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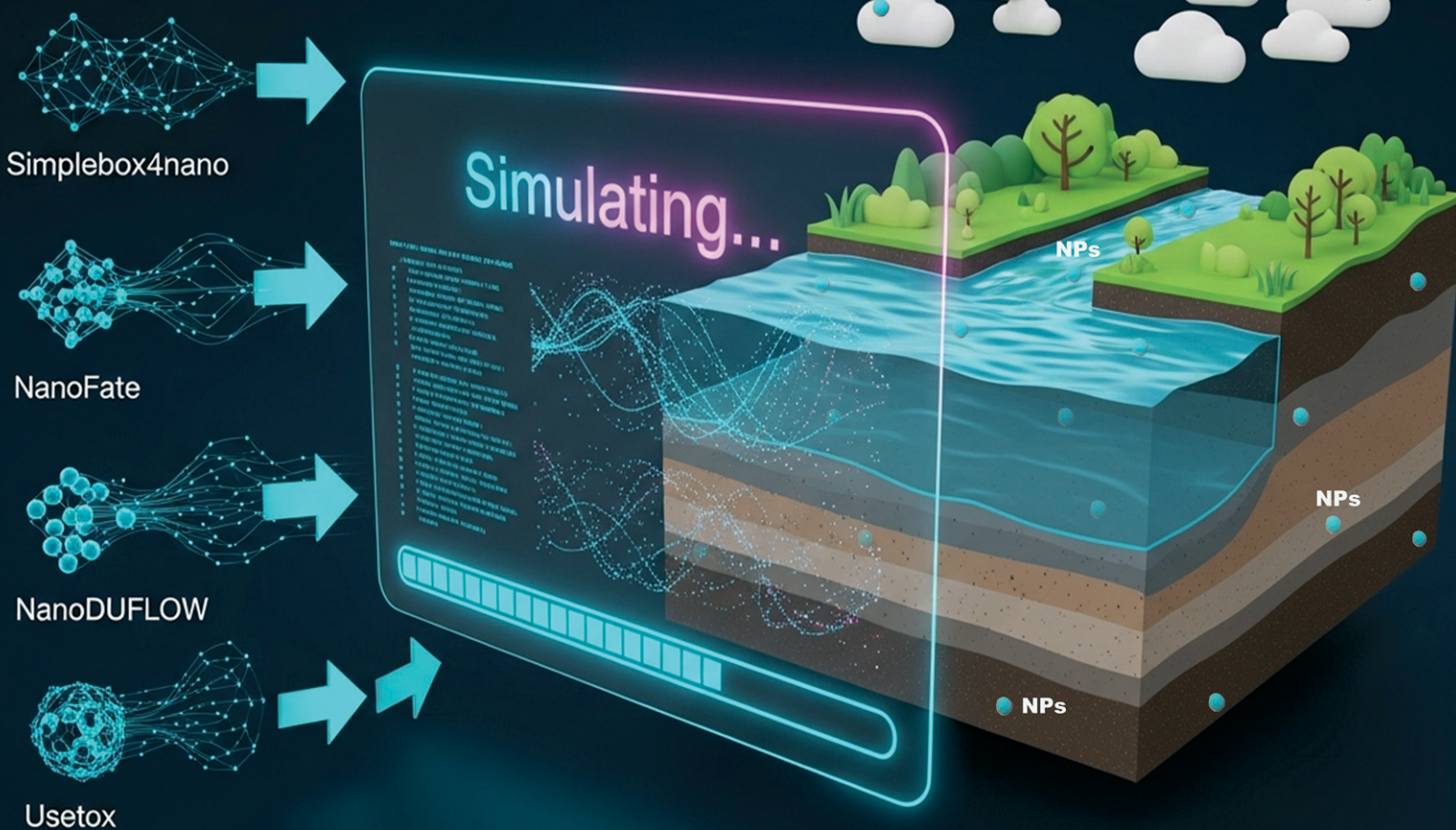
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Fate Models of Nanoparticles



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Fate models of nanoparticles in the environment: a critical review and prospects†

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The increasing use of nanoparticles (NPs) has raised concerns about their risks to the environment. However, the dynamics of the fate of NPs and their interplay with organisms make it challenging to perform an accurate and process-based hazard and risk characterization. Thus, it is crucial to estimate the concentrations of NPs after they are transported and transformed for their risk assessment (*i.e.*, evaluating the fate of NPs). This will provide more accurate results than using the mass of released NPs. However, experimental limitations make it challenging to directly quantify and track NPs. Hence, using mathematical models to simulate the fate of NPs has become a promising alternative, but previous reviews failed to systematically evaluate the strengths and weaknesses of these models. Accordingly, this review is the first to analyze and evaluate the fate models of NPs from a mathematical perspective. Specifically, we discuss the calculation methods and parameters for quantifying the transport processes and transformation reactions of NPs in environmental compartments (including water, soil, sediment, and atmosphere) used by different models and categorize and compare these processes in each compartment. Besides, this study provides recommendations for the further development of fate models of NPs and proposes an optimal modeling procedure for simulating the fate of NPs. The procedure provides the optimal simulation equations and parameters for each transport and transformation process in each compartment, intending to quantify these processes and the fate of NPs, explicitly considering the knowledge of uncertainties. Furthermore, we provide suggestions for constructing fate models for novel NPs and applying machine learning in these models to improve the fate models of NPs and environmental risk assessment.

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Environmental significance

The large-scale application of various NPs, including new nanomaterials, such as nanoplastics and nanopesticides, has raised concerns about their potential environmental risks in recent years. Thus, there is a pressing need to conduct accurate and reliable risk assessments of NPs as they can easily enter living cells and pose threats to various organisms and human health. A full understanding of the fate of NPs is a prerequisite for their risk assessment. Hence, this research is crucial for both environmental protection and ecological governance. Furthermore, the development of NP fate models will not only help assess the environmental risks of traditional nanoparticles but can also be applied to novel nanoparticles. Therefore, this research has a wide range of applications.

1. Introduction

Nanoparticles (NPs) have at least one dimension in the range of 1 to 100 nm in length and are commonly used in a variety

of applications such as paints, coatings, tires, clothing, energy, water treatment, and biomedicine.¹ Typical NPs include nano titanium dioxide (TiO₂ NPs), nanosilver (Ag NPs), and carbon nanotubes (CNTs). The global market for nanoproducts is expected to continuously expand in the future.^{2,3} NPs are produced during the manufacturing and use of various types of nanoproducts. Consequently, some are released directly into the water, atmosphere, and soil, while most are treated at sewage treatment plants and waste incineration plants before being released into the natural environment.⁴ Thus, there is a pressing need to assess the potential environmental and health risks associated with NPs as they can easily enter living cells and pose threats to

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various organisms and human health. However, evaluating the environmental and health risks of NPs requires the changes in their concentration in various environmental media to be initially determined, and thus, it is crucial to determine the fate of NPs in various environmental media.

After entering the natural environment, NPs undergo a variety of transport and transformation processes, which together determine their fate, and clarifying their fate is the premise of assessing their environmental risks. An in-depth investigation into the environmental fate of pollutants can help us identify their flow paths and dynamic changes. This will enable the more accurate assessment of the environmental risks posed by these pollutants and guide targeted interventions to address their environmental impact.⁵ Direct field observations and laboratory simulations are more commonly used to determine the environmental fate of NPs than model simulations. However, both approaches have their limitations, as follows: (1) field observations are challenging due to technical difficulties and the high cost of evaluating natural resources, making it difficult to observe NPs throughout the environmental system. (2) Laboratory simulations are constrained by limited human, material, and financial resources, leading to a restricted experimental scale. As a result, the data obtained is limited, and mathematical models are still necessary for further prediction and estimation. In conclusion, developing environmental fate models for NPs has become a more efficient and economically viable solution. The use of mathematical models to simulate, predict and evaluate the distribution, transport and transformation behavior of NPs in natural environments is not only easy to perform and cost-effective, but also flexible in changing the simulation area and comparing the effects of different variables on the environmental fate of NPs. Also, they provide theoretical guidance and directional suggestions for researchers to conduct experimental studies and field observations in the future.

Researchers first studied fate models for metals and organics, where the classical fate models for organics include the EQUilibrium criterion and multimedia activity model for ionics (MAMI). The EQUilibrium criterion is a fugacity-based steady-state model that can simulate the fate of non-ionic organics,⁶ while MAMI is an activity-based dynamic model that can simulate the fate of both ionic and non-ionic organics.⁷ The classic fate model for metals is TRANSPEC-II, which is a coupled metal form steady-state model.⁸ Additionally, the SimpleBox model developed by Meesters *et al.*⁹ is a concentration-based nested multi-medium fate model containing several environmental compartments, including air, freshwater, freshwater sediment, ocean, marine sediment, and three soil types (urban, agricultural, and others), which is capable of modeling the fate of non-ionic and ionic organic matter and metals.

Owing to the growing market share of nanomaterials, researchers have begun to focus on fate models of NPs. Meesters *et al.*¹⁰ improved SimpleBox to make it applicable to

NPs, and accordingly proposed the first multimedium model (*i.e.*, SimpleBox4Nano (SB4N)) for evaluating the environmental fate of engineered nanoparticles. This model considers the transformation of NPs in five environmental compartments, including air, rainwater, surface water, soil, and sediment, and the transport of NPs between them. Within each compartment, NPs are present in three forms, *i.e.*, free dispersion, heterogeneous aggregation with smaller natural particles, and attachment to larger natural particles. The final result of the model is the mass concentration of the three forms of NPs in each environmental compartment in the steady state. In 2019, Meesters *et al.*¹¹ analyzed the sensitivity of SB4N to determine the impact of the different physicochemical properties of NPs on the model. They discovered that the conversion rate constant and attachment efficiency are the most crucial factors affecting the environmental fate and exposure simulations of NPs. Furthermore, some researchers have directly modeled the fate of NPs based on their properties. However, researchers initially focused only on the fate behavior of NPs in aqueous environments, while few focused on their fate in soil or the atmosphere. Gradually, the multimedia model was developed to consider the fate of NPs in water, soil, the atmosphere, and sediment together. In 2017, Garner *et al.*¹² developed a dynamic multimedia fate and transport model (nanoFate) to predict the time-dependent accumulation of engineered nanomaterials in the environment. This model is comprised of four environmental compartments, *i.e.*, air, water, soil, and sediment. It considers more detailed transport and transformation processes, as well as the dimensions and characteristics of each environmental compartment. It also considers daily hydrometeorological data such as precipitation, wind speed, and river flow, thus improving the regional specificity of the model.

At the same time, comprehensive fate models for both traditional materials such as organics and metals and emerging materials such as nanoparticles are emerging. For example, USEtox¹³ can characterize the impacts of chemical release on freshwater organisms and human health in a life cycle assessment. This model uses the physicochemical properties of NPs as input parameters to simulate the transport between life phases, as well as the loss rate, and can output parameters that characterize the environmental fate, exposure, and toxicity of NPs. Eckelman *et al.*¹⁴ used USEtox to assess and compare the aquatic ecotoxicity of carbon nanotubes throughout their life cycle and found that their ecotoxicity impacts of their production phase, which is roughly equivalent to the ecotoxicity impact of releasing all of carbon nanotubes into water.

The above-mentioned models are all comprehensive multimedia fate models, and most of them are based on the classical fate models with a mature modeling framework. These models not only have broad applicability but also high reliability. Based on these models, recent reviews on NP fate models mainly focused on the factors that influence the transport and transformation behaviors of NPs in

environmental compartments. For example, Rawat *et al.*¹⁵ summarized the recent progress in the factors affecting the fate and transport of NPs in terrestrial environments, and Rex *et al.*¹⁶ provided a comprehensive evaluation of the fate and transformation behaviors of NPs in aqueous environments. Abbas *et al.*¹⁷ presented a comprehensive review of the transformation of NPs in different environmental compartments, including aquatic, terrestrial, and atmospheric environments. However, these reviews still lack information on the following four aspects: (i) lack of systematic strength, weakness, opportunity and threat (SWOT) evaluation of existing fate models, which hinders the optimization and refinement of the existing models and the further development of new modeling frameworks; (ii) lack of quantitative analysis and comparison of different parameters of multiple fate models, which is not helpful for the further optimization of parameters and models, and makes it difficult to understand the complex transport and transformation mechanisms of NPs; (iii) the focus is on specific environmental compartments, seldom considering multiple environmental compartments, which reduces the authenticity and accuracy of the use of fate models to visualize the fate of NPs; and (iv) lack of quantification of the fate behavior and transport and transformation processes of NPs using models, focusing on the overview of the description and portrayal of the fate behavior and transport and transformation processes of NPs obtained through experiments.

Therefore, this study reviews the models used to simulate the fate of NPs in natural environments over the last two decades, including models focusing on aqueous environments and multimedia models. We describe and evaluate in detail the transport and transformation processes that occur in natural environments and their simulation formulas, analyze the challenges faced by the fate models of NPs, and offer suggestions for the future development and application of the models.

2. Literature survey

In September 2024, we searched the Web of Science using the keywords “nano” and “fate”, which yielded 5167 articles on. Subsequently, 4212 articles were excluded, including reviews and articles that did not align with this topic. We further read the abstracts and excluded 831 articles that investigated the fate of NPs through experiments. Finally, 124 articles related to the study of NPs fate models were obtained (Fig. 1a). We analyzed the development of the fate model based on changes in the number of articles. Since 2008, researchers have focused their attention on the fate of NPs. From 2015 to 2019, the number of publications in the modeling category increased (Fig. 1b), and models such as dynamic material flow models¹⁸ focusing on the release of NPs and nanoFate were proposed during this period. In fact, the number of experimental articles related to the fate of NPs has consistently been much higher than that on modeling

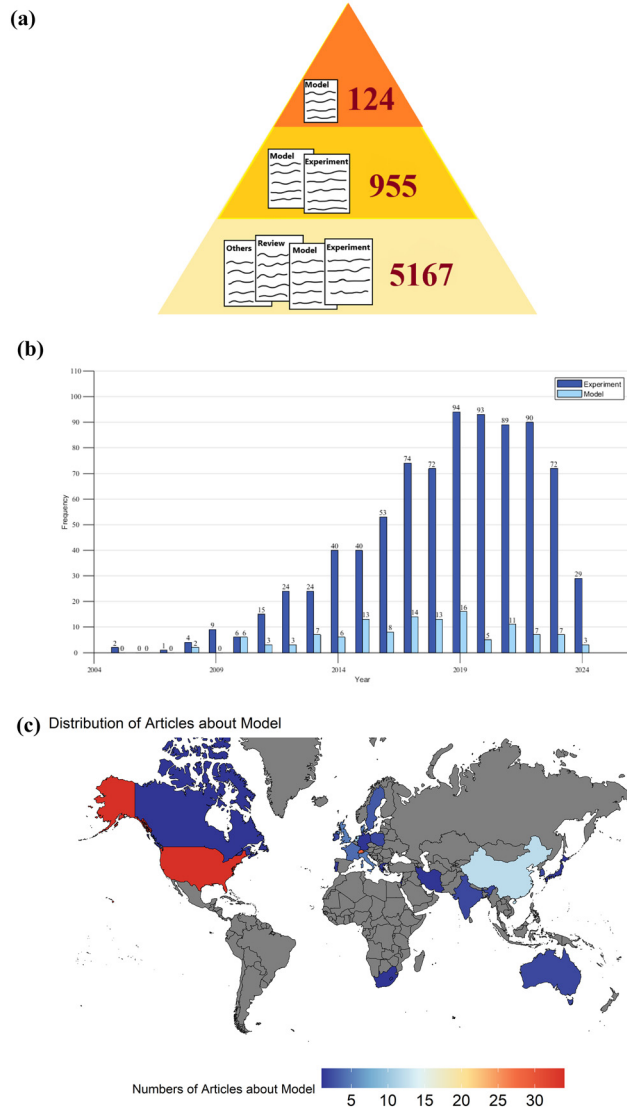


Fig. 1 (a) Articles retrieved with the keywords “nano” and “fate”. In September 2024, a total of 5167 articles was found on the Web of Science. A total of 4212 articles were excluded from the review articles and articles that did not match this topic; 831 experimental articles were further excluded by reading the abstracts, and finally, we obtained 124 articles that conducted research on fate models of NPs. (b) Number of experimental and model articles published each year from 2004 to 2024. The figure is a multi-group bar chart, where the left column represents the number of experimental articles published per year and the right column represents the number of models published per year. It is clear that the number of experimental articles published per year is higher than the number of model articles. (c) Distribution of authors of model articles by country. The country distribution was counted based on the country of the institution to which the first author of the article belonged.

articles for two decades (Fig. 1b). After 2019, the number of research articles on fate modeling showed a decline, but the number of experimental articles increased (Fig. 1b). We speculate that there may be two reasons for this. One is that the research hub for nanomaterials has shifted to micro- and nano-plastics in recent years, but researchers lack a deep

understanding of micro- and nano-plastics, and thus they have started to focus on experimental investigation again. The second reason is that when researchers attempt to use models to simulate the fate process, they need experimental data to modify the models and parameters, and experimental results are needed to validate the final simulation results of the models. Thus, the focus has shifted back to experimental simulation.

The distribution of the country affiliations of the authors of the 124 articles on the environmental fate models of NPs (Fig. 1c) shows that the United States has the most published articles, followed by Switzerland. These two countries contributed nearly half of the total number of articles on environmental fate models of NPs, which mainly involve the material flow analysis model (MFA) and USEtox model. The third and fourth countries are China and the Netherlands, but there is a significant gap between the number of articles published by these two countries and the first two countries. The statistics also indicate that research on the development of fate models is primarily focused in North America and Europe. Although there are studies on fate models from Asia, most of these studies are local practices of existing models and there is a lack of development and improvement of the models.

We further visualized the keywords of the searched articles (Fig. 2) and found that fate is often associated with release, exposure, and toxicity. The fate behavior of NPs in aqueous environments received more attention than in the atmosphere and soil environments, probably because aqueous environments are the main sinks of NPs.¹⁹ Researchers have especially focused on the aggregation, dissolution, and transport of NPs. Ag NPs and TiO₂ NPs are widely used in various products due to their excellent properties, and thus have become the most common research objects when studying the environmental fate of NPs. ZnO

NPs and CNT are also commonly studied. With the advancement of science and technology, emerging nanomaterials such as micro- and nano-plastics have gradually entered this research field. Besides, the keyword bioavailability also appeared frequently, although it may not be as relevant to the environmental fate of NPs and more relevant to the application of NPs. For example, drug delivery using nanocarriers is a crucial application of NPs, which improves drug uptake due to the small size of NPs, making it easier for them to enter cells. In addition, NPs enhance the dissolution and improve the targeting of drugs, significantly increasing the bioavailability of drugs.²⁰

3. Overview of models

Early models of the fate of NPs only considered transport and transformation processes in freshwater, gradually expanding to other environmental compartments. For example, in 2008, Blaser *et al.*²¹ analyzed the risk to freshwater ecosystems from Ag NPs in NPs released from textiles and plastics. They evaluated the fate and predicted the environmental concentrations of Ag NPs in river systems in the EU25 in 2010 and estimated the predicted no-effect concentration (PNEC) of Ag NPs by analyzing the available toxicity data, thus providing a risk assessment of the environmental exposure to Ag NPs. The classical fate model for NPs proposed by Praetorius *et al.*²² in 2012, which initially focused only on the concentration of NPs in surface water, could predict the steady-state concentration after fate behavior, focusing on the hetero-aggregation of suspended sediment and NPs, and investigated the effect of various parameters of suspended sediment on the fate of NPs. In 2015, Sani-Kast *et al.*²³ improved Praetorius's model by incorporating the spatial

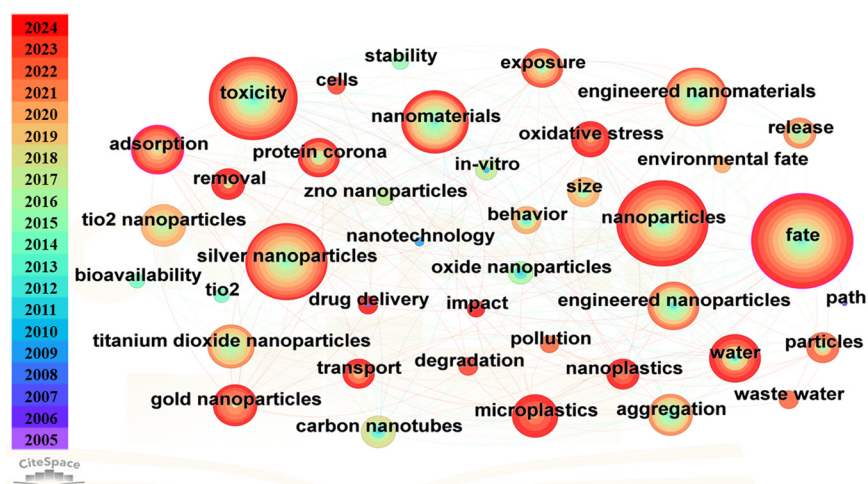


Fig. 2 Network built using the keywords extracted from retrieved articles using CiteSpace. We used CiteSpace to create a yearly graph for the visual analysis of the articles. The nodes in the graph represent the keywords of these articles, and different colors represent different years (if a color appears in the outer ring of the keyword, it means that there are articles containing this keyword published in that year). The outer ring of the year wheel of some keywords is wrapped in purple, which indicates that the keyword is highlighted.

variability of the aquatic environment, combining river systems with different environmental conditions, and using clustering analysis to identify the key features affecting the fate of NPs. In 2021, Gao *et al.*²⁴ modeled the multimedia fate and transport of Ag NPs with two spatial resolutions based on the model developed by Praetorius *et al.* They compared the effect of spatial resolution on the simulation results using the spatial distribution of Ag NPs in the Xiangjiang region of China as an example and found that a high spatial resolution significantly improves the accuracy of the simulation results.

In 2014, Dumont *et al.*²⁵ proposed the GWAVA model, which is capable of simulating monthly concentrations of Ag NPs and ZnO NPs in European surface waters at a spatial resolution of 6×9 km. Their model simulates NPs moving from households to rivers, considering processes such as dilution, downstream transport, evaporation, extraction, and deposition. This model is highly applicable to rivers, lakes, reservoirs, and wetlands. In 2015, de Klein *et al.*²⁶ proposed the NanoDUFLOW model by linking processes of NPs to a spatially explicit hydrological model, DUFLOW. This model uses the Dommel River in the Netherlands as the default scenario to explain the homogeneous and heterogeneous aggregation, dissolution, and degradation of NPs, as well as their deposition, resuspension, and burial in deeper sedimentary layers.

The Water Quality Analysis Simulation Program (WASP) is a classic water quality analysis simulation program with a spatially resolved dynamic mass balance fate and transport modeling framework, which allows users to simulate the concentrations of toxic substances in surface water and sediment with complexity at spatial and temporal scales (<https://www.epa.gov/hydrowq/water-quality-analysis-simulation-program-wasp>). It is currently updated to version 8 (WASP8), where a new state variable, nanoparticles, has been added to WASP8. It can evaluate the fate of NPs and considers transport processes such as deposition, erosion, and resuspension of NPs, as well as transformation processes such as sulfation, oxidation, dissolution, and heteroaggregation.²⁷ Han *et al.*²⁸ successfully simulated the photoconversion and transport of graphene oxide in Brier Creek, Georgia, USA using WASP8. Avant *et al.*²⁹ continued their research by using WASP8 to examine the fate and transport of multi-walled carbon nanotubes (MWCNT), graphene oxide (GO), and reduced graphene oxide (rGO) in four aquatic ecosystems in the southeastern United States (Briar River, North Carolina; Lake Waccamaw, North Carolina; Lake Baco, Florida; and Yadkin River, North Carolina). Ross *et al.*³⁰ also used WASP8 to simulate the fate and transport of copper oxide nanoparticles (CuO NPs) and copper ions in Lake Waccamaw, North Carolina over an 11 year period from January 1, 2000 to January 1, 2011. WASP8 also considers light attenuation and photo-transformation processes compared to previous models, employing a new structure to simulate the light intensity and light responses in a water column.³⁰

Given that environmental compartments are often interconnected, it is biased to only consider the behavior of NPs in one environmental compartment when assessing their environmental risk. To more accurately and thoroughly assess the fate of NPs, it is optimal to develop a multimedia model that can consider multiple environmental compartments. The typical multimedia fate models include Simplebox4nano, nanoFate, and USEtox. Simplebox4nano uses first-order kinetics to estimate the background concentration of NPs in the environmental system. It uses first-order rate constants to relate the substance concentration to the transfer process, and then uses simple matrix algebra to solve the associated system of mass balance equations. The SB4N model simulates the processes roughly, and most of the transport and transformation processes are quantified by first-order reaction rate constants. However, it is a fresh attempt to consider the “rainwater” compartment separately, which is well worth studying and referencing. NanoFate is designed based on a series of mass balance equations that account for the transport of NPs between environmental compartments and their transformation into non-nano forms, using a set of ordinary differential equations to link the various transport and transformation processes in each compartment. NanoFate considers a wider range of processes but fewer transformation processes. Additionally, the environmental compartments are not detailed enough, causing the spatial resolution of the model to be insufficient. USEtox constructs a fate matrix to quantify the transport of NPs between compartments, and the elements of the matrix include the residence time of NPs in each compartment as well as the transport time between compartments.³¹ Fate factor (FF) is a characterization factor in USEtox that quantifies the fate of NPs in the environment and describes their distribution and degradation.³² In calculating the FF, Salieri *et al.*³³ adapted the USEtox model to more thoroughly consider various transport processes of NPs, including hetero-aggregation, precipitation, convection, resuspension, burial, and interlayer transfer between sedimentary layers. The FF was calculated for TiO₂ NPs with varying particle sizes, considering the specificity of NPs. Pu *et al.*³¹ further considered pseudo-settlement processes. Pseudo-settlement refers to settling that does not accurately reflect the situation but is theoretically calculated. They focused on the nano-specific behavior of NPs in freshwater compartments and calculated nano copper (Cu NPs) equivalents in freshwater on 17 subcontinents. Temizel-Sekeryan and Hicks.³⁴ combined the principles of colloidal science with the USEtox model to evaluate Ag NPs in a life cycle assessment and proposed two methods for calculating the parameter FF and conducting sensitivity analyses for both methods. USEtox enables the evaluation of the fate of NPs more conveniently, but it may not be detailed enough. Additionally, NanoFASE (a four year Horizon 2020 project and member of the EU NanoSafety Cluster) developed a framework for combining the soil–water–sediment transport, transformation, and biosorption of NPs. The NanoFASE WSO model predicts the spatial and temporal

variations in the concentration of NPs within a catchment, providing detailed predictions of PECs in different parts of the catchment. It works by dividing the catchment into a series of “cells”, each with its own set of environmental compartments. This model is more detailed than NanoFate and considers more processes, even mentioning the impact of bioturbation on the fate of NPs, and has a higher spatial and temporal resolution, but it does not consider the atmosphere as an environmental compartment.

Additionally, some researchers have also attempted to combine the USEtox and SimpleBox models to assess the environmental fate behavior and toxicity of NPs. For example, Ettrup *et al.*³⁵ integrated the USEtox 2.0 model and the SimpleBox4nano model, and used the SB4N model to calculate the FF for a comprehensive evaluation of TiO₂ NPs. In 2018, Salieri *et al.*³⁶ attempted to improve the combination of the USEtox model and the SB4N model. They combined the air compartment and the rainwater compartment in the SB4N model and considered the sum of the NPs of the three morphologies in the final output. This combination deserves recognition and represents an improvement of the USEtox model, compensating for its lack of detail, while maintaining its concise modeling framework.

After summarizing the temporal evolution of the fate models, we further categorized them according to the nanoparticle types studied, environmental media considered and simulation scenarios (Table 1). It is clear that TiO₂ NPs are the most widely studied NPs, and almost all fate models have studied it, including Praetorius *et al.*, NanoDUFLOW, USEtox, SimpleBox4nano, nanoFate, and Usetox4nano. The research area covers Europe and the United States, and the environmental compartments studied are comprehensive. Next, Ag NPs have been simulated by Praetorius *et al.*, GWAVA, NanoDUFLOW, and USEtox. Regrettably, the current

research on the fate behavior of Ag NPs is limited to water compartments and has not been thoroughly studied in multiple media. In addition, CuO NPs have been simulated by WASP8 and nanoFate, CeO₂ NPs simulated by NanoDUFLOW and nanoFate, and ZnO NPs simulated by GWAVA and nanoFate. These NPs have been thoroughly evaluated in the multimedia fate model. Additionally, the fate of carbon-based NPs, including GO, rGO, CNT, and MWCNT, can be estimated using WASP8 or USEtox.

4. Details of processes for the fate of NPs

The study of the environmental fate of NPs usually begins by dividing the natural environment into compartments, and then the transport and transformation processes of NPs within and between each compartment are investigated separately.^{10,12,13} Some researchers focused on the compartments of freshwater, seawater, soil, atmosphere, and sediment,¹⁰ some ignored the seawater compartment,^{16,19,20} and some divided the environment into more detailed compartments.^{12,13} In this study, we consider four types of compartments, including the water environment (including freshwater and seawater), the soil environment (including urban, natural, and agricultural soils), the atmosphere (including air, aerosols, and rainwater) and the sediment environment (including freshwater and seawater sediments). This division facilitates a clear and concise categorization of various transport and transformation processes, and encompasses most of the environmental compartments considered in the studies of fate models. In this study, the release of NPs to each environmental compartment is considered as the initial concentration. Subsequently, NPs will undergo transport and transformation processes that

Table 1 Summary of fate models based on nanoparticles and environmental media

NPs	Model	Media	Scenario	References
TiO ₂ NPs	Praetorius <i>et al.</i>	Water	Rhine river	22
	Praetorius <i>et al.</i>	Water	Rhône river	23
	NanoDUFLOW	Water	Dommel river	26
	USEtox	Water	—	33
	SimpleBox4nano	Air, water, soil, sediment	Switzerland	10
	NanoFate	Air, water, soil, sediment	San Francisco bay	12
	USEtox4nano	Water	—	35
	USEtox4nano	Air, water, soil, sediment	—	36
Ag NPs	Praetorius <i>et al.</i>	Water	Xiang river	24
	GWAVA	Water	Europe	25
	NanoDUFLOW	Water	Dommel river	86
	USEtox	Water	—	34
CuO NPs	WASP8	Water	Lake Waccamaw	30
	NanoFate	Air, water, soil, sediment	San Francisco bay	12
Cu NPs	USEtox	Water	—	31
CeO ₂ NPs	NanoDUFLOW	Water	Dommel river	26, 86
	NanoFate	Air, water, soil, sediment	San Francisco bay	12
ZnO NPs	GWAVA	Water	Europe	25
	NanoFate	Air, water, soil, sediment	San Francisco bay	12
GO, rGO, CNT, MWCNT	USEtox	Water	—	14
	WASP8	Water	Brier Creek, USA	28
	WASP8	Water	Briar river, Lake Waccamaw, Lake Baco, and Yadkin river	29

affect their final fate, and the concentration of NPs in each environmental compartment at this time is regarded as the steady-state concentration. It is more informative to use such steady-state concentration to assess the environmental risk of NPs. Fig. 3 shows the transport and transformation process of NPs within and between each environmental compartment, which we primarily introduced.

4.1 Similar processes for the fate of NPs: aggregation and advection

Aggregation occurs after NPs enter each environmental compartment.^{10,12} Aggregation refers to the formation of clusters of NPs, and particle–particle interactions (*i.e.*, aggregation) lead to changes in the shape and size of the particles, and the size of the particles affects the environmental fate and toxicity of NPs. In general, aggregation is mainly determined by the properties of the particles, such as size, shape, chemical composition, surface charge, and surface roughness.³⁷ Furthermore, particle aggregation in water environments is influenced by factors such as ionic strength, pH, and NOM. It is also impacted by certain environmental factors in soil and atmospheric environments.³⁸ Aggregates formed due to interactions between identical NPs are homogeneous, while aggregates formed between NPs and other environmental components are heterogeneous.³⁹ Hetero-aggregation can occur between NPs and suspended particulate matter (SPM), or between NPs

and aerosols. Particles stick together to form aggregates during collisions with a probability expressed in terms of attachment efficiency. Given that the number of natural particles in the environment is much larger than the number of NPs, heterogeneous aggregation is more likely to occur than homogeneous aggregation, which is why homogeneous aggregation is often overlooked in studies on the environmental fate of NPs. However, for a more accurate model, we suggest considering homogeneous aggregation.

Smoluchowski first provided the mathematical foundation for the description of aggregation dynamics in 1917, and since then the von Smoluchowski equation (eqn (1)) is commonly used to describe aggregation and has been applied in a variety of fate models,⁴⁰ as follows:

$$\frac{dn_k}{dt} = \frac{1}{2} \sum_{i=1}^{k-1} \alpha_{i,j} K_{i,j} n_i n_j - n_k \sum_{i=1}^{\infty} \alpha_{i,k} K_{i,k} n_i \quad (1)$$

where n_i denotes the concentration of particles of size class, i , t denotes time, $\alpha_{i,j}$ denotes the attachment efficiency of particles i and j , and $K_{i,j}$ denotes the collision efficiency of particles i and j . The von Smoluchowski equation is applicable to both homogeneous and heterogeneous aggregation, but it also needs to determine the attachment and collision efficiencies between particles, which makes the calculations more complex but reflects the mechanism of the aggregation process. However, some fate models simplify the simulation of the aggregation process, for example, nanoFate

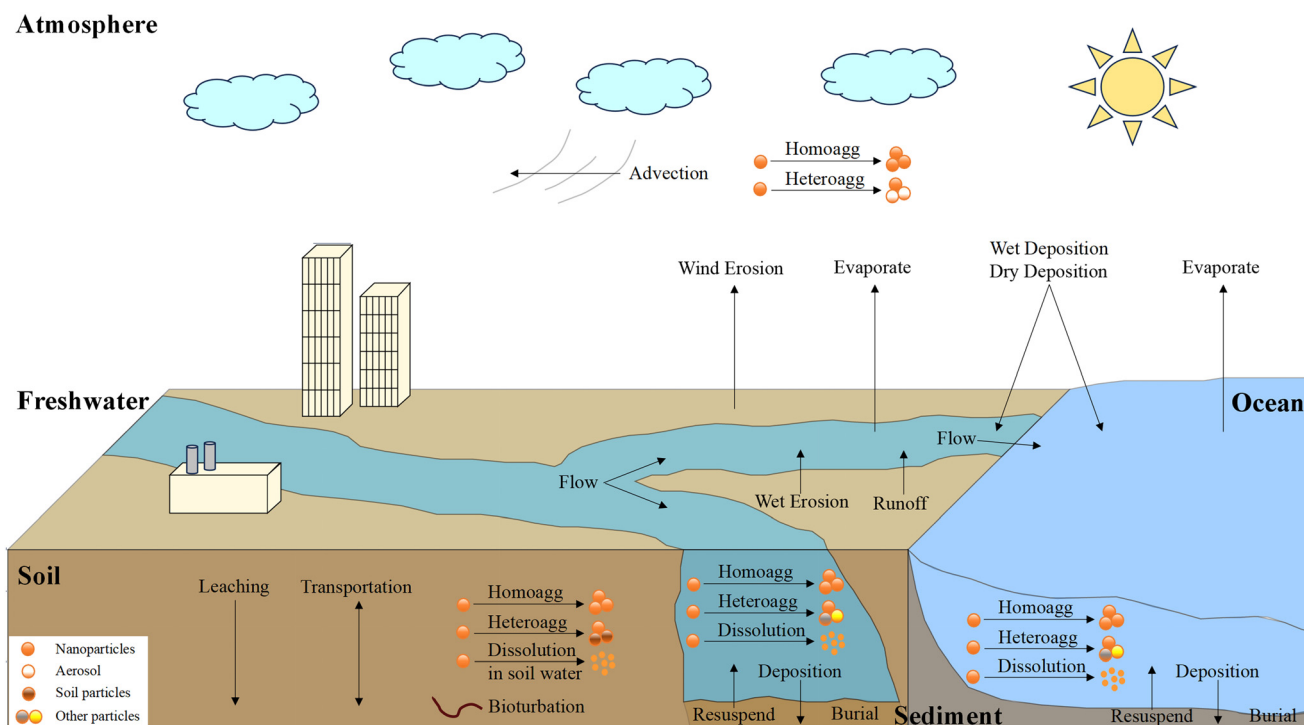


Fig. 3 Transport and transformation processes for NPs in various environmental compartments. Transport and transformation processes in aquatic environments include aggregation, advection, dissolution, deposition, resuspension, and burial. The processes occurring in the soil environment include wind erosion, water erosion, runoff, aggregation, dissolution, and advection. The atmospheric processes include aggregation, attachment, advection, dry deposition, and wet deposition.

assumes that the aggregation rate is a pseudo-primary rate constant, and SB4N also assumes that the aggregation process follows primary kinetics. These factors may result in bias and uncertainty in the final calculations.

Advection is a process for the movement of NPs caused by medium movement, and thus it can occur in water compartments, sediment compartments and atmospheric compartments. In the water compartment, the advection process mainly involves exchanging NPs in the water column and suspended sediments between freshwater and seawater. The sediment contain NPs that are transported from freshwater to seawater sediment due to sediment mobilization. In the atmosphere, it refers to the flow of NPs in and out of the system. NanoDUFLOW calculates the flow, water level, and mean flow rate for each time step in each river reach using DUFLOW Modeling Studio (v3.8.7), a software package that uses Preissmann's scheme to solve the Saint-Venant continuous momentum equation with initial-value and marginal-value conditions to determine water level and flow rate.^{41,42} Most studies assume that the advection rate is a primary reaction rate constant.^{10,12} The advection rate of NPs can also be calculated from the flow rate and the concentration of NPs, which is a more generalized calculation method that is applicable to all compartments, and the flow rate and concentration data are easily available.

4.2 Transformation of NPs

4.2.1 Dissolution. The dissolution of NPs is essentially a transformation from a compound form to a dissolved ionic form or other compounds, depending on the environmental conditions. Dissolution is a surface-controlled process that is primarily influenced by the properties of the particles (*e.g.*, chemical properties and surface area) and the properties of the water environment (*e.g.*, pH and NOM concentration).⁴³ For example, NPs with smaller surface areas, such as CuO NPs⁴⁴ and Ag NPs,⁴⁵ typically have higher solubility. For instance, most metal and metal oxide NPs, including Ag NPs,⁴⁵ TiO₂ NPs,⁴⁶ and ZnO NPs,⁴⁷ have increased solubility under extreme pH conditions. Based on this, some researchers have conducted experiments to investigate the dissolution kinetics of NPs, but fewer models focus on the dissolution process, which is likely due to their focus on insoluble NPs (*e.g.*, TiO₂ NPs and CeO₂). The dissolution process simulation varies greatly among different fate models. SB4N is calculated separately for dissolved concentrations of NPs with varying solubility (soluble and almost insoluble). NanoFate considers the equilibrium dissolved concentration of each type of NPs at a specific pH and corrects the estimated dissolved concentration if it exceeds the equilibrium concentration. The model provides the first-order dissolution rates of CuO NPs and ZnO NPs for all pH values of freshwater, marine, and soil waters. Most fate models, such as NanoDUFLOW and Praetorius *et al.*,²² use a first-order rate constant to quantify the dissolution process. However, the dissolution rate is proportional to the

surface area of the particles, not their mass, and thus assuming it follows first-order kinetics is not reasonable. Quik *et al.*⁴³ suggested adding another first-order removal rate constant to model the process of removing NPs from water through dissolution. In fact, the simulation of the dissolution process needs to be further improved in the future based on the results of experiments, which is due to the fact that the solubility of NPs varies depending on the different properties of different environmental media and the estimation of the dissolution rate of NPs through experiments is more accurate.

4.2.2 Sulfidation. Sulfidation refers to the process by which metal NPs combine with sulfide ligands to form metal sulfides.¹⁷ Under hypoxic conditions, Ag NPs easily react with dissolved sulfides in water to form silver sulfide nanoparticles,⁴⁸ which in turn alter their toxicity and bioavailability. The parabolic rate model (eqn (2)) originally proposed by Jander⁴⁹ is the optimal method for simulating this process.⁵⁰

$$F_{\text{Ag}} = \left(1 - \sqrt{\frac{k}{r^2}}\right)^3 \quad (2)$$

where F is the metallic Ag fraction, r is the radius of the Ag NPs, k is the rate constant and t is the time. NanoFASE WSO model considers the formation of metal sulfide between CuO NPs and bisulfide (HS^-), and the sulfidation rate is calculated using eqn (3):⁵¹

$$F_{\text{CuO},t} = e^{-kt} \quad (3)$$

where $F_{\text{CuO},t}$ is the remaining fraction of CuO at time t of the reaction of CuO with HS^- , k is the pseudo first-order reaction rate coefficient and t is the time. This equation has been validated through experiments and can simulate the sulfidation of CuO NPs well. These two methods (eqn (2) and (3)) are currently our most recommended ones.

4.2.3 Phototransformation. Phototransformation refers to a series of reactions that occur in NPs under illumination, including photo-oxidation, photo-catalytic reduction, and photo-induced chemical structural changes.⁵² WASP8 includes a phototransformation module, and Han *et al.*²⁸ used it to simulate the phototransformation process of GO (eqn (4)), as follows:

$$k = \sum_{\lambda=1}^{10} \frac{k_{\text{ph}}}{\Delta} \lambda \left(\sum_{\lambda_1}^{\lambda_2} \frac{1 - 10^{-A\lambda}}{E_{\text{ph},\lambda}} \right) I_{\text{av},\lambda} \quad (4)$$

where k is the rate constant, k_{ph} is the observed photoreduction rate constant, $\Delta\lambda$ is the bandwidth, λ_1 , λ_2 are bandwidths, $E_{\text{ph},\lambda}$ is the energy of a photon of wavelength λ , A is the absorption coefficient of a GO solution at wavelength λ and $I_{\text{av},\lambda}$ is the flux of light. Currently, only a few fate models consider this process. However, the toxicity of many nanoparticles is altered after phototransformation,⁵³ and thus this process should not be disregarded. In the future,

this process should be given more consideration when constructing fate models.

4.3 NPs in the water environment and sediment environment

The water and sediment environments include freshwater (rivers, lakes, wetlands, and reservoirs), marine, mixed freshwater and marine zones (estuaries, *etc.*), and freshwater and marine sediments. Researchers primarily focus on freshwater, seawater, and sediment, while mixed freshwater and seawater zones are often overlooked due to the difficulty in modeling complex environmental conditions in mixed freshwater and seawater zones. Even if studies consider the mixed freshwater and seawater zone, it is often divided into freshwater and seawater zones.¹² Sediment also includes suspended sediment, and thus when studying the fate behavior of NPs in the water and sediment environments, it is important to fully consider the transport processes between the water column, sediment, and suspended sediment. The main transport processes in the water and sediment environments commonly considered in fate models are aggregation, advection, dissolution, deposition, resuspension, and burial. The detailed simulation equations for these processes are presented in Table 2.

4.3.1 Deposition. NPs are deposited into sediment compartments through gravity settling as free particles, small aggregates, or heterogeneous aggregates. Particle size and aggregated particle size are the main factors affecting deposition, and when aggregates are formed, particle aggregates become more easily deposited by gravity as they become larger in size.⁴³ The deposition of NPs is also largely influenced by environmental factors such as pH, ionic strength, initial NP concentration, natural colloids, and aquatic organisms. For example, NOM or other stabilizers have been found to reduce the deposition rate in aqueous suspensions through experiments. The deposition of NPs is also affected by their chemical composition. Carbon NPs deposit the fastest, followed by metal and metal oxide NPs.^{43,54,55} Furthermore, different morphologies (free particles, small aggregates, or heterogeneous aggregates) exhibit different deposition rates, but studies usually assume they are first-order reaction rates, and there are also studies that calculate the deposition rates using Stokes' law^{12,29,43} (eqn (5)), as follows:

$$k_{\text{sed,ss}} = \frac{2(\rho_p - \rho_w)}{\mu} \times g \times R_p^2 \quad (5)$$

where ρ_p denotes the suspended sediment density, ρ_w denotes the density of seawater or freshwater in each compartment, μ denotes the dynamic viscosity, g denotes the gravitational acceleration, and R_p denotes the particle radius. This calculation method follows the particle deposition process mechanism, and it can be seen that the deposition rate is controlled by the balance between the resistance that keeps the particles suspended and the gravity of the particles. Therefore, it is recommended to use this method to measure

Table 2 Equations usually used in different fate models for transformation and transport in the water and sediment environments. Table S2† provides the specific meanings of the symbols

Water	Flow	Dissolution	Sedimentation	Aggregation		Sediment		
				Hetero-aggregation	Homo-aggregation	Resuspension	Burial	Advective transfer
SimpleBox4Nano		$k_{\text{dis}} = -\frac{\ln C_0/C_t}{t}$		$k_{\text{agg}} = f_{\text{col}}(\text{NP}, \text{NC}) \cdot \alpha_{\text{agg, NP, NC}} \cdot N_{\text{nc}}$		$k_{\text{res}} = \frac{v_{\text{res}} \cdot \text{AREA}_{\text{sw}}}{V_{\text{sc}}} \cdot \text{FR}_{\text{SE}}$	$k_{\text{bur}} = \frac{v_{\text{bur}} \cdot \text{AREA}_{\text{SE}}}{V_{\text{w}}}$	
NanoDUFLOW	DUFLOW modeling studio	$\frac{dC}{dt} = -k_{\text{dis}} C_0$	$k_{\text{sed}} = \frac{2(\rho_p - \rho_w)}{9\mu} \cdot g \cdot R_p^2$	$\frac{dn_j}{dt} = -\alpha_{\text{hete}} n_j \sum_i K_{j, \text{SSI}} n_{\text{SSI}} + \frac{1}{2} \alpha_{\text{hom}} K_{i,j} n_i n_j \frac{\rho_{\text{af}}^3}{\rho_j g_j^3}$	$\frac{dn_j}{dt} = -\frac{1}{2} \alpha_{\text{hom}} K_{j,j} n_j n_j + \frac{1}{2} \alpha_{\text{hom}} K_{i,j} n_i n_j \frac{\rho_{\text{af}}^3}{\rho_j g_j^3}$	$R_j = R_j \max \left(\frac{\tau}{\tau_{\text{crit}}} - 1 \right)$	$\frac{dC}{dt} = -k_{\text{bur}} C$	DUFLOW modeling studio
NanoFate	$k_{\text{flow}} = V \cdot C_0$	$\frac{dC}{dt} = -k_{\text{dis}} C_0$	$k_{\text{sed}} = \frac{2(\rho_p - \rho_w)}{9\mu} \cdot g \cdot R_p^2$	$\frac{dC}{dt} = -k_{\text{het}} C_{\text{ss}} C_0$				
Praetorius <i>et al.</i>	$k_{\text{flow}} = v \frac{A_{\text{w}}}{V_{\text{w}}}$		$k_{\text{sed}} = \frac{2(\rho_p - \rho_w)}{9\mu} \cdot g \cdot R_p^2$	$k_{\text{agg}} = \alpha_{\text{het}} \cdot k_{\text{coll}, i, j} \cdot C_{\text{particle}}^{\text{SPM}, i}$			$k_{\text{bur}} = \frac{v_{\text{bur}}}{h}$	$k_{\text{trans}} = \frac{v_{\text{max}}}{n_{\text{sed}}}$
GWAVA	$\frac{dn_j}{dt} = -\frac{1}{2} \alpha_{\text{hom}} K_{j,j} n_j n_j + \frac{1}{2} \alpha_{\text{hom}} K_{i,j} n_i n_j \frac{\rho_{\text{af}}^3}{\rho_j g_j^3}$					$k_{\text{res}} = \frac{v_{\text{res}}}{h}$		

particle deposition. In addition, we can attempt to use depth-integrated models⁵⁶ in the future to simulate the deposition of NPs in water. This method accurately simulates the deposition of suspended fine sediments and may be more accurate for simulating the deposition of NPs with small-size characteristics.

4.3.2 Resuspended and burial. After NPs are deposited in the sediment compartment, they may re-enter the water compartment through resuspension, or they may be buried to be removed from the system. Resuspension is the transport of NPs from the sediment compartment back into water under the influence of turbulence. NanoDUFLOW describes resuspension by a critical shear stress level based on the equations of Krone and Partheniades.⁵⁷ When the critical shear stress (τ_{crit}) is exceeded, the resuspension flux (R_j) is calculated based on the quotient of the actual shear stress (τ) and the critical shear stress (τ_{crit}) as well as the resuspension rate constant (eqn (6)), as follows:

$$R_j = R_{j\text{max}} \left(\frac{\tau}{\tau_{\text{crit}}} - 1 \right) \quad (6)$$

SB4N corrects the deposition rate by treating the resuspension process as a deposition resistance, and the resuspension rate can be calculated separately for free particles, small aggregates, and hetero-aggregates. Instead, NanoFate provides default rates for the resuspension of NPs in freshwater and seawater, and thus the results are somewhat crude. To calculate the resuspension rate of NPs more accurately, the methods of NanoDUFLOW or SB4N are recommended. Burial involves adding additional sediment to existing sediment, causing it to be removed from the system. Burial is often viewed as a primary loss process, and thus most researchers typically use a primary reaction rate constant to quantify this process.

4.3.3 Others. In addition to the processes described above, NanoFate also considers the transfer of NPs from the ocean surface to the aerosol zone through bubbles created by breaking waves caused by strong winds. The reaction rate of this process is calculated by multiplying the enrichment factor, the rate of bubble formation, and the coastal area over which this process occurs.¹² Praetorius *et al.*²² divided the water compartment into moving and stagnant zones, and thus the exchange of NPs between the moving and stagnant zones will also be considered. NanoFASE WSO models the transport and transformation processes of NPs in different water environments. The simulation of the movement of estuarine advection considers the influence of the tides and the transfer of NPs between the surface and lower waters of lake, the two types of spillways of reservoirs (with controlled and uncontrolled flow) are modeled separately, and the evaporation and cliff erosion processes of ocean are additionally considered. The evaporation process is also included in the USEtox model. Evaporation is the process by which seawater is converted into water vapor, and then rises into the atmosphere, which plays a crucial role in the water cycle. The evaporation of seawater has a significant impact

on the concentration of NPs in water. Given that NPs may not evaporate in the same proportion as water, this can lead to an increase in pollutant concentrations in seawater in a short period of time. These processes can be quantified through experimental data. However, the current research on simulating the fate of NPs in the water and sediment environments is extensive, and thus future research should concentrate on the identification of the uncertainty types and correction of the kinetic/reaction parameters. Furthermore, if we want to model the fate of NPs more accurately and in greater detail, we need to divide the individual environmental compartments into layers, and then consider layer-to-layer transfer.

4.4 NPs in the soil environment

NPs are mostly released into soil and landfills during the production, use, and end-of-life phases of nanoproducts, with a small portion is released into the atmosphere and aquatic environments.⁵⁸ This is because NPs that enter landfills will partially enter the soil after treatment, NPs released into the atmosphere will partially combine with other atmospheric components to settle in the terrestrial environment, and NPs entering the aquatic environment will return to the soil due to processes such as bubble bursting. The presence of inhomogeneous mixtures of gases, liquids, and soils, as well as organic matter and microbiota makes soil environments more complex than other environmental compartments, especially unsaturated soils.¹² After entering the soil system, NPs can be bioavailable to plants or adsorbed on mineral surfaces and undergo reactions such as homogeneous aggregation, heterogeneous aggregation, dissolution, deposition, adsorption, oxidation, reduction, sulfation, and photochemistry. Soil environments are often considered in layers such as surface soil, deep soil, and pore water, and thus some fate models also consider the transfer of NPs between different layers of soil.¹² The main fate processes of NPs in the soil environment are considered in the fate model, including wind erosion, water erosion, runoff, aggregation, dissolution, and advection. The detailed simulation equation information for each process is provided in Table 3.

4.4.1 Wind erosion. The erosion of the top layer of soil due to strong winds when the soil is relatively dry is known as wind erosion (dry erosion). Chepil *et al.*⁵⁹ divided the factors affecting wind erosion into three categories including air factors (wind speed, turbulence, air density, viscous coefficient, *etc.*), surface factors (roughness, ground cover, obstacles, temperature, topography, *etc.*), and soil factors (soil structure depending on the organic matter content, calcium carbonate content, and mechanical composition, bulk density, water content, *etc.*). NPs can be removed from the soil system into the air through the direct or indirect action of air flows. Given that urban systems often lack open, spacious, and uncovered surfaces, wind erosion mainly occurs on natural and agricultural soils. Garner *et al.*¹² first used jump equations and vertical flux conversions to

Table 3 Equations usually used in different fate models for transformation and transport in the soil environment. Table S3† provides the specific meanings of the symbols

Soil	SimpleBox4Nano	NanoFate
Wind erosion	$k_{\text{ero}} = \frac{v_{\text{ero}} \cdot \text{AREA}_s}{V_{\text{soilsolids}}}$	$F_a = A_c \frac{p}{g} \sum_{u_*} u_* (u_*^2 - u_{*t}^2) \cdot \Delta T \cdot K_c$
Wet erosion		$A = R \times K \times \text{LS} \times C \times P$
Runoff	$k_{\text{runoff}} = \frac{\text{FR}_{\text{runoff}} \cdot p_0 \cdot \text{AREA}_s}{V_{\text{soilporewater}}}$	$Q = \frac{(P_R - 0.2S)^2}{P_R + 0.8S}$
Attachment	$k_{\text{att}} = \lambda_{\text{filter}} \cdot \alpha_{\text{att,NP,grain}} \cdot \eta_{0,\text{NP,grain}} \cdot U_{\text{Darcy}}$	
Leaching	$k_{\text{leach}} = \frac{\text{FR}_{\text{leach}} \cdot p_0 \cdot \text{AREA}_s}{V_{\text{soilporewater}}}$	$6.25 \times 10^{-5} \text{ m}^3 \text{ m}^{-2}$
Dissolution	$k_{\text{dis}} = -\frac{\ln C_0/C_t}{t}$	$\frac{dC}{dt} = -k_{\text{dis}} C_0$
Hetero-aggregation	$k_{\text{agg}} = f_{\text{col}}(\text{NP}, \text{NC}) \cdot \alpha_{\text{agg,NP,NC}} \cdot N_{\text{nc}}$	$\frac{dC}{dt} = -k_{\text{het}} C_{\text{ss}} C_0$

estimate the total soil transport between soil and aerosols (eqn (7) and (8)), and then calculated the amount of NPs in the soil being transported.

$$Q_{\text{Tot}} = A \frac{p}{g} \sum_{u_*} u_* (u_*^2 - u_{*t}^2) \Delta T \quad (7)$$

$$F_a = Q_{\text{Tot}} K \quad (8)$$

where Q_{Tot} is the horizontal mass flux, F_a is the vertical mass flux (representing the mass of soil leaving the surface per unit of time), A is an acausal fitting parameter (typically 1), p denotes the air density, g denotes the gravitational acceleration, u_* denotes the wind shear rate, u_{*t} denotes the critical shear rate, and K is a constant. Strong winds blow, causing materials such as loose dust and gravel on the soil surface to be carried away, and fine-grained materials such as NPs will also be easily carried away, affecting the concentration of NPs in the soil. Although many models can simulate wind erosion, the calculation of wind erosion in the fate model requires dividing space and time, and there are few wind erosion models that can satisfy this requirement. As a result, it is necessary to improve the current wind erosion equation, while maintaining a good performance and applying it to the fate simulation of NPs.

4.4.2 Wet erosion. Water erosion (wet erosion) occurs when soil materials are separated and transported due to rainfall, runoff, irrigation, as well as snow and ice melt. The main factors that influence soil water erosion include rainfall characteristics, soil factors, topography, climate, and land use.⁶⁰ Based on these factors, the revised soil loss equation (RUSLE, eqn (9)) has been widely used in recent years to estimate soil loss due to water erosion,⁶¹ as follows:

$$A = R \times K \times \text{LS} \times C \times P \quad (9)$$

where R represents the erosive power of rainfall runoff, K represents the erosive power of soil, which determines the sensitivity of soil to erosion based on its texture and composition, LS is the slope length factor, representing the impact of slope steepness and length on erosion, C is the crop management factor, responding to the effect of agricultural and control practices on erosion, and P

represents the effect of support practices on the erosion rates. Soil loss can be assessed in the future using spatial distribution models such as WATEM/SEDEM,⁶² Limburg soil erosion model (LISEM),⁶³ and water erosion prediction project (WEPP) model.⁶⁴

4.4.3 Runoff. When the precipitation rate exceeds the rate of water infiltration into the soil or when the soil pores have been completely saturated, surface water that has not been infiltrated converges and flows to form surface runoff. Runoff allows for the transfer of NPs from surface soil to surface water, which is mainly influenced by factors such as topography, climate, and meteorology.⁶⁵ Methods that have been applied in fate models of NPs to calculate the runoff volume include the SCS runoff equation¹² and the CERF⁶⁶ model. The SCS runoff equation (eqn (10) and (11)) is based on the premise that the flow of water into and out of the system is equal, that is,

$$\text{Runoff} = \text{Rainfall} - \text{Losses} \quad (10)$$

$$Q = P - (I_a + F) \quad (11)$$

where Q denotes the amount of direct runoff, P is the amount of rainfall, I_a is the sum of all losses before runoff, and F is the amount of retention after runoff. CERF⁶⁶ is a regionalized rainfall runoff model for predicting river flow time series, and NanoFASE WSO model calculates runoff using the output of its section on runoff. Both calculations are good choices and can model runoff using data such as rainfall, and the output results vary with time. Researchers have started using deep learning, neural networks, *etc.* to estimate the runoff volume. For example, Kratzert *et al.*⁶⁷ simulated rainfall runoff using the long short-term memory (LSTM) network and predicted the runoff volume based on available data. As a result, in the future, emerging computational methods such as machine learning and neural networks can be applied to simulate processes in the fate model.

4.4.4 Transportation. Soil is a porous medium and the transport of NPs in soil depends on their particle size and pore size. The transport of NPs in saturated porous media can be described using the convective diffusion equation

(eqn (12)), which assumes no source and sink and is related to DLVO interactions:⁶⁸

$$\frac{\partial C}{\partial t} + u \cdot \nabla C = \nabla \left[D \cdot \nabla C + \frac{DC}{k_B t} \nabla \varphi_{DLVO} \right] \quad (12)$$

where C is the concentration of NPs and D is the diffusion coefficient of NPs. The DLVO theory can be used to evaluate the gravitational and repulsive potential interactions between NPs or between NPs and the pore surface of the rock, and φ_{DLVO} represents the total potential energy of the interaction. Soils are not all saturated, and in the case of partially saturated porous media, the soil saturation varies based on geographical location. Yechezkel *et al.*⁶⁹ investigated the transport of Ag NPs using column experiments and model simulations. Jayaraj *et al.*⁷⁰ developed a three-dimensional (3D) mathematical model to simulate the transport and retention of NPs in a partially saturated pore space with an angular cross-section. Studies on the transport of different forms of NPs (free particles as well as particles encapsulated by other substances) in porous media also highlight the importance of studying the fate of NPs in porous media such as soil.

4.4.5 Others. In addition to the above-mentioned processes, transport and transformation processes also occur in soil such as attachment, filtration, leaching, dissolution, and bioturbation. Firstly, through the process of diffusion and deposition, NPs may attach to the exposed soil surface. This process can be directly quantified using the attachment efficiency. Secondly, soil is a porous medium with narrow pores that can physically filter particles by forming wedges. This process is heavily influenced by particle size, with a significantly higher likelihood of large particles being stuck in the narrow pores. Subsequently, this portion of NPs is retained in the soil, and thus the retention is modeled as an irreversible first-order loss process. The amount of retention can also be determined through soil column experiments. The dissolution of NPs in soil water is calculated the same as in surface water. Consequently, the NPs dissolved in soil water will infiltrate with the water to deeper soils (*i.e.*, leaching), and then may be transferred to deeper soils. The attachment and retention of NPs on soil particles can significantly impact their concentration, and thus it is necessary to consider these processes. Furthermore, the movement of numerous soil organisms, such as

earthworms, through the soil also affects the distribution of NPs and may transfer NPs from unsaturated to saturated conditions. They also have the potential to take up NPs, causing changes in the concentration of NPs in the soil. Therefore, we suggest that future fate models of soil environments should consider these processes. In addition, researchers can also attempt to learn and employ processes from the well-studied aquatic environment.

4.5 NPs in the atmosphere environment

After NPs are released into the atmosphere, some particles will remain as free particles or form homogeneous aggregates with other particles, while others attach to aerosols to form heterogeneous aggregates. NPs in various forms may be suspended in the atmosphere or may undergo deposition, and be removed from the atmosphere to soil or surface water. Deposition in the atmosphere is classified as dry deposition and wet deposition, while wet deposition is associated with rainfall. SB4N divides the atmosphere into dry air and rainwater, and then wet deposition is considered as a process in the rainwater compartment. Since the number of NPs released into the atmosphere is small and their residence time is short compared to water and soil, some researchers do not focus on the fate of NPs in the atmosphere, and the multimedia model NanoFASE WSO model focuses only on water and soil. The size distribution and particle concentration of NPs in the atmosphere are primarily influenced by the environmental conditions such as atmospheric temperature, relative humidity (RH), and turbulence.⁷¹ In addition, photochemically induced reactions, mainly driven by free radicals, and UV radiation also play a role in transforming NPs in the atmosphere.²¹ The transport and transformation processes of NPs in the atmosphere in the model mainly include aggregation, attachment, advection, dry deposition, and wet deposition, and the detailed simulation equations for each process are listed in Table 4.

4.5.1 Dry deposition. The process of removing particles from the atmosphere through gravity settling, interception, impaction, diffusion, Brownian motion, and turbulence is known as dry deposition.^{72,73} The rate of dry deposition depends primarily on the gravitational settling velocity of the NPs, which is proportional to the diameter and density of the

Table 4 Equations usually used in different fate models for transformation and transport in the atmosphere environment. Table S4† provides the specific meanings of symbols

Air	SimpleBox4Nano	NanoFate
Dry deposition	First-order rate constant	$k_{\text{dep}} = \frac{2(\rho_p - \rho_a)}{9\mu} \times g \times R_p^2$
Wet deposition	First-order rate constant	
Advection		$Q_{\text{adv}} = V_w \times h \times \sqrt{a}$
Hetero-aggregation	$k_{\text{agg}} = f_{\text{coag(NP,nuc)}} \cdot \alpha_{\text{agg,NP,nuc}} \cdot N_{\text{nuc}} + f_{\text{coag(NP,acc)}} \cdot \alpha_{\text{agg,NP,acc}} \cdot N_{\text{acc}}$	$\frac{dC}{dt} = -k_{\text{het}} C_{\text{ss}} C_0$
Attachment	$k_{\text{att}} = f_{\text{coag(NP,coarse)}} \cdot \alpha_{\text{att,NP,coarse}} \cdot N_{\text{coarse}}$	

particles.⁷⁴ Stokes' law can be used to solve the deposition rate (eqn (13)), as follows:

$$k_{\text{dep}} = \frac{2(\rho_p - \rho_a)}{9\mu} \times g \times R_p^2 \quad (13)$$

where k_{dep} is the deposition rate, ρ_p is the density of aerosols or NPs, ρ_a is the density of air, μ is the dynamic viscosity of air, g is the acceleration of gravity, and R_p is the radius of the aerosol or the average radius of aggregation of NPs. The deposition rates calculated using this method are significantly impacted by the diameter and density of the aerosol, as well as the density and viscosity of the atmosphere, which can reflect regional specificity. SB4N calculates the dry deposition rate as a function of particle size and density (eqn (14)), as follows:

$$v = \frac{1}{R_A + R_s} + v_{\text{terminal}} \quad (14)$$

where R_A is aerodynamic resistance is caused by the resistance above the surface, which is different for land and water, R_s is surface resistance for atmospheric particles, which is determined by the efficiency of Brownian motion, interception and gravitational impact, and v_{terminal} is the terminal velocity of atmospheric particles. The two methods for calculating the deposition efficiency are similar, but SB4N assumes a fixed value for the drag force above the land and water surfaces, and therefore the rates obtained lack some dynamics compared to that obtained from Stokes' law.

4.5.2 Wet deposition. Wet deposition is the process of removing atmospheric particles associated with precipitation (rainfall or snowfall) through gravity settling, Brownian settling, and turbulent coalescence with water droplets.⁷² Wet deposition is the primary process for removing nanoscale particles from the atmosphere and is influenced by the intensity, frequency, and type of precipitation, as well as the properties of the particle. NanoFate calculates the wet deposition rates of free particles and heterogeneous aggregates separately. SB4N assumes the rate to be a first-order rate constant, and uses the precipitation rate to estimate the diameter of raindrops to determine the rate constant for the wet deposition of NPs from rainwater into soil or surface water. Given that rainwater is also a medium, some of the NPs are also dissolved in the raindrops, but the amount is very small. Thus, many studies choose to overlook this process. Furthermore, we can also use eqn (15) and (16) to simulate the wet deposition of NPs when constructing fate models.⁷⁵

$$k_w = \frac{3E(r_{\text{rain}}, r)P}{4r_{\text{rain}}} \quad (15)$$

$$p = 1 - e^{-k_w t} \quad (16)$$

where k_w is the scavenging coefficient, r_{rain} is the radius of a raindrop, r is the radius of NPs, $E(r_{\text{rain}}, r)$ is the collision efficiency, P is the rain intensity, p is the probability of wet

deposition of NPs and t is time. This method models the wet deposition of NPs as a random event, providing a more realistic simulation of the dynamic behavior of NPs, but the calculations become more complex.

4.6 Connections between compartments

After obtaining the rate constants describing the transport and transformation of NPs in each environmental compartment through the quantitative methods described above, it is necessary to link the processes in and between environmental compartments to obtain the final steady-state concentrations of NPs after their environmental fate. Researchers have mainly connected the above-mentioned processes through matrices^{10,35} or differential equations,^{12,22,25,26} and the representative models are SimpleBox4nano and NanoFate, respectively. SimpleBox4nano uses a matrix (eqn (17)) that consists of first-order rate constants for all relevant transport and transformation processes of NPs to relate emission concentrations, steady-state concentrations, and transfer processes, as follows:

$$m = -A^{-1}e \quad (17)$$

where m (kg) is a vector consisting of the steady-state mass of NPs in various forms (including free, aggregated, *etc.*) after their fate behavior in each environmental compartment, e (kg d⁻¹) consists of the mass of NPs in various forms released into each environmental compartment, and A (d⁻¹) denotes a matrix consisting of rate constants. NanoFate relates different environmental compartments by using a series of ordinary differential equations (eqn (18)), as follows:

$$\frac{dVC_i}{dt} = (K_{21} - K_{12}) \cdot C_2 + (K_{31} - K_{13}) \cdot C_3 + (K_{41} - K_{14}) \cdot C_4 - K_1 \cdot C_1 + Q_1 \quad (18)$$

where C_i (kg m⁻³) denotes the concentration of NPs in each compartment, V (m³) denotes the volume of the compartment, K_{ij} (m³ d⁻¹) denotes the rate constant for the transfer of NPs from compartment i to compartment j , K_i (m³ d⁻¹) denotes the rate constant for the transformation process (*e.g.*, dissolution) of NPs in compartment i , and Q_i (kg d⁻¹) denotes the emission of NPs per unit time in compartment i .

In fact, both computational methods essentially involve solving a set of equations to determine the steady-state concentrations of NPs in the environment, and both require the calculation of a series of rate constants and transfer coefficients as preparation. The difficulties associated with using the algebra solving computational method include the size of the data and the matrix inverse operation. Alternatively, solving a system of ordinary differential equations with multiple unknowns simultaneously is also challenging, but these computations can be performed using MATLAB. We believe that matrices are easier to solve than differential equations, but they are not dynamic enough. However, differential equations can reflect the changes in the concentrations of NPs over time in a flexible and time-effective manner. We also encourage researchers to use both

approaches to simulate the same area, enabling the comparison of their accuracy and complexity and improving the reliability of the final results. The simulation of fate is complete and the steady-state concentrations of NPs in each environmental compartment can be determined, which can then be used to assess the risk of NPs.

5. Challenges and future development in fate models for nanoparticles

5.1 Challenges and possible solutions

After conducting comprehensive research and analyzing past research results, we found that fate models still have six shortcomings, as follows: (i) the model framework is not ideal and it is challenging to simulate complex natural environments such as river networks and the junction of freshwater and seawater. Many models overlook these special environmental compartments, which makes the model unable to accurately reflect the situation and affects the accuracy of the simulation results. (ii) The fate models are still not dynamic enough. The flexibility of the model is limited by the fact that its parameters are mostly fixed constants (*e.g.*, first-order rate constants) and lack dynamic adjustment mechanisms. In addition, the continuity assumption and deterministic structure of the system of ordinary differential equations make it challenging to handle discrete events or sudden input changes directly. (iii) There is uncertainty in both the modeling framework and the input parameters. Uncertainties in the model framework mainly pertain to the formulas used for quantifying transport and transformation processes. Although most of these formulas have been approved by researchers, there are still uncertainties and these formulas should be continually optimized and improved. The input parameters of the model, which may have some deviations, include various physical and chemical parameters, as well as environmental parameters. (iv) It is challenging to achieve the same spatial and temporal resolution in simulation results as in observation results. Simulation results are often measured in days, whereas observation results can be measured in hours and minutes. Although it is possible to subdivide the individual environmental compartments into smaller sections, it may not accurately simulate the variation in concentrations with spatial location in the actual environment. As a result, the size of the data obtained through model simulation will be smaller than the size of the data obtained through actual observation. (v) Current researchers have not given enough attention to modeling the environmental fate of emerging NPs such as nanoplastics and nanopesticides. Many fate models for NPs are not applicable to them, and thus the assessment of their environmental risks is still lacking. Researchers have made some attempts to simulate the fate of nanoplastics, but little attention has been paid to nanopesticides, and their

specificity remains poorly understood. (vi) These models often lack comparative validation with actual data and only the simulation results of a few models are compared to previous studies. However, this comparison is often not on the same spatial and temporal scale, making the comparison results not reliable enough.

In response to these shortcomings, we may be able to take the following three approaches to address and supplement them. Firstly, based on the existing fate models and available parameters, we propose an optimal modeling process for simulating the fate of NPs, including environmental compartments such as water, sediment, atmosphere, and soil (Fig. 4). In the optimal process, based on the experience of past research and the compositional characteristics of the natural environment, the three largest environmental compartments (water and sediment, atmosphere, and soil) are further divided into eleven smaller environmental compartments, including air, aerosols, surface soil, deep soil, soil water, river and river sediment, lake and lake sediment, and ocean and ocean sediment. To improve the spatial resolution of the model, these small environmental

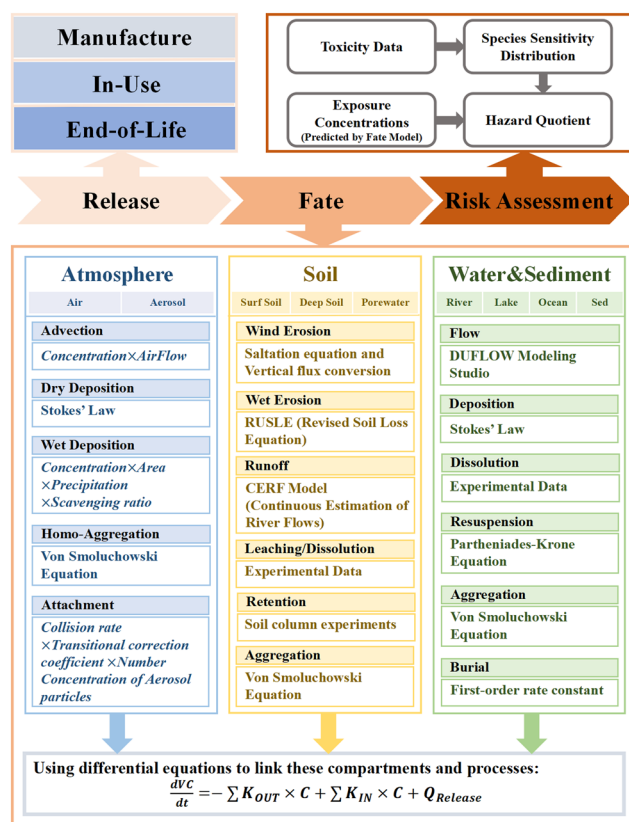


Fig. 4 Optimal choices for modeling transport and transformation processes and the fate of nanoparticles (NPs) in various environmental compartments, including the processes we recommend considering each compartment and their quantification methods. We also suggest that researchers use a system of differential equations to link different environmental compartments. The “×” in the figure represents the multiplication sign, “surf” represents surface, and “sed” represents sediment. The equations and models mentioned in this figure are also provided in the main text.

compartments are partitioned again into smaller subsections to simulate the transport and transformation processes of NPs in different environmental subsections, including aggregation, attachment, deposition, erosion, and advection. The final steady-state concentrations of NPs are calculated using a set of ordinary differential equations that link different environmental compartments. The species sensitivity distribution model and the hazard quotient method are also recommended for risk assessment.

Secondly, machine learning methods can be used to correct the simulation of the distribution of NPs in complex environments and refine the temporal and spatial units used in the simulation. In fact, machine learning methods have been used by researchers to assess the distribution of NPs in the environment. Money and Barton *et al.*⁷⁶ created an updated FINE model for predicting the concentration of Ag NPs in water. Bilal and Liu *et al.*⁷⁷ proposed a method for rapidly assessing the distribution of NPs based on Bayesian networks, which simulated the distribution of six NPs in eight regions based on simulated data obtained from the MendNano model based on a wide range of geographic and meteorological parameters, as well as the release rates of NPs into the main environmental compartments, such as water, air, and soil. These research results show that machine learning methods can help assess and predict the concentration of NPs in certain regions, and we can gain some inspiration from them. Besides, we can use machine learning to directly correct the model framework and parameters, and analyze the sensitivity of simulation results to different parameters, which not only reduces the uncertainty of the parameters but also helps us better understand the mechanism of the fate of NPs. For example, Yu and Zhao *et al.*⁷⁸ applied an interpretable model of the LightGBM algorithm with the RuleFit algorithm to investigate the interactions among nanomaterials, plants and soil, and then determined the effects of parameters such as metal oxide nanoparticle concentration, plant subclasses, clay content, and metal oxide nanoparticle composition on the uptake of NPs by roots through *post hoc* interpretation.

Thirdly, nanoplastics are distinct from classical NPs. Initially, plastic degradation needs to be modeled, and the second step is that the presence of biofilms needs to be considered. Furthermore, with reference to the seasonal distribution of microplastics, it may also be necessary to model the seasonal distribution of nanoplastics. Besseling and Quik *et al.*⁷⁹ improved the NanoDUFLOW model by considering the specificity of nanoplastics and using this spatially and temporally resolved hydrological model to simulate the fate of nanoplastics in a freshwater system, successfully predicting the exposure concentrations. In 2020, Sieber *et al.*⁸⁰ used a dynamic probabilistic material flow analysis to quantify the release of rubber particles from tire decomposition to the road, and subsequently into soil and surface water in Switzerland, which serves as a reference for simulating the release of nanoplastics. In 2021, Kim *et al.*⁸¹ developed a fate model that combined a flocculation

dynamics model to simulate the fate of nanoplastics in freshwater. Unfortunately, this model only considered changes due to vertical transfer (vertical transport and transformation) and did not take into account the effects of horizontal transfer (advection and diffusion). In 2022, Domercq *et al.*⁸² proposed a framework to simulate the transport and homing of nanoplastics in aquatic systems based on the model proposed by Praetorius *et al.* Nanoplastics of five particle sizes and four particle morphologies were considered. In 2023, Quik and Meesters *et al.*⁸³ improved the SimpleBox model by additionally accounting for plastic fragmentation and explication, as well as adapting the differential settling algorithm to explain that plastics with densities less than water do not settle, thus obtaining a multimedium model that can estimate the environmental fate of micro- and nano-plastics. Researchers have only focused on nanoplastics for a short period of time, and thus there may be processes (*e.g.*, flocculation) that have not been fully considered in models. Furthermore, there are many fate models for NPs that can be adapted to evaluate the fate of nanoplastics, and further development of fate models focused on nanoplastics is needed in the future. In the case of nanopesticides, it is crucial to first understand their properties, and then try to improve the models of NPs for the preliminary simulations of the fate of nanopesticides. In fact, there is still a long way to go in evaluating the fate of novel nanomaterials using models.

5.2 Future development and implication

(1) Adding more modules to the fate model. More modules may need to be added to improve fate models in the future, such as the diffusion process of NPs when they enter the environment. This is because most existing fate models assume that NPs are instantly dispersed after entering each environmental compartment, and thus the diffusion process of NPs can be considered to obtain a more accurate spatial and temporal distribution of NPs in each compartment. Besides, although fate models have already divided the entire natural environment into several parts, each compartment still needs to be further divided into more detailed compartments, such as in NanoFASE WSO model (rivers, soil, *etc.* are divided into smaller compartments), to improve the spatial resolution of the model.

(2) Tracking of the entire process model. NPs are released into the environment at every stage of their life cycle, from the time they are produced and put on the market, until they are scrapped at the end of their life. After entering the natural environment, NPs will undergo numerous physical and chemical reactions, be transported, transformed into other forms of particles, and eventually enter organisms to produce toxic effects. However, researchers often only consider a single process, such as the release process or the fate process, or the toxicity assessment process, and rarely connect these processes. There is no model that can track NPs throughout the entire process, leading to the

fragmentation of the various stages of risk assessment of NPs and making it difficult to simulate the full-process simulation of the real situation. Hence, there is an urgent need to develop multimedia fate models that can fully assess the full cycle of release, fate, and toxicity of NPs.

(3) Deeper application of machine learning in fate models.

Machine learning, as a branch of artificial intelligence technology, has been applied in various fields such as healthcare, finance, and transportation. In possible solutions, we also mentioned that machine learning can improve the spatio-temporal resolution of models and reduce the uncertainty of their structure and input parameters. Machine learning methods can also optimize the physical parameters of fate models, *i.e.*, selecting and correcting model parameters, expanding the scale of the data input to the model to improve the efficiency of the model simulation and analysis of the data, and helping the model to realize real-time analysis of the data and instant feedback. In addition, common interpretable models in machine learning can also promote the understanding of environmental fate mechanisms of NPs and the determination of the correlation between unknown parameters and the final results. Therefore, some difficulties that still exist in the fate models, such as the complexity and large-scale data, uncertainty in the model framework and parameters, and inadequate real-time dynamics of output results, can be addressed through machine learning methods. For instance, Bayesian inference is commonly applied to parameter estimation in systems of ordinary differential equations (ODEs).^{84,85} The core of some fate models is ODEs, and thus Bayesian inference can be used to estimate parameters and quantify their uncertainty. In the future, the application of machine learning in the development of fate models for NPs should be deeper, allowing a more comprehensive, efficient, and accurate simulation of the environmental fate of NPs.

6. Conclusion

This review provides a comprehensive overview and summary of the fate model of NPs, analyzed and discussed in-depth the factors affecting the fate of NPs in each compartment, and organized and discussed the calculation formulas and parameters of the transport and transformation processes of NPs. Our recommendations for researchers on the optimal modeling process to simulate the fate of NPs address questions such as how to reasonably divide environmental compartments, how to simulate the transport and transformation process of NPs in environmental compartments as realistically as possible, how to obtain reliable final steady-state concentrations of NPs, and how to conduct risk assessment. Although the fate models of NPs still face many challenges, it is expected that future fate models of NPs will be developed in a more comprehensive, detailed, and broader direction through continuous improvement and refinement. The parameters

of transport and transformation will be more detailed, the range of environmental systems will be more extensive, the input parameters and output results will be more dynamic, and the prediction results of the model will be more accurate and closer to the actual situation. Based on these findings, the environmental risk of NPs will be more accurately assessed.

Data availability

No primary research results, software or code have been included, and no new data were generated or analysed as part of this review.

Author contributions

Ruiyu Zhang: formal analysis, visualization, writing – original draft preparation, writing – review & editing. Xiaoxin Zheng: supervision, writing – review & editing. Wenhong Fan: supervision, writing – review & editing, funding acquisition. Xiangrui Wang, Tianhui Zhao, Xiaoli Zhao, Willie J. G. M. Peijnenburg, Martina G. Vijver: writing – review & editing. Ying Wang: conceptualization, supervision, writing – review & editing, funding acquisition.

Conflicts of interest

The authors declare that they have no actual or potential competing financial interests.

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