Transport of nanoparticles in porous media and associated environmental impact: a review.

YUSUF, E.O., AMBER, I., OFFICER, S. and OLUYEMI, G.F.

2024

© 2024 The Authors. Published by Elsevier B.V. on behalf of Kuwait University. This is an open access article under the CC BY license (<u>http://creativecommons.org/licenses/by/4.0/</u>).



This document was downloaded from https://openair.rgu.ac.uk



Contents lists available at ScienceDirect





Journal of Engineering Research

journal homepage: www.journals.elsevier.com/journal-of-engineering-research

Transport of nanoparticles in porous media and associated environmental impact: A review.



Esther O. Yusuf^{a,*}, Ityona Amber^a, Simon Officer^b, Gbenga F. Oluyemi^a

^a School of Engineering, Robert Gordon University, Aberdeen AB10 7GJ, United Kingdom

^b School of Pharmacy and Life Sciences, Robert Gordon University, Aberdeen AB10 7GJ, United Kingdom

ARTICLE INFO	A B S T R A C T	
Keywords: Nanoparticles Remediation Transport Environment Porous media	The release of nanoparticles into the environment occurs at different stages during their life cycle, with signif- icant harmful effects on the human (e.g., lung inflammation and heart problems) and the ecosystem (e.g., soil and groundwater contamination). While colloids (particles >1 micrometre) behaviour in porous media is influenced by filtration, nanoparticles (<100 nanometres) behaviour is driven by Brownian motion and quantum effects. Recognising these disparities is essential for applications like groundwater remediation and drug de- livery, enabling precise strategies based on the differing transport dynamics of colloids and nanoparticles. The extent of the impact of nanoparticle release on the environment is strongly influenced by their type, size, con- centration, and interaction with porous media. The main factor preventing the use of nanoparticles for envi- ronmental remediation and other related processes is the toxicity arising from their uncontrolled distribution beyond the application points. Finding a suitable dosing strategy for applying nanoparticles in porous media, necessary for the correct placement and deposition in target zones, is one of the significant challenges researchers and engineers face in advancing the use of nanoparticles for subsurface application. Thus, further studies are necessary to create a model-based strategy to prevent nanoparticle dispersion in a porous media. In general, this review explores the transport of nanoparticles in porous media concerning its application for environmental remediation. The aim of this study is captured under the following:	
	 a) Identifying the properties of nanoparticles and porous media to develop an innovative remediation approach to reclaim contaminated aquifers effectively. b) Identify critical parameters for modelling an effective strategy for nanoparticle-controlled deposition in porous media. This would require a general understanding of the onset and mapping of the different nanoparticle depositional mechanisms in porous media. c) Identify existing or closely related studies using model-based strategies for controlling particulate transport and dispersion in porous media, focusing on their shortcomings. 	

1. Introduction

Nanoparticles have emerged as promising materials for environmental remediation due to their unique properties (small size and large surface area) [44,54,15]. Nanoparticles are particles with a diameter between 1 and 100 nm; however, the term is sometimes used for larger particles, up to 500 nm or fibres and tubes less than 100 nm in only two directions. The use of nanoparticles in environmental remediation has been extensively studied in recent years, and various types of nanoparticles (e.g., iron oxide and silver nanoparticles) have been developed for different applications, such as removing heavy metals in aquifers and wastewater treatment. Nanoremediation is an emerging industry with documented application covering numerous US and European clean-up sites [24]. Nanoremediation is widely used for groundwater treatment, with additional extensive research being carried out for wastewater treatment [44,15]. Some nano-remediation methods, particularly nano-zerovalent iron for groundwater clean-up, have been deployed at full-scale clean-up sites, while other methods remain in research phases [44]. Iron-based nanoparticles are one of the most widely used for environmental remediation due to their high surface area and ability to

* Corresponding author. E-mail address: e.yusuf@rgu.ac.uk (E.O. Yusuf).

https://doi.org/10.1016/j.jer.2024.01.006

Received 27 July 2023; Received in revised form 3 January 2024; Accepted 4 January 2024 Available online 9 January 2024 2307 1977 (© 2024 The Authors – Published by Elevier B.V. on behalf of Kuwait Univ

^{2307-1877/© 2024} The Authors. Published by Elsevier B.V. on behalf of Kuwait University. This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/).

oxidise and reduce multiple pollutants. They are effective in the degradation of dyes and the removal of nitrate, hexavalent chromium, arsenate, arsenite, and total phosphates [34,15,78]. Other types of nanoparticles have also been investigated for environmental remediation, such as Co₃O₄ nanoparticles that have shown potential for the environmental remediation of antibiotic-resistant and pathogenic bacteria [9]. Metal and semiconductor nanoparticles (e.g., zinc oxide nanoparticles) have been fabricated for environmental remediation applications, particularly groundwater [55].

The effectiveness of nanoparticles in environmental remediation depends on several factors, including the in-situ location, the type of pollutants to be treated, and the specific nanoparticles used [13]. However, despite the promising results obtained in laboratory studies, the use of nanoparticles in environmental remediation is still limited to laboratory setups. Therefore, there is a need for more practical field testing on using nanoparticles for environmental remediation and quantifying any associated impacts [79]., Using nanoparticles in environmental remediation would inevitably lead to the release of nanoparticles into the environment and subsequent ecosystems, raising concerns about nanoparticles' potential environmental impact. Recently, the European Union (EU) commissioned a study on the application of nanoparticles for environmental remediation, which focussed on facilitating practical, safe, economic, and exploitable nanotechnology for in situ remediation [24]. This study was commissioned out of concern relating to the potential environmental impact of nanoparticles acting as a secondary source of contamination, especially in soils or porous media and aquifers, which serve as portable drinking water sources. Therefore, it is essential to carefully evaluate the potential environmental impact of nanoparticles before their widespread use in environmental remediation [13,15,78].

The transport of nanoparticles in porous media is still of considerable concern, with the large-scale application of nanoparticles (such as field tests or application) for remediation or subsurface applications likely to result in their abundant release and retention. This is a cause of concern, and the reason for this can be examined from two perspectives:

- a) Using nanoparticles for subsurface application can lead to an undesirable distribution of the particles beyond the points of interest, potentially migrating into groundwater aquifers [11,15,71,89].
- b) The transport of nanoparticles in porous media is often accompanied by retention, which can occur through different mechanisms such as entrapment, ripening, adsorption, aggregation, blocking, straining, attachment and detachment, as shown in Fig. 1 below [44,87].
- c) The controlled emplacement in porous media of nanoparticles requires an in-depth understanding of nanoparticle properties, properties of porous media, fluid, and the interplay of these factors (nanoparticles, porous media, and liquid).

Given that these nanoparticles can be toxic, they can become a source of environmental contamination. Currently, in subsurface water, nanoparticles of various types have been discovered, ranging in concentration from micrograms to picograms per litre, and size, from tens to hundreds of nanometres [41,44]. For example, in Europe, the silver and titanium oxide nanoparticles' concentration in subsurface water was detected to be 1.5 ng/L and 2.2 μ g/L, respectively [44]. The concentrations of silver nanoparticles in the Isar River in Germany and Dutch water were estimated at 8.6 and 0.8 ng/L, respectively [44]. Due to concerns about the uncontrolled migration of nanoparticles, the application of nanoparticles for subsurface applications such as nanoremediation has been restricted in the United Kingdom [11]. However, the environmental application of nanoparticles at a field scale is already standard practice in the USA and some countries in the EU despite its toxic nature [11]. In the case of groundwater remediation, the deposition of nanoparticles is considered favourable as the retained nanoparticles would not act as secondary carriers for existing pollutants [67]. In other words, contaminants (such as heavy metals) attached to the nanoparticles would remain trapped with the particles on the retention sites in the porous media while ensuring that the groundwater aquifer is free from heavy metals. However, the conditions in a porous media may change over time, leading to the detachment of nanoparticles and the attached pollutants or the complete separation of the contaminants back into the aquifer system [35,44]. For example, an increase in the pH of a porous media containing migrating polystyrene nano-plastics would



Fig. 1. Retention mechanisms associated with the transport of nanoparticles in porous media [44].

lead to greater electrostatic repulsion between the nanoparticles and nanoparticle-porous media interaction [44,59]. Under these circumstances, there would be a reduction in the attachment or retention of nanoparticles onto the porous media surface. Thus, the retained nanoparticles would eventually be released back into the main flow stream in the porous media. Therefore, the challenge faced by researchers and engineers to advance the use of nanoparticles for subsurface application is finding a suitable dosing strategy for the application of nanoparticles in porous media, which is necessary for the correct emplacement and deposition of nanoparticles in target zones [44,15,87]. The rest of the paper will focus on the following:

- a) Discussion of nanoparticle transport in porous media the effect of nanoparticle size and concentration, mechanism of nanoparticle retention and impact of physiochemical conditions of the porous media on retention.
- b) Nanoremediation and the potential release of nanoparticles and secondary contamination of the environment.

2. Transport of nanoparticles in porous media

Understanding nanoparticles' transport in porous media is crucial in designing and operating an effective environmental remediation strategy. When using in situ nano-remediation, the design and effectiveness of the remediation strategy are considered for two reasons:

- a) The nanoparticles employed might be more harmful or mobile than the parent compound.
- b) The fate of the nanoparticles during in situ transport can affect the effectiveness and cost of the remediation process.

2.1. Deposition dependency on nanoparticle size

The effect of nanoparticle size on nanoparticle retention in porous

media is influenced by various factors such as particle-collector interaction, surface chemistry, and solution chemistry. Experimental results suggest that particle size may not significantly affect deposition in clean bed filtration under unfavourable deposition conditions [61]. However, nanoscale particle dimensions can favour aggregation kinetics, altering the transport and retention of nanoparticles in porous media [73]. Physical and true filtration impeded the transport of nanoparticles in porous media [26]. Surface potential and aggregate size dominate nanoparticle interactions with each other and surfaces, affecting their transport and retention in porous media [33]. The impact of mean collector grain size on nanoparticle retention has been studied, showing that nanoparticles can travel through porous media of different sizes [49]. Similarly, Mattison et al. [49] investigated the mobility of multi-walled carbon nanotubes (MWCNTs) through porous media. They found that MWCNTs travelled through porous media of varying grain sizes, resulting in significant retention. On the other hand, Lin et al. [43] found that the transport properties of iron oxide nanoparticles through sand and soil columns were poor for particles with diameters of 30-100 nm compared to larger particles. These studies highlight the complex interplay between nanoparticle size and porous media characteristics in determining retention. Furthermore, Shaniv et al. [70] studied the relationship between the size of polystyrene nanoparticles (PS-NPs) and their retention in porous media, as shown in Fig. 2. The study showed that size and surface functional groups affect the transport of PS-NPs through saturated soil. Unmodified 110 nm and 50 nm PS-NPs demonstrated similar transport patterns in the soil. However, a maximum elution value of 90% from the soil was found for the 50 nm PS-NPs, compared to a maximum value of \sim 45% for 110 nm PS-NPs. The breakthrough curve for 190 nm PS-NPs demonstrated a maximum % elution value of 60% from the soil. PS-NPs with surface functional groups display different mobility profiles: carboxylated PS-NPs demonstrated a plateau of 40% elution from the soil. In contrast, aminated PS-NPs were eluted only in small amounts and showed a spike elution pattern from the column. These findings are attributed to the effects of common soil constituents, such as calcium cations and humic



Fig. 2. Illustration of the relationship between the size of PS-NPs and the retention type in porous media [70].

acids, on the size and charge of the PS-NPs with surface functional groups. Overall, PS-NP mobility in the soil can vary widely, depending on PNP properties, such as size and surface chemistry and matrix properties, such as the type of porous medium and its composition. These findings suggest that knowledge of inherent characteristics (size, surface charge, surface functional groups) of PNPs is required to elucidate the behaviour of such particles in soil-water environments. Further research is needed to fully understand and predict the impact of nanoparticle size on retention in porous media, as understanding the relationship between nanoparticle size and retention can help map the different types of retention mechanisms in porous media.

Different studies on nanoparticle retention and deposition mechanisms in porous media have attempted to map nanoparticle retention mechanisms, as Bianco et al. [15] and Ling et al. [44] reported. However, such procedures for mapping nanoparticle retention mechanisms over various environmental water chemistries and nanoparticle properties have been considered impracticable due to their cumbersome and time-consuming nature [45,83]. Thus, the current interest lies in generalising nanoparticle retention behaviour, focusing on aggregation/accumulation of the flowing particles. This is evident in models such as the one-dimensional form of the advection-dispersion-reaction equation in Eqs. (1) to (3), which are fitted to the effluent concentration profile of nanoparticles exiting a porous media with a parameter dedicated to particle aggregation.

$$\frac{dC}{dt} + \frac{\rho_{b}}{\theta_{W}} \left(\frac{dS_{1}}{dt} + \frac{dS_{2}}{dt} \right) = D \frac{\partial^{2}C}{\partial x^{2}} - v \frac{dC}{dx}$$
(1)

$$\frac{\rho_{b}}{\theta_{W}}\left(\frac{dS_{1}}{dt}\right) = k_{att1}C - k_{det}\rho_{b}S_{1}$$
⁽²⁾

$$\frac{\rho_{b}}{\theta_{W}}\left(\frac{dS_{2}}{dt}\right) = k_{att2}C$$
(3)

Where *C* is the nanoparticle concentration, ρ_b is the porous media bulk density, θ_W is the dimensionless volumetric water content, S_1 and S_2 are the concentrations of nanoparticles attached to the surface of the porous media, k_{att1} and k_{att2} are the attachment coefficient, k_{det} is the detachment coefficient and *D* is the coefficient of hydrodynamic dispersion. The parameter k_{att} is used to generalise the retention of nanoparticles in porous media. However, this does not indicate the size dependency of nanoparticle retention or the various types of retention taking place. Therefore, while this approach of fitting Eq. (1) to the effluent profile of nanoparticles simplifies the study of nanoparticle fate or behaviour in porous media, this k_{att} parameter does not account for the following:

- a) The type of aggregation between nanoparticles in porous media homoaggregation or heteroaggregation.
- b) The relationship between the type of nanoparticle deposition in the porous media and the aggregation type.

Besides the aggregation type, incorporating other retention mechanisms is crucial in understanding the relationship between aggregation and deposition in porous media. However, in general, the understanding of the role of nanoparticle size in the detailed mapping of the depositional and retention mechanism in porous media is limited.

Furthermore, solution chemistry, including ionic strength and valence, affects nanoparticle aggregates' electrokinetic properties and the extent of their transport and retention in porous media [18]. Adsorption onto solid surfaces can impede nanoparticle transport, and the choice of polymer coatings can affect nanoparticle adsorption and retardation in porous media [69]. Particle-solid interactions, including van der Waals attraction and electrostatic repulsion forces, control the adsorption of stable nanoparticles in porous media [88]. The surface modifiers of nanoparticles can stabilise their transport in granular porous media [62].

2.2. Mechanism of nanoparticle transport and deposition in porous media

The transport of nanoparticles in porous media is significantly affected by the material composition of the media, pore structure and material grain size [44]. The material makeup (sand or carbonate) of the porous media may hinder the deep propagation of nanoparticles through various deposition mechanisms such as blocking, straining, and preferential flow, thus controlling the deposition of nanoparticles. Ly et al. [47] conducted a comparative analysis of the transport of titanium oxide nanoparticles in homogeneous and heterogeneous columns. The homogeneous column was made of fine sand, while the heterogeneous column was a coarse and fine sand mix. It was observed that the titanium oxide nanoparticles had a higher penetration rate and transport speed in the heterogenous column due to the effect of preferential flow. This preferential flow of nanoparticles in a heterogenous column was also investigated by Chen et al. [16,17]. However, Chen et al. [16,17] carried out their work using a layered heterogeneous column (also consisting of coarse and fine sand) to study the transport of graphene oxide nanoparticles. It was observed that the graphene oxide nanoparticles remained mainly at the boundary of the coarse-fine sand, which indicated that particle transfer in a porous media consisting of coarse and fine sand would be detrimental to the transport of the graphene oxide nanoparticles. This outcome was in contrast to the findings of Lv et al. [47] on the effect of porous media heterogeneity on nanoparticle deposition. These contrasting results could be due to the type and properties of the nanoparticles employed (titanium oxide and graphene oxide) since similar heterogeneous porous media was used [75]. A similar work carried out by Chrysikopoulos and Fountouli [20] investigated the simultaneous transport of titanium dioxide (TiO₂) nanoparticles and formaldehyde (FA) in quartz sand-packed columns under water-saturated and unsaturated conditions. Their results showed TiO2 retention occurred in both scenarios, influenced by flow rate and solution ionic strength. However, in water-saturated columns, TiO2 mass recoveries rose with the flow rate. Furthermore, their co-transport experiments showed no distinct relationship between mass recoveries and flow rate. Also, Formaldehyde transport was hindered by TiO₂ presence, especially at high ionic strength. The study provides valuable insights into the fate and transport of TiO2 nanoparticles and FA in porous media, vital for environmental risk assessment. In another study by Sotirelis & Chrysikopoulos [74] and Syngouna et al. [77], the dynamic interaction of graphene oxide nanoparticles with quartz sand and montmorillonite (MMT) colloids at pH 7 and ionic strength of 2 mM was explored. It was observed that MMT's kinetic attachment to quartz sand is minimally affected by pH. At the same time, graphene oxide nanoparticles attach more to MMT than quartz sand, with the coexistence enhancing the total graphene oxide nanoparticles' mass on quartz sand and MMT. The authors' findings strengthen the understanding of graphene oxide nanoparticles' behaviour in subsurface formations, especially in the presence of colloids, which is vital for designing efficient environmental remediation strategies. Nonetheless, the effect of the degree of heterogeneity of porous media on nanoparticle's controlled emplacement in a target location needs to be well studied. Most of the reported works on nanoparticle-controlled deposition have focused on homogenous porous media, which have some level of heterogeneity. Changes in porous media properties, such as grain size and pore structure, have been reported to impact permeability and porosity, directly influencing nanoparticle transport [76,84]. Chen et al. [19] and Velimirovic et al. [82] elucidated this impact on permeability and porosity, which showed that nanoparticles favourably flow in zones with high permeabilities. Velimirovic et al. [82] reported using a column of coarse sand with 40% porosity to study the transport of nanoparticles. The transport rates were observed to be higher, positively correlated with the porosity and permeability of the porous media. However, the work of Chen et al. [19] was carried out in a fractured porous media with the pressure at the entry point increasing due to low permeability resulting in a significant anisotropy preventing further nanoparticle transport in the media.

Furthermore, it was observed by the authors that injecting nanoparticles whose size was equal to the medium grain size leads to trapping of these particles by blocking or straining, which leads to reduced permeability. The phenomenon of blocking and straining are just a couple of the mechanisms by which nanoparticles are retained, and this can be grouped further into "nanoparticle-nanoparticle" and "nanoparticle-pore" interactions (Fig. 3); however, exploring how the relationship between nanoparticle size and pore size can be used to map and distinguish this retention type from others needs to be better understood.

Most research on the mechanisms of nanoparticle deposition in porous media has yet to be able to capture and quantify all known mechanisms for nano-deposition. Meng & Yang [51] reviewed the nanoparticle transport phenomena in porous media and identified the filtration mechanisms, the underlying interaction forces, and the factors dominating nanoparticle transport behaviour in porous media. They found that various factors, including the size and shape of the nanoparticles, the properties of the porous media, and the flow conditions influence the transport of nanoparticles in porous media. In addition, Meng & Yang [51] reported that the filtration mechanisms by which nanoparticles are deposited include straining, interception, and diffusion. However, this filtration mechanism must give a holistic picture of all known interaction mechanisms of nanoparticles in porous media.

The various mathematical modelling of nanoparticle deposition in porous media has consistently accounted for the different types of deposition mechanisms using a single kinetic term. According to Loria et al. [46] and Dowd et al. [22], the transport of nanoparticles in porous media can be described by a convective-dispersive mass-transfer equation (see Eqs. (1) to (3)) that includes a kinetic term for first-order particle deposition. The convective term represents the transport of nanoparticles due to the fluid flow, while the dispersive term represents the spreading of nanoparticles due to diffusion. The kinetic term means the deposition of nanoparticles onto the porous media surface. The deposition rate is proportional to the concentration of nanoparticles and the surface area of the porous media. According to the authors, the general kinetic term was used to capture all known mechanisms of nanoparticle deposition and is obtained when such models are fitted to the breakthrough curve generated from the concentrations of nanoparticle effluent exiting the porous media. This tends to limit the understanding of the role the pore structure of the porous media plays in shaping the various types of retention mechanisms of nanoparticles. Furthermore, Wu and Schwartz [86] found that multiple factors, including the size and shape of the nanoparticles, the pore structure of the media, and the flow conditions influence the transport of nanoparticles in porous media. They established that pore accessibility and cavity escape are essential factors limiting nanoparticle transport in porous media. However, their work needs to be done using the understanding of the pore structure in mapping the various deposition mechanisms of nanoparticles in porous media. A similar knowledge concerning the formation of aggregates in flowing suspension of nanoparticles in porous media based on changing particle size can distinguish aggregates formed from those trapped and retained. Therefore, the nanoparticle, rock grain, and pore size can map the various retention mechanisms, such as blocking, straining, adsorption etc., that occur during transport in porous media. This review found that although there is limited understanding of the mapping of nanoparticle retention mechanisms, a complete understanding would ensure the following:

- a) An understanding of the relative occurrence of nanoparticle retention types and prediction of the time and location of occurrence in a porous media.
- b) Determination of the conditions that control the relative occurrence of the various retention types in a porous media.
- c) Developing a strategy to control nanoparticle deposition in porous media using understanding (a) and (b).

Bianco et al. [15] pointed out that the approach for the controlled deposition or retention of nanoparticles for heavy metal removal would only make economic sense if the retained nanoparticles having contaminants adsorbed on them were immobilised entirely at the point of deposition. This will prevent the deposited nanoparticles from acting as a secondary source of contamination if they are desorbed from the surface of the porous media.

2.3. Modelling the controlled deposition of nanoparticles in porous media

Modelling the controlled deposition of nanoparticles in porous media is crucial for understanding their transport properties and assessing their efficacy and environmental impact in various applications [61]. The transport and deposition of nanoparticles in porous media are influenced by several factors, including flow rate, surface chemistry, size, particle-collector interaction, pH, and ionic strength([27,61,73,33,49, 40,92,93]; Tosco et al., 2012; Xiao et al., 2011; [12]; He et al., 2009; Bradford & Torkzaban, 2015; Fei et al., 2022; Zhou et al., 2023; Fan et al., 2022; Ruo et al., 2022; Huang et al., 2023; Junin & Gbadamosi, 2018; [37,85]; Liao et al., 2023; Reguera et al., 2022; Patino et al.,



Fig. 3. Interaction mechanisms of nanoparticles with porous media [68].

2020). The classical filtration theory is often used to model the transport of nanoparticles in porous media. According to this theory, the retention of nanoparticles in porous media can be attributed to three mechanisms: direct interaction of nanoparticles with the media (interception), sedimentation due to gravity, and diffusion due to Brownian motion [92]. However, experimental results have shown that other factors, such as particle-collector interaction and pH, also play significant roles in nanoparticle transport and deposition [61,33].

The size and concentration of nanoparticles can affect their transport in porous media. Studies have shown that particle size distribution, concentration, and magnetic attraction can influence the transport of nanoparticles in sand columns [61]. Additionally, the stability of nanoparticle dispersions in aqueous suspensions, which is governed by solution pH and ionic strength, can impact the mobility, aggregation, and deposition of nanoparticles in porous media [73]. In addition, the surface potential of nanoparticles and the pH of the solution can also influence their aggregation and transport in porous media. Research has demonstrated that surface potential and aggregate size dominate nanoparticle interactions with each other and surfaces, and pH can affect the size distributions of nanoparticle aggregates [33]. Furthermore, nanoparticles have been shown to inhibit precipitation and deposition and enhance perdurability against asphaltene damage in porous media [27]. The mobility of nanoparticles in porous media is influenced by their physical properties and the characteristics of the porous media itself. The grain size of the porous media can impact the transport of nanoparticles, as demonstrated by studies on the impact of porous media grain size on the transport of multi-walled carbon nanotubes [49]. Moreover, the porous media's heterogeneity, roughness, and pore water velocity can affect the retention and release of colloids and nanoparticles (Bradford & Torkzaban, 2015; Fan et al., 2022).

Numerical simulation and mathematical modelling have been employed to gain insights into the behaviour of nanoparticles in porous media. Continuum-based models (Table 1) have been developed to describe the transport of nanoparticles in porous media and account for various transport mechanisms, such as irreversible deposition, attachment/detachment, agglomeration, physical straining, site-blocking, ripening, and size exclusion [12].

These models have successfully described the simultaneous occurrence of multiple transport mechanisms and can be scaled across different experimental setups and aquifers [12]. For example, Katzourakis and Chrysikopoulos [38] developed a model investigating nanoparticle migration in porous media by incorporating Smoluchowski's

Table 1

Continuum models used for describing nanoparticle transport in porous media [12].

Transport Model	Mechanisms	Fitting Parameters
$\frac{\rho_b}{\theta_W} \left(\frac{dS}{dt} \right) = k_{att} C$	Attachment	k _{att}
$\frac{\rho_b}{\theta_W} \left(\frac{dS}{dt} \right) = k_{att} C - \frac{\rho_b}{\theta_W} k_{det} S$	Attachment/Detachment	k _{att} , k _{det}
$\frac{\rho_{\rm b}}{\theta_{\rm W}} \left(\frac{{\rm d}S}{{\rm d}t} \right) = {\rm k}_{\rm att} {\rm C} - \frac{\rho_{\rm b}}{\theta_{\rm W}} f_r {\rm k}_{\rm det} {\rm S}$	Attachment and dual site detachment	k_{att}, k_{det}, f_r
$dS dS_1 dS_2$	Dual site attachment/	katt1, katt2, kdet1,
$\frac{dt}{dt} = \frac{dt}{dt} + \frac{dt}{dt}$	detachment	k _{det2}
$\frac{\rho_b}{\theta_W} \left(\frac{dS_1}{dt} \right) = k_{att1} C - k_{det1} \rho_b S_1$		
$\frac{\rho_b}{\theta_W} \left(\frac{dS_2}{dt} \right) = k_{att2} C - k_{det2} \rho_b S_2 \label{eq:eq:electropy}$		
$\frac{\mathrm{d}\mathbf{C}}{\mathrm{d}\mathbf{t}}\left(1+\frac{\rho_{\mathrm{b}}}{\theta_{\mathrm{W}}}K_{d}\right) = \mathbf{D}\frac{\partial^{2}\mathbf{C}}{\partial x^{2}} - \mathbf{v}\frac{\mathrm{d}\mathbf{C}}{\mathrm{d}x}$	Attachment, adsorption (retardation)	k _{att} , <i>K</i> _d
$+\mathbf{k}_{att}\mathbf{C}$	Dalaana (taa aa taalaatiaa	1 (
$\frac{\rho_{\rm b}}{\theta_{\rm W}} \left(\frac{{\rm d}S}{{\rm d}t} \right) =$	Release after perturbation	K _{rel} , J _{nr}
$\mathbf{k}_{rel}\frac{\rho_{\mathbf{b}}}{\theta_{\mathbf{W}}}\left(\mathbf{S}\!-\!\mathbf{S}_{\mathbf{eq}}\right)\!\boldsymbol{H}_{o}\left(\mathbf{S}\!-\!\mathbf{S}_{\mathbf{eq}}\right)$		
$\mathbf{S}_{eq} = f_{nr} \mathbf{S}_i$		

population balance equation and the advection-dispersion-attachment equation. The model considers nanoparticle collisions, leading to aggregated structures with varying mobility and reactivity. Particles may be suspended or attached to the solid matrix reversibly or irreversibly. Simulation results revealed exponential aggregation with increasing initial particle number and emphasise the influence of the initial particle diameter distribution on aggregate size and mobility. The model underscores the critical importance of considering realistic initial conditions for understanding nanoparticle behaviour in porous media, contributing to a comprehensive understanding of their transport dynamics.

However, these models used to study particle retention in porous media have certain limitations that should be considered. One limitation is using single-fitting parameters to describe the multiple retention mechanisms. Also, the models depicted in Table 1 only fit specific mechanisms, meaning that accurate modelling of the various mechanisms of nanoparticle retention would require more than one equation, which would require significant computing time and power. A further limitation is the assumption of idealised conditions in the models. Many models assume uniform and homogeneous porous media, neglecting the heterogeneity and complexity of real-world porous media [52]. This simplification may not accurately represent particles' transport and retention behaviour in natural systems. The heterogeneity of porous media can significantly affect particle deposition and retention, and neglecting this aspect can lead to inaccurate predictions [81]. Another limitation is the assumption of favourable colloid/collector interactions in some models. These models may need to adequately capture the behaviour of particles under unfavourable conditions, where significant particle deposition and retention can occur [52].

The interactions between particles and the porous media can be influenced by factors such as pH, ionic strength, and surface charge heterogeneity, which are only sometimes considered in the models [32]. The models also often assume that particle deposition follows exponential decay with travel distance, which may only sometimes be true. Laboratory-scale column experiments have shown that the retained particle profiles can decay non exponentially, indicating the presence of heterogeneity in the interactions between particles and sediment grains [81]. Incorporating this variability into the models can improve their accuracy in predicting particle deposition and retention [81]. Furthermore, the models may need to fully account for the effects of particle size, concentration, and surface chemistry on particle transport and retention. Experimental studies have shown that these factors can significantly influence the fate and transport of particles in porous media [83,91]. Neglecting these factors in the models can lead to inaccurate predictions of particle behaviour. Additionally, the models may not consider the influence of physicochemical conditions on particle transport in porous media. The physicochemical properties of particles and the surrounding fluid can affect their interactions with the porous media and influence their transport behaviour [31]. Current models often need more mechanistic insights to predict nanoparticle transport under different physicochemical conditions [31]. Moreover, the models may need to capture nanoparticles' complex behaviour in porous media fully. The transport of nanoparticles can be influenced by various factors, including aggregation, straining, and surface interactions [63,80]. Current models often rely on empirical parameters and may not comprehensively understand nanoparticle transport in porous media [31].

2.4. The effect of physiochemical conditions on the deposition of nanoparticles

Various physiochemical conditions influence the transport of nanoparticles in porous media. Several studies have investigated the effects of different factors on nanoparticle transport and deposition in porous media. One crucial factor that affects nanoparticle transport is solution chemistry. The ionic strength of the solution has been found to have a significant impact on nanoparticle deposition. For example, Jin et al. [36] studied the transport and deposition behaviour of single-walled carbon nanotubes (SWNTs) in a porous medium. They found that increasing solution ionic strength resulted in increased SWNT deposition. Similarly, Chen et al. [18] investigated the transport and retention kinetics of titanium dioxide (TiO2) nanoparticles in saturated porous media. They found that solution chemistry, precisely ionic strength and ion valence, influenced the electrokinetic properties of the nanoparticles and the resulting extent of nanoparticle transport and retention. The presence of other ions in the solution can also affect nanoparticle transport. Lewinski et al. [42] discussed the cytotoxicity of nanoparticles and highlighted the importance of understanding the properties of nanoparticles and their effect on the body before clinical use. Lecoanet & Wiesner [40] compared the transport of fullerenes and oxide nanoparticles in a porous medium and found that despite significant differences in surface chemistry and size, the fullerenes exhibited similar breakthrough behaviour at higher flow rates. The surface properties of nanoparticles also play a crucial role in their transport in porous media. The hydrophobicity of nanoparticles can impact their transport and retention. Mayegowda et al. [50] investigated the effect of the hydrophobicity of fluorescent carbon nanoparticles on transport in porous media. They found that temperature-sensitive hydrophobicity influenced the transport and retention of carbon-based nanoparticles. Guzman et al. [33] studied the influence of surface potential on the aggregation and transport of titania nanoparticles. They found that surface potential and aggregate size dominated nanoparticle interactions with each other and surfaces. Flow rate is another critical factor that affects nanoparticle transport in porous media. Lecoanet and Wiesner [40] observed that the transport of fullerenes and oxide nanoparticles in a porous medium exhibited different breakthrough behaviour at different flow rates. Solovitch et al. [73] investigated the concurrent aggregation and deposition of TiO2 nanoparticles in a sandy porous medium and found that flow rate influenced nanoparticle deposition and mobility. The physicochemical parameters of solution chemistry, such as pH and the presence of natural organic matter, can also influence nanoparticle deposition and mobility in porous media. Solovitch et al. [73] mentioned that these parameters control particle aggregation, which may subsequently influence the balance between the free migration of particles and deposition. Afolabi & Yusuf [3] discussed the use of nanoparticles to inhibit asphaltene damage and highlighted the importance of understanding the impact of nanoparticles on asphaltene deposition. The grain size of the porous media can also affect nanoparticle transport. Zhang et al. [90] mentioned that nanoparticle retention is expected to increase in finer-grained porous media, although some studies have indicated that grain size has little effect on nanoparticle transport. In summary, the transport of nanoparticles in porous media is influenced by various physicochemical conditions, including solution chemistry, surface properties of nanoparticles, flow rate, and

the physicochemical parameters of solution chemistry. Understanding these factors is crucial for predicting and controlling nanoparticle transport in porous media.

3. Nano-remediation and potential impact of secondary contamination

Nanoremediation is an innovative and promising technology that utilises nanomaterials for the remediation of environmental pollutants in various matrices such as soil, water, and air. It involves the application of reactive nanomaterials to transform and detoxify pollutants, leading to the purification of water and air resources, as shown in Fig. 4 [30].

Nanomaterials have gained attention in the field of remediation due to their unique properties, including their small size, high surface areato-volume ratio, and functionalizable surfaces, which enable high reactivity, targeting of specific species, and efficient transport for in situ application [5,2,56]. One of the key advantages of nanoremediation is its potential cost-effectiveness compared to traditional remediation methods. It offers more efficient and rapid removal of pollutants, reducing the overall costs associated with remediation processes [29,7]. Nanoremediation has been proposed as a more cost-effective technology for in situ soil and groundwater remediation, addressing site remediation challenges and improving overall efficiency [53]. It can potentially provide a new and effective solution for environmental clean-up, playing a significant role in pollution prevention, detection, monitoring, and remediation [60]. Nanoremediation techniques employ various types of nanomaterials, including nanoscale zero-valent iron (nZVI), carbon nanotubes (CNTs), metallic nanoparticles, magnetic nanoparticles, and graphene oxide nanoparticles (nGOx) [8]. These nanomaterials have been extensively studied and applied in the remediation of contaminants such as heavy metals, organic pollutants, and petroleum compounds [14,4]. For example, nZVI has been widely used to remediate groundwater contaminated with chlorinated solvents and heavy metals [28]. nGOx has shown effectiveness in reducing or increasing the availability of arsenic and metals in polluted soils [14]. However, it is important to consider the potential risks associated with nanoremediation. Nanomaterials should not pose any additional environmental or human health risks [21,58,57]. The environmental impact of micro/nanomachines and nanomaterials should be thoroughly assessed to ensure their safety and minimise any negative effects [30]. The potential risks of nanoremediation include mobilising nanoparticles in interstitial waters and the water column, which may pose a risk to marine biota [21,57]. Additionally, the interaction between nanomaterials, microorganisms, and contaminants should be carefully studied to understand the potential positive and negative effects [23,65,6]. One of the main concerns of nanoremediation is the potential toxicity of nanomaterials. Nanomaterials, including nanoremediation scaffolds, can positively and



Fig. 4. Remediation mechanisms of iron and iron sulphide nanoparticles for groundwater clean-up [8].

negatively affect natural ecosystems and human health [72]. Nanomaterials' high reactivity and small size can increase bioavailability and potential toxicity to organisms [10]. Studies have shown that nanomaterials can negatively affect soil microbial communities Lacalle et al. [39] and soil microbial biomass and activity [10]. Additionally, the long-term environmental impact of nanoremediation using nZVI has raised concerns [25]. Another concern is the potential for the release and mobility of nanomaterials in the environment. Nanomaterials can be mobile and potentially migrate to other locations, leading to unintended environmental impacts [66]. The mobility and transformations of nanomaterials in natural environments can pose risks to ecosystems and organisms [21]. It is important to conduct proper evaluation and full-scale ecosystem-wide studies to understand the fate and impacts of nanomaterials before implementing nanoremediation on a mass scale [48,1]. Furthermore, the interaction of nanoparticles with soil organic matter can hamper the effectiveness of nanoremediation for soil remediation [39]. Nanoparticles can interact with soil organic matter and form aggregates, reducing their reactivity and effectiveness in removing contaminants [39]. This can limit the efficiency of nanoremediation and may require higher doses of nanomaterials to achieve desired remediation outcomes [39]. In addition to these concerns, a comprehensive risk assessment and evaluation of nanoremediation technologies are needed. The potential risks and benefits of nanoremediation should be carefully evaluated in a case-specific context [8]. Field-scale validation of remediation results and suitable market development initiatives are necessary to increase the acceptability and popularity of nanoremediation technologies [8]. It is also important to consider the potential risks of using nanomaterials in natural environments, including their mobility, transformations, and potential ecotoxicity [64]. Developing environmentally friendly nanotechnologies and nanomaterials is crucial to ensure the sustainability and eco-safety of nanoremediation. The design and synthesis of new eco-friendly engineered nanomaterials (ENMs) can contribute to developing safe and effective remediation technologies [21]. Eco-friendly nanotechnologies and nanomaterials are recommended for sustainable and eco-safe nanoremediation, considering the potential environmental risks and adopting consensus recommendations [21]. Using polysaccharide-based materials for water nano-treatment is one example of environmentally sustainable and eco-safe nanoremediation [21].

4. Conclusion

Due to size disparities, colloid and nanoparticle transport in porous media exhibit distinct behaviours. Colloids, larger particles with diameters exceeding 1 micrometre, follow traditional filtration and straining mechanisms. Their movement is influenced by porous media characteristics such as pore size and geometry. In contrast, nanoparticles, typically smaller than 100 nanometres, navigate porous structures through intricate interactions, including Brownian motion and surface interactions. Quantum effects become pronounced at this scale, influencing transport dynamics. Understanding these fundamental distinctions is crucial for applications ranging from groundwater remediation to drug delivery systems, as it enables tailored approaches based on the unique transport mechanisms of colloids and nanoparticles. In addition, their transport in porous media is a complex phenomenon influenced by factors such as concurrent aggregation and deposition, surface chemistry, solution chemistry, immobile zones, confinement, flow velocity, and physicochemical properties. Understanding and overcoming these limitations is crucial for successfully applying nanoparticles in various fields, including environmental remediation, oil recovery, and drug delivery. However, several limitations and challenges are associated with nanoparticle transport in porous media. One limitation is the concurrent aggregation and deposition of nanoparticles in porous media. Another limitation is the influence of surface chemistry and solution chemistry on nanoparticle transport and retention. Immobile zones or areas of low flow in porous media can also impact nanoparticle transport and retention. The transport of nanoparticles in porous media is also influenced by flow velocity. As flow velocity decreases, the retention and mobility of ENPs can be affected due to the prevalence of diffusion over advection. Furthermore, the physicochemical properties of nanoparticles play a crucial role in their transport behaviour. Current particle transport models often need to consider the influence of physicochemical conditions and different retention mechanisms on nanoparticle transport in porous media, limiting their predictive capabilities. New approaches are needed to overcome these limitations and improve our understanding of nanoparticle transport in porous media. This would require developing a model-based approach essential to prevent the uncontrolled dispersal of nanoparticles in a porous media. The developed method is also expected to differ from previous works in incorporating the effect of monovalent and divalent ions and natural destabilising agents. This would ensure a more accurate prediction of the locational occurrence of nanoparticle deposition and accumulation and eliminate the tendency for an earlier or later forecast of nanoparticle aggregation. In addition, the developed model would also consider the effect of nanoparticle migration towards the bottom of the porous media, especially when the concentration is above a particular threshold value. Incorporating this threshold value as part of the prediction methodology is expected to improve the location accuracy of the model in estimating the point of nanoparticle deposition in the porous media.

In general, the developed approach for predicting the location of nanoparticle deposition and accumulation in a porous media would help achieve the following:

- a) Innovative nano-remediation approach within the framework of environmental nanotechnology for effective reclamation of contaminated aquifers through a controlled deposition.
- b) A general understanding of the onset and mapping of the different nanoparticle depositional mechanisms in a porous media.

In the future, this review recommends the following for future work in advancing nano-remediation for environmental clean-up:

- a) First, investigate the effect of temperature, salinity, particle size and concentration on the aggregation kinetics of nanoparticles and identify the time for maximum aggregate formation.
- b) Examine the long-term stability of the nanoparticle aggregates under changing experimental conditions (such as temperature, salinity, and pH) and ascertain conditions for disaggregation where possible.
- c) Estimate the optimum nanoparticle concentration necessary for the maximum deposition based on the maximum aggregate formation and the average pore size of the porous media.
- d) Develop a mapping approach to categorise the various types of nanoparticle retention mechanisms in porous media and predict the onset of these mechanisms based on the pore and nanoparticle aggregate size.
- e) Develop an approach for the controlled emplacement of nanoparticles at a targeted location and evaluate the accuracy of the predictive control of this approach through transport experiment studies.

Declaration of Competing Interest

The authors declare that there is no conflict of interest regarding the publication of this article.

Acknowledgement

The authors want to acknowledge the financial grant (PTDF/ED/ OSS/PHD/EOY/1821/20) from the Petroleum Technology Development Fund (PTDF) Nigeria for this research work. Also, the authors acknowledge the comments and contributions of the various anonymous

reviewers of this article.

References

- R.O. Afolabi, A new model for predicting fluid loss in nanoparticle modified drilling mud, Journal of Petroleum Science and Engineering 171 (2018) 1294–1301, https://doi.org/10.1016/j.petrol.2018.08.059.
- [2] R.O. Afolabi, Enhanced oil recovery for emergent energy demand: challenges and prospects for a nanotechnology paradigm shift, Int Nano Lett 9 (2019) 1–15, https://doi.org/10.1007/s40089-018-0248-0.
- [3] R.O. Afolabi, E.O. Yusuf, Nanotechnology and global energy demand: challenges and prospects for a paradigm shift in the oil and gas industry, J Petrol Explor Prod Technol 9 (2019) 1423–1441, https://doi.org/10.1007/s13202-018-0538-0.
- [4] R.O. Afolabi, E.O. Yusuf, Modification of the Vipulanandan rheological model with correlation for temperature and electrolyte effect on drilling muds, Advanced Powder Technology 31 (1) (2020) 312–322, https://doi.org/10.1016/j. apt.2019.10.023.
- [5] R.O. Afolabi, O.D. Orodu, I. Seteyeobot, Predictive modelling of the impact of silica nanoparticles on fluid loss of water based drilling mud, Applied Clay Science 151 (2018) 37–45, https://doi.org/10.1016/j.clay.2017.09.040.
- [6] R.O. Afolabi, T.F. Ogunkunle, O.A. Olabode, E.O. Yusuf, Dataset on the beneficiation of a Nigerian bentonite clay mineral for drilling mud formulation, Data in Brief 20 (2018) 234–241, https://doi.org/10.1016/j.dib.2018.07.071.
- [7] R.O. Afolabi, E.O. Yusuf, C.V. Okonji, S.C. Nwobodo, Predictive analytics for the Vipulanandan rheological model and its correlative effect for nanoparticle modification of drilling mud, Journal of Petroleum Science and Engineering 183 (2019) 106377, https://doi.org/10.1016/j.petrol.2019.106377.
- [8] M.Y. Alazaiza, A. Albahnasawi, G.A. Ali, M.J. Bashir, N.K. Copty, S.S. Amr, M. F. Abushammala, T. Al Maskari, Recent Advances of Nanoremediation Technologies for Soil and Groundwater Remediation: A Review, Water 13 (16) (2021) 2186, https://doi.org/10.3390/w13162186.
- [9] A. Anele, S. Obare, J. Wei, Recent Trends and Advances of Co3O4 Nanoparticles in Environmental Remediation of Bacteria in Wastewater, Nanomaterials 12 (7) (2022), https://doi.org/10.3390/nano12071129.
- [10] M. Anza, O. Salazar, L. Epelde, I. Alkorta, C. Garbisu, The Application of Nanoscale Zero-Valent Iron Promotes Soil Remediation While Negatively Affecting Soil Microbial Biomass and Activity, Frontiers in Environmental Science 7 (2019) 435715, https://doi.org/10.3389/fenvs.2019.00019.
- [11] P. Babakhani, The impact of nanoparticle aggregation on their size exclusion during transport in porous media: one- and three-dimensional modelling investigations, Sci. Rep. 9 (2018) 14071.
- [12] P. Babakhani, J. Bridge, R.A. Doong, T. Phenrat, Continuum-based models and concepts for the transport of nanoparticles in saturated porous media: A state-ofthe-science review, Adv Colloid Interface Sci 246 (2017) 75–104.
- [13] A. Bansal, Nanotechnology in environmental clean-up, Mater. Res. Proc. 145 (2023) 281–310.
- [14] D. Baragaño, R. Forján, L. Welte, J.L. Gallego, Nanoremediation of As and metals polluted soils by means of graphene oxide nanoparticles, Scientific Reports 10 (1) (2020) 1–10, https://doi.org/10.1038/s41598-020-58852-4.
- [15] C. Bianco, J.E. Higuita, T. Tosco, A. Tiraferri, R. Sethi, Controlled deposition of particles in porous media for effective aquifer nanoremediation, Sci. Rep. 7 (2017) 12992.
- [16] C. Chen, J. Shang, X. Zheng, K. Zhao, C. Yan, P. Sharma, K. Liu, Effect of physiochemical factors on transport and retention of graphene oxide in saturated media, Environ. Pollut. (2018) 168–176.
- [17] F. Chen, X. Yuan, Z. Song, S. Xu, Y. Yang, X. Yang, Gram-negative Escherichia coli promotes deposition of polymer capped silver nanoparticles in saturated porous media, Environ. Sci. Nano 5 (2018) 1495–1505.
- [18] G. Chen, X. Liu, C. Su, Transport and retention of TiO2 rutile nanoparticles in saturated porous media under low-ionic-strength conditions: measurements and mechanisms, Langmuir 27 (9) (2011) 5393–5402, https://doi.org/10.1021/ la200251v. Epub 2011 Mar 29. PMID: 21446737.
- [19] Y. Chen, J. Ma, Y. Li, L. Weng, Enhanced cadmium immobilisation in saturated media by gradual stabilisation of goethite in the presence of humic acid with increasing pH, Sci. Total Environ. 648 (2019) 358–366.
- [20] C.V. Chrysikopoulos, T.V. Fountouli, Cotransport of titanium dioxide nanoparticles and formaldehyde in saturated and unsaturated columns packed with quartz sand, Vadose Zone J. 22 (1) (2023) e20175, https://doi.org/10.1002/vzj2.20175.
- [21] I. Corsi, M.F. Desimone, J. Cazenave, Building the Bridge From Aquatic Nanotoxicology to Safety by Design Silver Nanoparticles, Frontiers in Bioengineering and Biotechnology 10 (2022) 836742, https://doi.org/10.3389/ fbioe.2022.836742.
- [22] R. Dowd, S. Lee, Y. Fan, K. Gerdes, Engineering the solid oxide fuel cell electrocatalyst infiltration technique for industrial use, Int. J. Hydrog. Energy 41 (33) (2016) 14971–14981.
- [23] C. Eduardo, J. Mario, M. Guadalupe, Use of Nanotechnology for the Bioremediation of Contaminants: A Review, Processes 8 (7) (2020) 826, https:// doi.org/10.3390/pr8070826.
- [24] European Commission, Taking Nanotechnological Remediation Processes from Lab Scale to End User Applications for the Restoration of a Clean Environment, European Commission, Stuttgart, 2017.
- [25] C. Fajardo, J. García-Cantalejo, P. Botías, G. Costa, M. Nande, M. Martin, New insights into the impact of nZVI on soil microbial biodiversity and functionality, J Environ Sci Health 54 (3) (2019) 157–167, https://doi.org/10.1080/ 10934529.2018.1535159.

- [26] J. Fang, X. Shan, B. Wen, J. Lin, G. Owens, Stability of titania nanoparticles in soil suspensions and transport in saturated homogeneous soil columns, Environmental Pollution 157 (4) (2009) 1101–1109, https://doi.org/10.1016/j. envpol.2008.11.006.
- [27] C. Franco, N. Nassar, M. Ruiz, P. Pereira-Almao, F. Cortés, Nanoparticles for inhibition of asphaltenes damage: adsorption study and displacement test on porous media, Energy Fuels 27 (6) (2013) 2899–2907.
- [28] A. Galdames, L. Ruiz-Rubio, M. Orueta, M. Sánchez-Arzalluz, J.L. Vilas-Vilela, Zero-Valent Iron Nanoparticles for Soil and Groundwater Remediation, International Journal of Environmental Research and Public Health 17 (16) (2020), https://doi.org/10.1016/j.apt.2019.10.023.
- [29] S.A. Ganie, S.H. Wani, R. Henry, G. Hensel, Improving rice salt tolerance by precision breeding in a new era, Current Opinion in Plant Biology 60 (2021) 101996, https://doi.org/10.1016/j.pbi.2020.101996.
- [30] W. Gao, S. Thamphiwatana, P. Angsantikul, L. Zhang, Nanoparticle Approaches against Bacterial Infections, Wiley Interdisciplinary Reviews. Nanomedicine and Nanobiotechnology 6 (6) (2014) 532, https://doi.org/10.1002/wnan.1282.
- [31] E. Goldberg, M. Scheringer, T. Bucheli, K. Hungerbühler, Prediction of nanoparticle transport behavior from physicochemical properties: machine learning provides insights to guide the next generation of transport models, Environ. Sci. Nano 2 (2015) 352–360.
- [32] S. Guo, M. Vieweger, K. Zhang, H. Yin, H. Wang, X. Li, S. Li, S. Hu, A. Sparreboom, B.M. Evers, Y. Dong, W. Chiu, P. Guo, Ultra-thermostable RNA nanoparticles for solubilizing and high-yield loading of paclitaxel for breast cancer therapy, Nature Communications 11 (1) (2020) 1–11, https://doi.org/10.1038/s41467-020-14780-5.
- [33] K.A.D. Guzman, M.P. Finnegan, J.F. Banfield, Influence of surface potential on aggregation and transport of titania nanoparticles, Environ. Sci. Technol. 40 (24) (2006) 7688–7693.
- [34] Z. Hu, H. Gao, S.B. Ramisetti, J. Zhao, E. Nourafkhan, P.W. Glover, D. Wen, Carbon quantum dots with tracer-like breakthrough ability for reservior characterisation, Sci. Total Environ. 669 (2019) 579–589.
- [35] D. Huang, Z. Ren, X. Li, Q. Jing, Mechanism of stability and transport of chitosanstabilized nano zerovalent iron in saturated porous media, Int. J. Environ. Res. Public Health 18 (2021) 5115.
- [36] C.Y. Jin, B.S. Zhu, X.F. Wang, Q.H. Lu, Cytotoxicity of titanium dioxide nanoparticles in mouse fibroblast cells, Chem Res Toxicol. 21 (9) (2008) 1871–1877, https://doi.org/10.1021/tx800179f. Epub 2008 Aug 5. PMID: 18680314.
- [37] V. Katzourakis, C. Chrysikopoulos, Modeling the transport of aggregating nanoparticles in porous media, Water Resour. Res. 57 (1) (2021) e2020WR027946.
- [38] V.E. Katzourakis, C.V. Chrysikopoulos, Investigating the effects of initial concentration and population distribution on the transport of aggregating nanoparticles in porous media, Adv. Water Resour. 178 (2023) 104475, https:// doi.org/10.1016/j.advwatres.2023.104475.
- [39] R.G. Lacalle, C. Garbisu, J.M. Becerril, Effects of the application of an organic amendment and nanoscale zero-valent iron particles on soil Cr(VI) remediation, Environ Sci Pollut Res 27 (2020) 31726–31736, https://doi.org/10.1007/s11356-020-09449-x.
- [40] H.F. Lecoanet, M.R. Wiesner, Velocity effects on fullerene and oxide nanoparticle deposition in porous media, Environ Sci Technol. 38 (16) (2004) 4377–4382, https://doi.org/10.1021/es035354f. PMID: 15382867.
- [41] F. Leuther, J. Kohne, G. Metreveli, H. Vogel, Transport and retention of sulfidized silver nanoparticles in porous media: the role of air-water interfaces, flow velocity and natural organic matter, Water Resour. Res. 56 (2020) 1–19.
- [42] N. Lewinski, V. Colvin, R. Drezek, Cytotoxicity of Nanoparticles, Small 4 (1) (2008) 26–49, https://doi.org/10.1002/smll.200700595.
- [43] S. Lin, M.P. Wiesner, Deposition of aggregated nanoparticles A theoretical and experimental study on the effect of aggregation state on the affinity between nanoparticles and a collector surface, Environ. Sci. 522 Technol. 46 (24) (2012) 13270–13277.
- [44] X. Ling, Z. Yan, Y. Liu, G. Lu, Transport of nanoparticles in porous media and its effect on the co-existing pollutants, Environ. Pollut. 283 (2021) 117098.
- [45] H.H. Liu, S. Surawanvijit, R. Rallo, G. Orkoulas, Y. Cohen, Analysis of nanoparticle agglomeration in aqueous suspensions via constant number monte carlo simulation, Environ. Sci. Technol. 45 (2011) 9284–9292.
- [46] H. Loria, P. Pereira-Almao, C. Scott, Model to predict the concentration of ultradispersed particles immersed in viscous media flowing through horizontal cylindrical channels, Ind. Eng. Chem. Res. 49 (4) (2010) 1920–1930.
- [47] X. Lv, B. Gao, Y. Sun, S. Dong, J. Wu, B. Jiang, X. Shi, Effects of grain size and structural heterogeniety on the transport and retention of nano-TiO2 in saturated porous media, Sci. Total Environ. 563-564 (2016) 987–995.
- [48] L. Marcon, J. Oliveras, V.F. Puntes, In situ nanoremediation of soils and groundwaters from the nanoparticle's standpoint: A review, Sci. Total Environ. 791 (2021) 148324, https://doi.org/10.1016/j.scitotenv.2021.148324.
- [49] N.T. Mattison, D.M. O'Carroll, R. Kerry Rowe, E.J. Petersen, Impact of porous media grain size on the transport of multi-walled carbon nanotubes, Environ Sci Technol. 45 (22) (2011) 9765–9775, https://doi.org/10.1021/es2017076. Epub 2011 Oct 21. PMID: 21950836.
- [50] S.B. Mayegowda, A. Roy, S. Pandit, S. Pandit, S. Pandit, S. Alghamdi, M. Almehmadi, M. Allahyani, N.S. Awwad, R. Sharma, Eco-friendly synthesized nanoparticles as antimicrobial agents: An updated review, Frontiers in Cellular and Infection Microbiology 13 (2023), https://doi.org/10.3389/fcimb.2023.1224778.
- [51] X. Meng, D. Yang, Critical review of stabilized nanoparticle transport in porous media, J. Energy Resour. Technol. 141 (7) (2019) 070801.

- [52] I.L. Molnar, J.I. Gerhard, C.S. Willson, The impact of immobile zones on the transport and retention of nanoparticles in porous media, Water Resources Research 51 (11) (2015) 8973–8994, https://doi.org/10.1002/2015WR017167.
- [53] S. Montalvo-Quiros, G. Aragoneses-Cazorla, L. Garcia-Alcalde, M. Vallet-Regí, B. González, J.L. Luque-Garcia, Cancer cell targeting and therapeutic delivery of silver nanoparticles by mesoporous silica nanocarriers: Insights into the action mechanisms by quantitative proteomics, Nanoscale 11 (10) (2019) 4531, https:// doi.org/10.1039/C8NR07667G.
- [54] S.K. Nune, Q.R. Miller, H.T. Schaef, T. Jian, M. Song, D. Li, B.P. McGrail, Transport of polymer-coated metal-organic framework nanoparticles in porous media, Sci. Rep. 12 (2022) 13962.
- [55] S. Obare, G. Meyer, Nanostructured materials for environmental remediation of organic contaminants in water, J. Environ. Sci. Health, Part A 39 (10) (2004) 2549–2582.
- [56] K.B. Orodu, R.O. Afolabi, T.D. Oluwasijuwomi, O.D. Orodu, Effect of aluminum oxide nanoparticles on the rheology and stability of a biopolymer for enhanced oil recovery, Journal of Molecular Liquids 288 (2019) 110864, https://doi.org/ 10.1016/j.molliq.2019.04.141.
- [57] O.D. Orodu, K.B. Orodu, R.O. Afolabi, E.A. Dafe, Dataset on experimental investigation of gum arabic coated alumina nanoparticles for enhanced recovery of nigerian medium crude oil, Data in Brief 19 (2018) 475–480, https://doi.org/ 10.1016/j.dib.2018.05.046.
- [58] O.D. Orodu, K.B. Orodu, R.O. Afolabi, E.A. Dafe, Rheology of Gum Arabic Polymer and Gum Arabic Coated Nanoparticle for enhanced recovery of Nigerian medium crude oil under varying temperatures, Data in Brief 19 (2018) 1773–1778, https:// doi.org/10.1016/j.dib.2018.06.075.
- [59] T. Pak, L. Fernando de Lima Luz Jr, T. Tosco, N. Archilha, Pore-scale investigation of the use of reactive nanoparticles for in situ remediation of contaminated groundwater source, Proc. Natl. Acad. Sci. 117 (24) (2020) 13366–13373.
- [60] S.S. Patil, U.U. Shedbalkar, A. Truskewycz, B.A. Chopade, A.S. Ball, Nanoparticles for environmental clean-up: A review of potential risks and emerging solutions, Environmental Technology & Innovation 5 (2016) 10–21, https://doi.org/ 10.1016/j.eti.2015.11.001.
- [61] T. Phenrat, H.-J. Kim, F. Fagerlund, T. Illangasekare, R.D. Tilton, G.V. Lowry, Particle size distribution, concentration, and magnetic attraction affect transport of polymer-modified Fe(0) nanoparticles in sand columns, Environ. Sci. Technol. 43 (13) (2009) 5079–5085.
- [62] I.R. Quevedo, N. Tufenkji, Influence of solution chemistry on the deposition and detachment kinetics of a CdTe quantum dot examined using a quartz crystal microbalance, Environ Sci Technol. 43 (9) (2009) 3176–3182, https://doi.org/ 10.1021/es803388u. PMID: 19534131.
- [63] T. Raychoudhury, N. Tufenkji, S. Ghoshal, Aggregation and deposition kinetics of carboxymethyl cellulose-modified zero-valent iron nanoparticles in porous media, Water Research 46 (6) (2012) 1735–1744, https://doi.org/10.1016/j. watres.2011.12.045.
- [64] S. Raza, A. Ansari, N.N. Siddiqui, F. Ibrahim, M.I. Abro, A. Aman, Biosynthesis of silver nanoparticles for the fabrication of non cytotoxic and antibacterial metallic polymer based nanocomposite system, Scientific Reports 11 (1) (2021) 1–15, https://doi.org/10.1038/s41598-021-90016-w.
- [65] Richard O. Afolabi, Oyinkepreye D. Orodu, Vincent E. Efeovbokhan & Oluwatosin J. Rotimi (2017) Optimizing the rheological properties of silica nano-modified bentonite mud using overlaid contour plot and estimation of maximum or upper shear stress limit, Cogent Engineering, 4:1, DOI: 10.1080/ 23311916.2017.1287248.
- [66] M. Riley, N. Suttie, C. Stevenson, J. Tellam, Magnetic susceptibility monitoring and modelling (MSMM): a non-invasive method for acquiring and modelling exceptionally large datasets from column experiments with manufactured nanoparticles, Colloids Surf. A: Physicochem. Eng. Asp. 563 (2019) 289–301.
- [67] A. Roy, A. Sharma, S. Yadav, L. Jule, R. Krishnaraj, Nanomaterials for remediation of environmental pollutants, Bioinorg. Chem. Appl. 2021 (2021) 1–16.
- [68] S.M. Rohaida Mohd Shafian I. Saaid N. Razali A. Fadhil Jahari S. Irawan Aggregation of Partially Hydrophilic Silica Nanoparticles in Porous Media: Quantitative and Qualitative Analysis Intech Open. doi: 10.5772/ intechopen.92101.
- [69] H. ShamsiJazeyi, C.A. Miller, M.S. Wong, J.M. Tour, R. Verduzco, Polymer-coated nanoparticles for enhanced oil recovery, Journal of Applied Polymer Science 131 (15) (2014), https://doi.org/10.1002/app.40576.
- [70] D. Shaniv, I. Dror, B. Berkowitz, Effects of particle size and surface chemistry on plastic nanoparticle transport in saturated natural porous media, Chemosphere 262 (2021) 127854, https://doi.org/10.1016/j.chemosphere.2020.127854.
- [71] H. Singh, F. Javadpour, Retention of nanoparticles: from laboratory cores to outcrop scale, Geofluids 2017 (2017) 8730749.

- [72] H. Singh, M.F. Desimone, S. Pandya, S. Jasani, N. George, M. Adnan, A. Aldarhami, A.S. Bazaid, S.A Alderhami, Revisiting the Green Synthesis of Nanoparticles: Uncovering Influences of Plant Extracts as Reducing Agents for Enhanced Synthesis Efficiency and Its Biomedical Applications, Int J Nanomedicine 18 (2023) 4727–4750, https://doi.org/10.2147/IJN.S419369. PMID: 37621852; PMCID: PMC10444627.
- [73] N. Solovitch, J. Labille, J. Rose, P. Chaurand, D. Borschneck, M.R. Wiesner, J. Y. Bottero, Concurrent aggregation and deposition of TiO2 nanoparticles in a sandy porous media, Environ. Sci. Technol. 44 (13) (2010) 4897–4902.
- [74] N.P. Sotirelis, C.V. Chrysikopoulos, Interaction between graphene oxide nanoparticles and quartz sand, Environ. Sci. Technol. 49 (22) (2015) 13413–13421, https://doi.org/10.1021/acs.est.5b03496.
- [75] A.S. Stefanarou, C.V. Chrysikopoulos, Interaction of titanium dioxide with formaldehyde in the presence of quartz sand under static and dynamic conditions, Water 13 (10) (2021) 1420, https://doi.org/10.3390/w13101420.
- [76] A. Suzuki, J. Cui, Y. Zhang, S. Uehara, K. Li, R.N. Horne, H. Ito, Experimental study of nano/microparticles transport to characterise structures in fractured porous media, Rock. Mech. Rock. Eng. 53 (2020) 4357–4365.
- [77] V.I. Syngouna, G.I. Giannadakis, C.V. Chrysikopoulos, Interaction of graphene oxide nanoparticles with quartz sand and montmorillonite colloids, Environ. Technol. 41 (9) (2020) 1127–1138, https://doi.org/10.1080/ 09593330.2018.1521876.
- [78] H. Thacker, V. Ram, P. Dave, Plant mediated synthesis of Iron nanoparticles and their applications: a review, Prog. Chem. Biochem. Res. 2 (3) (2019) 84–91.
- [79] L. Thangavelu, G. Veeraragavan, S. Mallineni, E. Devaraj, P. Parameswari, N. Syed, D. Chellappan, Synthesis, characterisation, and applications of bioinorganic-based nanomaterials for environmental pollution hazards, Bioinorg. Chem. Appl. (2022) 1946724.
- [80] L. Tian, X. Shi, L. Yu, J. Zhu, R. Ma, X. Yang, Chemical composition and hepatoprotective effects of polyphenol-rich extract from Houttuynia cordata tea, Journal of Agricultural and Food Chemistry 60 (18) (2012) 4641–4648.
- [81] N. Tufenkji, J.A. Redman, Interpreting deposition patterns of microbial particles in laboratory-scale column experiments, Environ. Sci. Technol. 37 (2003) 616–623, https://doi.org/10.1021/es025871i.
- [82] M. Velimirovic, C. Bianco, N. Ferrantello, T. Tosco, A. Cassaso, R. Sethi, T. Hofmann, A large scale 3-D study on transport of humic acid-coated goethite nanoparticles for aquifer remediation, Water 12 (2020) 1207.
- [83] C. Wang, A.D. Bobba, R. Attinti, C. Shen, V. Lazouskaya, L. Wang, Y. Jin, Retention and transport of silica nanoparticles in saturated porous media: effect of concentration and particle size, Environ. Sci. Technol. 46 (2012) 7151–7158.
- [84] H. Wang, J. Xin, X. Zheng, M. Li, Y. Fang, T. Zheng, Clogging evolution in porous media under the coexistence of suspended particles and bacteria: insights into the mechanisms and implications for groundwater recharge, J. Hydrol. 582 (2020) 124554.
- [85] X. Wang, X. Yang, S. Chen, Q. Li, W. Wang, C. Hou, S. Wang, Corrigendum: zinc oxide nanoparticles affect biomass accumulation and photosynthesis in arabidopsis, Front. Plant Sci. 7 (2016) 559.
- [86] H. Wu, D. Schwartz, Nanoparticle tracking to probe transport in porous media, Acc. Chem. Res. 53 (10) (2020) 2130–2139.
- [87] X. Xin, J.D. Judy, F. Zhao, S.L. Goodrich, B.S. Sumerlin, P.J. Stoffella, Z. He, Transport and retention of polymeric and other engineered nanoparticles in porous media, NanoImpact 24 (2021) 100361.
- [88] D. Xue, H. Wang, Y. Zhang, Specific and sensitive colorimetric detection of Al3+ using 5-mercaptomethyltetrazole capped gold nanoparticles in aqueous solution, Talanta 119 (2014) 306–311. https://doi.org/10.1016/j.talanta.2013.11.012.
- [89] S. Ying, Z. Guan, P.C. Ofoegbu, P. Clubb, C. Rico, F. He, J. Hong, Green synthesis of nanoparticles: Current developments and limitations, Environmental Technology & Innovation 26 (2022) 102336, https://doi.org/10.1016/j.eti.2022.102336.
- [90] X. Zhang, Y. Song, H. Gong, C. Wu, B. Wang, W. Chen, J. Hu, H. Xiang, K. Zhang, M. Sun, Neurotoxicity of Titanium Dioxide Nanoparticles: A Comprehensive Review, Int J Nanomedicine 5 (18) (2023) 7183–7204, https://doi.org/10.2147/ LJN.S442801. PMID: 38076727; PMCID: PMC10710240.
- [91] Y. Zhang, D. Yang, Y. Kong, et al., Synergetic Antibacterial Effects of Silver Nanoparticles@Aloe Vera Prepared via a Green Method, Nano Biomedicine and Engineering 2 (4) (2010) 252–257, https://doi.org/10.5101/nbe.v2i4.p252-257.
- [92] Q. Zhao, C.E. Finlayson, D.R. Snoswell, A. Haines, C. Schäfer, P. Spahn, G. P. Hellmann, A.V. Petukhov, L. Herrmann, P. Burdet, P.A. Midgley, S. Butler, M. Mackley, Q. Guo, J.J. Baumberg, Large-scale ordering of nanoparticles using viscoelastic shear processing, Nature Communications 7 (1) (2016) 1–10, https://doi.org/10.1038/ncomms11661.
- [93] Y. Zhou, Y. Kong, S. Kundu, et al., Antibacterial activities of gold and silver nanoparticles against *Escherichia coli* and bacillus Calmette-Guérin, J Nanobiotechnol 10 (2012) 19, https://doi.org/10.1186/1477-3155-10-19.