to be 0.12 m/s, representing a modest water movement capable of transferring suspended nanoparticles through advection mechanisms. Environmental conditions were maintained at 25 °C and a neutral pH of 7.0, which are representative values found in many freshwater habitats. The choice of these parameters was based on the fact that temperature and pH have a major influence on the stability of nanoparticles, aggregation behavior, rates of dissolution, and transport properties[5].

The simulation has been run for a duration of 180 days to examine environmental behavior in the short and long term. Three commonly used engineered nanoparticles were selected for investigation: silver nanoparticles

(AgNPs), titanium dioxide nanoparticles (TiO2-NPs), and zinc oxide nanoparticles (ZnO-NPs). These nanoparticles were chosen because of their ubiquitous use in consumer products, industrial processes, and environmental technologies, and their frequent detection in environmental monitoring investigations. For the simulation, the initial nanoparticle concentration of each nanoparticle type was set to 100 mg/L. It was expected that the concentration was uniform over the entire water column. The advection-diffusion equation was utilized to predict the transport of nanoparticles in the aquatic environment, and particle aggregation kinetics were used to analyze the clustering of particles over time. Sedimentation rates were calculated, and the deposition of nanoparticles in the bottom sediments was predicted by using Stokes' Law[6]. The major environmental processes were examined in the simulation: transport by water flow, diffusion, aggregation of nanoparticles to bigger particles, sedimentation to the benthic layer, and concentration reduction by removal mechanisms. The nanoparticle concentrations were estimated and recorded at preset time intervals (0, 30, 60, 90, and 180 days). The obtained data were evaluated to find out the trends in concentration, accumulation pattern of sediments, and comparative behavior of AgNPs, TiO 2 -NPs and ZnO-NPs.

Simulated Dataset and Interpretation

A simulated collection was created based on theoretical transport, aggregation, and sedimentation models to predict the environmental behavior of manufactured nanoparticles. The dataset gives insights into the effect of the physicochemical features of nanoparticles on their mobility, persistence, and accumulation in aquatic environments during 180 days. For comparison, three commonly used engineered nanoparticles, silver nanoparticles (AgNPs), titanium dioxide nanoparticles (TiO 2 -NPs) and zinc oxide nanoparticles (ZnO-NPs), were selected due to their vast industrial and commercial applications[7,8].

4.1 Physicochemical Properties of Nanoparticles

The environmental behavior of nanoparticles is strongly influenced by their intrinsic physicochemical properties, including particle size, density, and surface charge. Table 1 summarizes the selected properties used in the simulation.

Table 1. Physicochemical Properties[9]

Nanoparticle	**Diameter (nm)**	**Density (g/cm³)**	**Zeta Potential (mV)**	**Nanoparticle**
AgNP	20	10.5	-35	AgNP
TiO_2	50	4.2	-20	TiO_2
ZnO	40	5.6	-18	ZnO

The transport behavior of nanoparticles is directly affected by the diameter of nanoparticles. Smaller nanoparticles often have a higher mobility, as they undergo less gravitational settling and greater Brownian motion. In this simulation, AgNPs showed the smallest diameter (20 nm), indicating the increased possibility of suspension and long-distance transmission in water. TiO 2 nanoparticles had the biggest diameter (50 nm); hence, they were more prone to aggregation and sedimentation. ZnO nanoparticles exhibited intermediate particle size properties.

Another important element influencing the fate of nanoparticles is the density. AgNPs had the highest density (10.5 g/cm³) followed by ZnO (5.6 g/cm³) and TiO_2 (4.2 g/cm³). High-density particles are subjected to larger gravitational forces, and so are more likely to settle when aggregation takes place. Sedimentation, however, is not only a function of density, but also of particle size and aggregation behavior. The zeta potential is a measure of the electrical charge present on the surface of nanoparticles and is an indicator of colloidal stability. The more negative the zeta potential value, the stronger the electrostatic repulsion between particles, which reduces aggregation. AgNPs had the largest negative zeta potential (-35 mV), indicating good stability and lower propensity for aggregation. In contrast, TiO_2 (-20 mV) and ZnO (-18 mV) showed weaker electrostatic stability, leading to a higher tendency for particle collisions and aggregation formation[10].

The physicochemical features indicate that AgNPs should be suspended in water for a longer time, while TiO_2 and ZnO nanoparticles are likely to agglomerate and settle down more swiftly.

4.2 Predicted Sedimentation Behavior

Sedimentation represents one of the most important mechanisms controlling nanoparticle removal from aquatic environments. The percentage of nanoparticles transferred from the water column to bottom sediments was estimated over time and is presented in Table 2.

Table 2. Predicted Sedimentation[11]

Particle	Day 30	Day 90	Day 180
AgNP	18%	34%	57%
TiO_2	26%	48%	71%

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ZnO	22%	43%	65%

The results show gradual buildup of nanoparticles in the sediments during the simulated period. On Day 30, TiO 2 nanoparticles had the highest sedimentation percentage (26%), followed by ZnO (22%) and AgNPs (18%). This pattern is indicative of the higher likelihood of TiO2 NPs to aggregate because of their bigger size and lower surface charge. By day 90, all forms of nanoparticles showed much greater silt accumulation. Almost half of TiO_2 nanoparticles (48%) were accumulated in sediments, as well as 43% for ZnO and 34% for AgNPs. These results show that the aggregation processes are enhanced with time, leading to larger particle clusters with increased settling velocities. The TiO_2 NPs showed the highest percentage of sediment accumulated (71%) after the 180-day simulation, indicating that most of the particles were taken from the water column. The sedimentation percentage of ZnO nanoparticles was 65% and AgNPs 57%. Although AgNPs have the maximum density, their strong electrostatic stability causes less aggregation and a longer suspension time than TiO_2 and ZnO nanoparticles. Such results show that aquatic sediments may act as long-term environmental sinks for manufactured nanoparticles. Once deposited, nanoparticles may remain in the sediments for a long time and may harm benthic creatures such as worms, crustaceans, and microbial communities[12].

4.3 Remaining Water Concentration

Changes in nanoparticle concentration within the water column were monitored throughout the simulation period. The results are shown in Table 3.

Table 3. Remaining Water Concentration (mg/L)[13]

Day	AgNP	TiO_2	ZnO
0	100	100	100
30	82	74	78
60	69	58	64
90	56	45	51
180	31	19	25

First, all varieties of the nanoparticles were added at the same concentration of 100 mg/L. Environmental processes acted on the particles, and concentrations slowly declined by sedimentation, aggregation, and removal mechanisms. After 30 days, the concentration of AgNP was reduced to 82 mg/L, which is an 18% reduction. TiO_2 content reduced more dramatically to 74 mg/L, a 26% decline. ZnO nanoparticles indicated an intermediate reduction to 78 mg/L. These results are in good agreement with the sedimentation trends presented in Table 2. Concentrations fell significantly by Day 90. The lowest concentrations for AgNPs in the water column were at 56 mg/L, whereas for TiO_2 and ZnO concentrations decreased to 45 mg/L and 51 mg/L, respectively. The persistence of AgNPs is due to their tiny particle size and better colloidal stability. On Day 180, AgNP concentration was 31 mg/L, indicating that ~31% of the initial nanoparticles were still floating in the aquatic environment. ZnO nanoparticles showed the highest residual concentration of 25 mg/L, whereas TiO2 showed the lowest remaining concentration of 19 mg/L. The lower TiO_2 content is because of its higher sedimentation and aggregation rates for the whole simulation period[14].

4.4 Comparative Analysis: Comparing the three nanoparticles, they exhibit different behavior in the environment. The small diameter and very negative zeta potential of AgNPs resulted in the greatest mobility and persistence in the water column. They showed great colloidal stability, even at high density, with low aggregation and delayed sedimentation. TiO 2 nanoparticles displayed the most rapid elimination from the water column. Their increased particle size and less electrostatic stabilization favored aggregation, leading to rapid deposition of sediment. Thus, TiO 2 nanoparticles were shown to have more accumulation in the sediments than the other types of nanoparticles. ZnO nanoparticles showed intermediate behavior between AgNPs and TiO2 nanoparticles. Their modest size, density, and surface charge led to sedimentation and transport properties that were not very mobile or fast to be removed. Simulated data indicate that the environmental fate is mostly governed by the size, density, and surface charge of the nanoparticles. The results indicate that physicochemical parameters should be taken into account when evaluating nanoparticle transport, permanence, bioavailability, and ecological risk in aquatic habitats[15].

5. Sample Calculation: The theoretical transport model was used to calculate the concentration of silver nanoparticles (AgNPs) by applying a first-order removal equation. This equation assumes that the removal rate of the nanoparticle from the aqueous column is proportional to its concentration at that time. Removal processes include sedimentation, aggregation, dissolution, and other transformation mechanisms occurring in the aquatic environment[16].

The initial concentration of silver nanoparticles was assumed to be:

$$C_0 = 100\, mg/L \quad \text{.....(E)}$$

where (C_0) represents the nanoparticle concentration at the beginning of the simulation.

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Therefore, the removal constant was selected as: $k = 0.0065\ day^{-1}$

This constant represents the combined effect of all removal processes affecting nanoparticle concentration over time.

The concentration of nanoparticles at any time (t) can be estimated using the first-order decay equation:

$$C = C_0 e^{-kt} \quad \text{.....(F)}$$

For a simulation period of 90 days: t = 90 days Substituting the values into the equation gives:

$$C = 100e^{-0.0065\times 90}$$

$$C = 100e^{-0.585}$$

$$C = 100(0.557)$$

C = 55.7 mg/L .....(G)

The calculated concentration after 90 days is therefore approximately 55.7 mg/L. This value closely matches the simulated concentration of 56 mg/L presented in Table 3, confirming the consistency and validity of the theoretical model. The result indicates that approximately 44.3% of the original silver nanoparticles have been removed from the water column through environmental processes during the 90 days[17].

The example demonstrates how first-order kinetic models can be used to predict nanoparticle persistence and transport behavior in aquatic environments. Such calculations are useful for estimating environmental exposure levels and assessing potential ecological risks associated with nanoparticle contamination.

6. Results: The simulation findings give useful information on environmental fate and transport of designed nanoparticles under the chosen environmental conditions. The analysis of concentration profiles, sedimentation patterns and physicochemical parameters reveals several fundamental trends that influence the behavior of nanoparticles in aquatic systems. Water column concentrations decrease progressively[18].

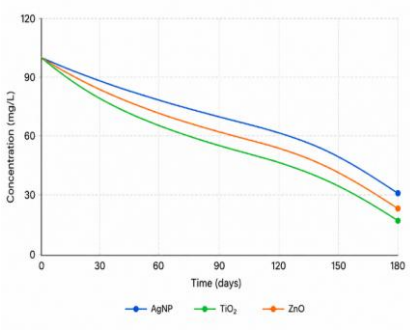

Figure-1, shows that the predicted nanoparticle concentration declines[19]

The model predicted a continued drop in nanoparticle concentrations over the 180 days of the experiment. Initially, all nanoparticles were added at a dosage of 100 mg/L. However, environmental processes such as aggregation, sedimentation, and removal eventually decreased their concentration in the water column. The concentrations of AgNPs, TiO_2 nanoparticles, and ZnO nanoparticles fell to 31 mg/L, 19 mg/L, and 25 mg/L, respectively, by the end of the simulation. This tendency especially reveals that nanoparticles are not permanent constituents of aquatic ecosystems but are continuously transformed and redistributed throughout time[20,21].

6.1 Increased Sediment Build-up Over Time: Sediment accumulation rose monotonically during the simulation. Their transfer from the water column to bottom sediments was enhanced with increasing settling velocity as a result of the aggregation of nanoparticles into bigger particles. The sedimentation percentages considerably increased from Day 30 to Day 180 for all types of nanoparticles. Results imply that sediments are an important sink for manufactured nanoparticles and could retain contamination long after water concentrations have abated. This could therefore result in long-term exposure of nanoparticle contaminants to sediment ecosystems[22].

6.2 Significant Effect of Particle Size on Transport Distance: Particle size was found to be an important element affecting the mobility and transport behavior of nanoparticles. Smaller nanoparticles had improved suspension stability and stayed suspended in the water column longer. The AgNPs with an average diameter of 20 nm demonstrated the highest persistence in water. In contrast, bigger particles such as TiO_2 nanoparticles (50 nm) had more frequent collisions and aggregation events and hence shorter transport distances and higher sediment deposition. The results reveal that nanoparticle size is a major factor in their environmental distribution and potential exposure routes[23].

6.3 Aggregation Speeds Up Elimination from Water: Aggregation was discovered as one of the most critical mechanisms governing the destiny of nanoparticles. Individual nanoparticles are very small in size and can remain suspended for long periods. However, when particles collide and combine, their effective size increases significantly. Bigger aggregates sink faster under the effect of gravity, decreasing the concentrations of nanoparticles in the water column. The simulation results showed that the nanoparticles with poorer electrostatic stability were easier to combine and had a higher removal rate. Thus, aggregation is an important step connecting nanoparticle movement and sedimentation.

6.4 Sediments as Long-Term Reservoirs: The results show that bottom sediments serve as long-term environmental sinks for manufactured nanoparticles. Nanoparticles may remain within sediments for months or even years after being deposited, depending on environmental circumstances. While sedimentation reduces the concentration of nanoparticles in surface waters, it does not eliminate environmental risk. Instead, contamination is transmitted to benthic environments where it might damage bacteria, water invertebrates, and benthic species. Secondary exposure pathways may also occur by remobilization of nanoparticles in the water column due to disturbance of sediments caused by flooding, dredging, or biological activity.

6.5 Enhanced Sedimentation of TiO_2 Nanoparticles: Among the three types of nanoparticles studied, the highest sedimentation rate was found for TiO 2 nanoparticles. By day 180, ~71% of TiO2 NPs had accumulated in the sediments compared to 65 % for ZnO NPs and 57 % for AgNPs. This phenomenon can be explained by the higher particle size and lower zeta potential of TiO2 nanoparticles, which favor aggregation and impair colloidal stability. As larger aggregates formed, settling velocities increased, leading to higher sediment deposition. Therefore, TiO_2 nanoparticles showed the lowest residual concentration in the water column at the end of the simulation. Thus, the results indicate that physicochemical parameters such as particle size, density, and surface charge are of critical importance for the environmental fate of designed nanoparticles. The results underscore the need to incorporate these elements into environmental risk assessment methods and regulatory frameworks for nanomaterials[24].

7. Ecological effects:

The expanding utilization of artificial nanoparticles in industry, medicine, agriculture, and consumer products has raised major worries about their possible consequences on environmental systems. Nanoparticles, once released into natural habitats, can interact with live species and ecological processes in complicated ways due to their small size, high surface reactivity, and ability to penetrate biological barriers. Awareness of these environmental ramifications is vital to identify ecological hazards and design sustainable nanotechnology practices.

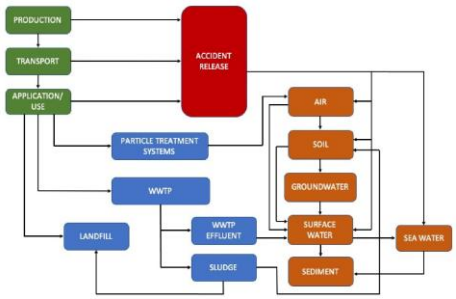

Figure 2 explores the Environmental risk evaluation of silver nanoparticles in aquatic environments[25].

Engineered nanoparticles can impact a diverse group of creatures in aquatic habitats, from bacteria and algae to fish and higher aquatic species. Algae are the main producers of the aquatic food chain and are essential for the creation of oxygen and the recycling of nutrients. Nanoparticle exposure could disrupt photosynthesis through altering cell structures or lowering light absorption efficiency, resulting in diminished algal growth eventually. Reducing algal populations can limit the energy available to higher trophic levels, disrupting the entire aquatic food chain. Moreover, many nanoparticles are capable of producing reactive oxygen species (ROS) that cause oxidative stress in aquatic organisms. Oxidative stress can damage proteins, lipids, and DNA in fish and may lead to impaired growth, lower reproductive ability, compromised immunological responses, and increased mortality. Nanoparticles may potentially interfere with aquatic microbial communities involved in organic matter decomposition and nutrient recycling. Changes in microbial community and activity can alter ecosystem function and lower the resilience of aquatic ecosystems to environmental perturbations[26]. Effects of nanoparticles are not just confined to aquatic systems. Soil ecology can also be greatly influenced when nanoparticles are introduced into the environment by wastewater irrigation, dumping of industrial wastes, agricultural applications, or atmospheric deposition. Soil microorganisms play a major role in the nutrient cycle, including nitrogen fixation, phosphorus mobilization, and breakdown of organic waste. Nano-sized materials can impede microbial activity and cause alterations in the nutrient cycle and decrease soil fertility. Long-term buildup of nanoparticles can reduce microbial diversity, which can alter ecosystem stability and reduce a soil's ability to support healthy plant development. Some

nanoparticles can also be taken up by plant roots and transferred to stems, leaves, and edible tissues. This absorption process may affect plant physiology, growth patterns and production and provide routes for nanoparticle entrance into terrestrial food webs. One of the main environmental problems related to manufactured nanoparticles is their potential for bioaccumulation and trophic transmission via the food chain. The plankton ingest the nanoparticles in the water; then they are eaten by small aquatic animals and fish. As nanoparticles migrate up the food chain, their concentration in biological tissue may grow (biomagnification)[27]. Humans can be exposed to NPs through contaminated seafood, agricultural products, or drinking water. The transfer mechanism can be described as

Water → Plankton → Fish → Humans. ……(H)

Continuous exposure through food consumption can pose hazards to human health, especially if nanoparticles tend to collect in vital organs such as the liver, kidneys, lungs, or brain. The long-term effects of prolonged exposure to nanoparticles are still under investigation, but some nanoparticles have been shown to cause cellular toxicity, inflammation, and oxidative stress when studied in current research. The manufactured nanoparticles have environmental impacts ranging from aquatic to terrestrial and biological systems. Their persistence, accumulation, and movement through ecosystems underscore the significance of extensive environmental monitoring and risk assessment. "Responsible management approaches such as controlled release of nanoparticles, green design of nanomaterials, and enhanced regulatory frameworks are needed to minimize potential ecological and human health impacts, while maintaining the benefits of nanotechnology.

8. Index of Risk Assessment: Assessment of environmental risks is an important component of the evaluation of potential dangers of manufactured nanoparticles. Nanoparticles can remain in environmental compartments and interact with live species, so it is vital to assess whether their concentrations surpass thresholds considered safe for ecosystems. The Risk Quotient (RQ) technique is among the most used approaches for environmental risk characterization[28].

The Risk Quotient is calculated using the following equation:

$$RQ = \frac{PEC}{PNEC} \quad \text{……..(I)}$$

where: RQ = Risk Quotient , PEC = Predicted Environmental Concentration, PNEC= Predicted No Effect Concentration

8.1 PEC (Predicted Environmental Concentration): represents the estimated concentration of nanoparticles present in a specific environmental compartment, such as water, soil, or sediment. PEC values are generally obtained through environmental monitoring, laboratory experiments, or predictive transport models.

8.2 PNEC (Predicted No Effect Concentration): represents the maximum concentration below which no significant adverse effects on organisms or ecosystems are expected. PNEC values are typically derived from ecotoxicological studies involving algae, aquatic invertebrates, fish, microorganisms, and plants[29].

For example: RQ=2.5

In this case, the predicted environmental concentration of nanoparticles is 25 mg/L, while the no-effect concentration is 10 mg/L. The resulting Risk Quotient is 2.5.

The interpretation of RQ values generally follows these criteria:

i. **R**
Q < 0.1: Negligible environmental risk

ii. **0.1**
≤ RQ < 1.0: Low to moderate environmental risk

iii. **R**
Q = 1.0: Threshold level of concern

iv. **R**
Q > 1.0: Significant environmental concern requiring further investigation

The calculated RQ value of 2.5 is more than 1, indicating that the nanoparticle concentration is over the threshold of ecological safety. This shows that under the simulated conditions, harmful effects on the ecosystem can occur. Potential implications include poisoning of aquatic creatures, disturbance of microbial ecosystems, diminished biodiversity, and long-term ecosystem alterations[30].

Risk evaluation of manufactured nanoparticles is particularly hard because toxicity is regulated not only by concentration but also by particle size, shape, surface coating, aggregation state, and environmental circumstances. Thus, conventional chemical risk assessment approaches may not adequately account for nanoparticle-specific behavior. The Risk Quotient technique, however, provides a valuable screening tool at the first level for identifying environmental dangers and for prioritization of management measures.

9. Discussion

The results of this theoretical work show that the destiny and transport of manufactured nanoparticles in the environment are controlled by a complex interaction of

hydrodynamic, physicochemical, and environmental factors. Nanoparticles behave differently than traditional pollutants because of their nanoscale size, high surface-area-to-volume ratio, and increased reactivity. Therefore, the environmental distribution of these compounds can only be predicted if numerous transport and transformation processes are considered simultaneously[31].

An important insight from the simulation is the significance of aggregation in determining the mobility of nanoparticles. At the beginning, nanoparticles stay scattered within the water column thanks to Brownian motion and electrostatic repulsion between particles. However, as particles collide and agglomerate, their effective size grows. Larger aggregates have higher gravitational forces and faster settling velocities, resulting in a decrease in nanoparticle concentrations in surface waters. This is why we see a gradual decrease in water-column concentrations during the 180-day simulated period[32].

The results also show the importance of physicochemical parameters in environmental behavior. The nanoparticles with bigger diameters and lower surface charge were more aggregated and sedimented. Titanium dioxide nanoparticles showed the largest sediment buildup, which was attributed to their large size and low zeta potential, which encouraged the development of aggregates. Contrary to the results of steel nanoparticles, silver nanoparticles were suspended for a longer time owing to their smaller particle size and more electrostatic stability. These results underline that the transport of nanoparticles cannot be explained simply based on their chemical composition and that particle-specific features need to be considered.

Another key result of the study is the identification of sediments as long-term environmental sinks. Although concentrations of nanoparticles in surface waters declined significantly over time, a huge proportion of the particles accumulated in bottom sediments. This indicates that sediment habitats may remain exposed for long periods even after contamination appears to have declined in the water column. Therefore, water sampling-based environmental monitoring programs may underestimate the real ecological dangers. Sediment-associated nanoparticles can be retained in the biologically active form, taken up by benthic organisms, and may cause food chain transfer and chronic exposure routes[33].

The study also shows that environmental circumstances can have a major impact on the fate of nanoparticles. Parameters such as pH, temperature, ionic strength, dissolved organic matter, and water flow parameters affect aggregation, dissolution, and transport processes. Changes in these variables can modify the behavior of nanoparticles and result in varied environmental effects. Therefore, risk assessments should consider environmental factors of a place rather than depending on data from laboratory studies.

The theoretical model provides useful insights, but there are a number of limitations that should be recognized. The model is based on relatively steady environmental conditions and biological absorption; seasonal variation or intricate interactions with other pollutants are not explicitly included. In natural environments, nanoparticles commonly coexist with organic contaminants, heavy metals, and microplastics. These interactions may affect transport and toxicity.

Therefore, future studies should include other parameters to improve forecast accuracy. The interaction of nanoparticles with natural organic matter should be studied as organic molecules might change surface characteristics and alter aggregation behaviour. The effects of seasonal variability, including temperature, rainfall, and hydrological variations, should be incorporated since they influence the transport paths and environmental persistence. Nanoparticle dispersal could be affected by weather patterns, flooding, and ecological responses as well, which may change with climate change[34].

Emerging research has also shown that interactions between microplastics and nanoparticles are important. Microplastics can operate as carriers for nanoparticles, boosting their movement through environmental compartments and raising the probability of biological exposure. Future environmental risk evaluations will need to understand these combined consequences.

Moreover, machine learning and artificial intelligence approaches offer intriguing potential for environmental modeling. Machine-learning algorithms can analyze huge datasets to discover complicated patterns and enhance forecasts of nanoparticle transit, accumulation, and ecological consequences. These approaches can give more accurate and adaptive tools for environmental management and decision-making[35].

So, this abstract illustrates that manufactured nanoparticles represent a unique class of developing pollutants, whose environmental behavior is governed by numerous interrelated processes. Comprehensive evaluation methodologies are necessary to fully comprehend their long-term ecological impacts.

10. Conclusion:

This theoretical work created and implemented an integrated environmental fate and transport model to examine the behavior of manufactured nanoparticles in aquatic systems. It combines advection, diffusion,

aggregation kinetics, sedimentation dynamics, and risk assessment in a comprehensive framework for the understanding of the movement and accumulation of nanoparticles in environmental compartments.

Simulation results showed that size, density, and surface charge of nanoparticles are important parameters affecting environmental transit and persistence. Smaller nanoparticles with greater colloidal stability stayed suspended in the water column for longer times, whereas bigger and less stable nanoparticles displayed increased aggregation and sedimentation. Among the studied nanoparticles, titanium dioxide nanoparticles had the highest potential to accumulate sediment, while silver nanoparticles had the maximum permanence in the aquatic environment.

The study also revealed that sediment compartments become more important over time, representing dominating sinks for nanoparticle accumulation. This result highlights the importance of incorporating sediment monitoring in environmental assessment programs, because surface water measurements alone may underestimate the long-term pollution levels and ecological consequences.

Elevated nanoparticle concentrations may surpass ecological safety limits, as suggested by risk quotient analysis, raising concerns about potential harmful impacts on aquatic species, microbial communities, and ecosystem functioning. Moreover, the possibility of bioaccumulation and trophic transfer raises concerns for long-term exposures via food webs, including potential human exposure.

Although the model is theoretical in nature, it gives useful insights into the environmental behavior of designed nanoparticles and provides a scientific basis for future experimental studies. The methodology can enable environmental risk assessment, regulatory decision-making, and the creation of safer nanomaterials with lower impacts on the ecology.

Thus, nanotechnology continues to grow internationally; understanding the environmental fate of designed nanoparticles will become more and more critical. To harness the full potential of nanotechnology while minimizing the hazards to human and environmental health, it will be necessary to combine advanced modelling methodologies, long-term monitoring programmes and sustainable design strategies for nanomaterials.

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