Simulation of the fate and transport of boron nanoparticles in two-dimensional saturated porous media

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MS received 24 June 2017; revised 14 November 2017; accepted 14 January 2018;
published online 1 December 2018

The wide production and application of engineered nanomaterials (ENMS) inevitably lead to their release in the groundwater environment. However, the release and transport of boron nanoparticles in the multi-dimensional subsurface remain largely unknown. In this work, a multi-dimensional numerical simulator for the transport of boron nanoparticles in the saturated porous media was first developed and validated. Hypothetical scenarios for the release of boron nanoparticles into a layered two-dimensional (2D) and heterogeneous 2D saturated porous media were then explored, and compared with the fullerene nanoparticles. The results demonstrated that the soil heterogeneity influenced the fate of nanoparticles, with high permeable layers and high aqueous-phase concentration. Besides, the boron nanoparticles tend to accumulate at the inlet zones, where it was closer to a nanoparticles source. Different layers of interface interaction also impact the concentration of nanoparticles. In general, the mobility and aqueous-phase concentration of fullerene nanoparticles were higher than those of the boron nanoparticles. In addition, the mobility of boron nanoparticles was found to be sensitive to release concentration, soil porosity and nanoparticle aggregate size.

Keywords. Boron nanoparticles; fullerene nanoparticles; mobility; subsurface; heterogeneity.

1. Introduction

According to an estimate by the United Nations Environment Programme (UNEP 2007), the production of engineered nanomaterials (ENMs) may reach 58,000 tons/yr by 2020. Due to the large production of ENMs in the current market (LuxResearch 2009; WWICS 2012; Joo and Zhao 2016) and their corresponding wide applications in various areas, such as optics, medicine, cosmetics,

electronics, manufacturing and biomedical technology (Mauter and Elimelech 2008), their release into the environment, especially the subsurface, has already attracted great environmental concern. A number of studies have investigated the aquatic toxicity and antimicrobial properties of ENMs and their potential effects on human health (Nakajima *et al.* 1996; Kamat *et al.* 2000; Sayers and Ryan 2005; Lyon *et al.* 2006). For instance, fullerene nanoparticle suspensions were found to be toxic

to juvenile largemouth bass and human cell lines (Oberdorster 2004; Sayes *et al.* 2005). Besides, due to their high sorption capacity of nanomaterials, ENMs could serve as carriers for toxic substances such as polycyclic aromatic hydrocarbons (Cheng *et al.* 2005; Yang *et al.* 2006). Potentially, ENMs may enter the water supply through a number of pathways, for instance, groundwater recharge with wastewater containing nanomaterials, agricultural use of biosolids containing ENMs, etc. After entering the environment, ENMs can interact with natural organic matter, resulting in stable aggregates that can travel very long distances, even as far as drinking water (Chen and Elimelech 2007; Espinasse *et al.* 2007; Hotze *et al.* 2010). To determine the risks associated with these emerging contaminants, it is important to understand the mobility of ENMs in the subsurface saturated porous media.

Due to the variations in the properties of nanomaterials and subsurface environment, the fate and transport of ENMs in the subsurface is a case-by-case issue. Boron nanoparticles, as a promising solid fuel and propellant (Liu *et al.* 2009), are widely used in military and civilian areas. The wide applications of boron nanoparticles would eventually lead to their release in the subsurface environment. Yet, the release and transport of boron nanoparticles in a multi-dimensional subsurface remains largely unknown. Previously, Liu *et al.* (2009) investigated the transport and deposition behaviours under various electrolyte concentrations and flow velocities in one-dimensional (1D) homogeneous column studies, and the experimental results show that the fate and transport of boron nanoparticles follows the classic clean-bed filtration theory (CFT model) (Liu *et al.* 2009). However, little information is provided regarding the transport of boron nanoparticles in the multi-dimensional subsurface environment, especially the heterogeneous subsurface. Furthermore, there is currently no modelling tool to facilitate the transport of boron nanoparticles in the subsurface field scale. Thus, one of the objectives of this study is to fill this research gap by exploring an appropriate numerical simulator to study the transport and retention of boron nanoparticles in the multi-dimensional saturated porous media.

Besides the boron nanoparticles, the fullerene nanoparticles nC_{60} have been chosen as the nanomaterial of comparison to help understand the differences in the transport behaviours of various nanomaterials. Fullerene nanoparticles are

comparably well studied by a number of researchers in 1D homogeneous columns (Oberdorster 2004; Cheng *et al.* 2005; Sayes *et al.* 2005; Chen and Elimelech 2006; Yang *et al.* 2006; Wang *et al.* 2008a,b). Based on various column experimental studies, Li *et al.* (2008) developed a 1D mechanistic model by incorporating a maximum retention capacity term to classic filtration theory, called maximum retention model (Li *et al.* 2008), which was able to simulate the transport of nC_{60} in 1D columns packed with various size fractions of Ottawa sands and flow rates (Li *et al.* 2008; Wang *et al.* 2008a). Later on, the model was extended to 2D and 3D numerical models (Cullen *et al.* 2010; Bai and Li 2012, 2014; Bai *et al.* 2013) to investigate the fate and transport of nC_{60} nanoparticles in the field scale. These studies found that the fate and transport of nC_{60} in subsurface is sensitive to subsurface heterogeneity, dispersivity, release scenarios, collision efficiency factor, maximum retention capacity, etc. Even though there have been some numerical simulators (Cullen *et al.* 2010; Bai and Li 2012, 2014; Bai *et al.* 2013) developed to explain the transport behaviour of nC_{60} in the multi-dimensional field scale, there is currently no study working on the fate and transport of boron nanoparticles in the multi-dimensional heterogeneous subsurface.

Field-scale heterogeneity of subsurface plays an important role during the transport and distribution of ENMs in the subsurface. The study by Cullen *et al.* (2010) investigated the impact of field-scale heterogeneities on the mobility of nC_{60} and multi-walled carbon nanotubes (MWCNT), and found that the distribution of nanoparticles in the heterogeneous field is much less uniform in the heterogeneous field than in the homogeneous field site, with preferable pathways in more permeable zones. Also, the results demonstrated that nanoparticles were less mobile in heterogeneous systems compared to the homogeneous systems with the same averaged hydraulic properties. In another study by Bai *et al.* (2013), the release of fullerene nanoparticles into a mildly heterogeneous site (Bachman Road site in Oscoda, Michigan, USA) (Christ *et al.* 2005) and a highly heterogeneous site (Columbus Air Force Base site in Mississippi, USA) (Barlebo *et al.* 2004) was addressed and compared. The results showed that the transport and distribution of fullerene nanoparticles is much more uncertain and harder to predict for the highly heterogeneous site than the mildly heterogeneous site. These studies (Barlebo *et al.* 2004;

Cullen *et al.* 2010; Bai *et al.* 2013) highlight the importance of subsurface heterogeneity on the transport and distribution of nanoparticles in groundwater. However, so far there is no study working on investigating the fate of boron nanoparticles in the multi-dimensional heterogeneous field site. This work would first address the impact of subsurface heterogeneity on the fate of boron nanoparticles in multi-dimensional saturated porous media, and then compare with that of nano-fullerenes (nC₆₀).

2. Nanoparticle transport modelling

Classic CFT model (Yao *et al.* 1971) was traditionally used to model nanoparticles transport in saturated porous media. Based on a number of 1D column studies, the work by Liu *et al.* (2009) also demonstrated that boron nanoparticles follow CFT model. According to the CFT model, the mass balance of boron nanoparticles in aqueous and attached phases could be described as follows:

$$\frac{\partial C}{\partial t} + \frac{\rho_b}{n} \frac{\partial S}{\partial t} - \nabla(\bar{\mathbf{D}} \cdot \nabla C) + \mathbf{V} \cdot \nabla C = 0, \quad (1)$$

$$\rho_b \frac{\partial S}{\partial t} = nk_{\text{att}} C, \quad (2)$$

$$k_{\text{att}} = \frac{3(1-n)v}{2d_c} \alpha \eta_0. \quad (3)$$

Here, C is the aqueous-phase concentration of boron nanoparticles [M/L³], S is the solid-phase concentration of boron nanoparticles [M/M], t is time [T], n is the soil porosity, ρ_b is the soil bulk density [M/L³], $\mathbf{V}$ is the pore water velocity vector [L/T], $\bar{\mathbf{D}}$ is the hydrodynamic dispersion tensor [L²/T], k_{att} is the boron nanoparticles attachment rate coefficient [1/T] (Ma *et al.* 2009), α is the collision efficiency factor, d_c is the mean grain size [L] and η_0 is the single collector efficiency (Tufenkji and Elimelech 2004).

Currently, there is no modelling tool for the fate and transport of boron nanoparticles in the multi-dimensional subsurface. In our previous work (Bai and Li 2012), a modular 3D transport model for multi-species (MT3DMS) (Zheng and Wang 1999) was successfully modified and validated to simulate the fate and transport of fullerene nanoparticles nC₆₀ in the subsurface field scale. Thus, this work aims at implementing the 1D

CFT model (equations 1–3) to multiple dimensions by further modifying our previous developed numerical simulator (Bai and Li 2012). MT3DMS is a multi-dimensional modelling tool for contaminant transport in groundwater, which is widely used to simulate advection, dispersion/diffusion and chemical reactions of contaminants in subsurface systems with various boundary conditions and external sources and sinks (Zheng and Wang 1999). This work utilised the non-equilibrium sorption model in MT3DMS as shown in the following equation:

$$\rho_b \frac{\partial S}{\partial t} = \beta \left(C - \frac{S}{K_d} \right). \quad (4)$$

Here, K_d is the distribution coefficient for sorbed phase [L³/M] and β is the first-order mass transfer rate between the dissolved and sorbed phases [1/T]. This non-equilibrium sorption module in MT3DMS could be modified to simulate the boron nanoparticles transport by setting β as:

$$\beta = nk_{\text{att}}. \quad (5)$$

Here, K_d in equation (4) was set to infinity so that the detachment rate did not have to be considered. Specifically, a subroutine for boron nanoparticles transport was developed and incorporated into the chemical reaction package of the MT3DMS program. The mass balance information for boron nanoparticles transport in the aqueous phase and attached phase was checked for each iteration.

The developed simulator for boron nanoparticles transport in subsurface was validated by comparing the results with the analytical solutions since there exist analytical solutions for 1D CFT model but not for 2D and 3D, and the results from the simulator are consistent with 1D analytical solutions under a range of collision efficiency and flow velocities. Figure 1 lists one example of the validation. Here, the boron nanoparticles with a concentration of 0.05 mg/l and the particle size of 100 nm was injected into a 16-cm long column packed with sand. The sand packed in the column has an average diameter of 1.2 mm and porosity of 0.37. The injection duration was 33.3 min with pore water velocity of 13.5 m/d and the collision efficiency for boron nanoparticles was 0.01. As illustrated in figure 1, the retention profile from the modified-boron MT3DMS was consistent with the analytical solution very well.

Figure 1. Comparison of boron-MT3DMS simulation result with the analytical solution for boron nanoparticles in a 1D sand column.

3. Nanoparticle release scenarios

Hypothetical scenarios for the release of boron nanoparticles and fullerene nanoparticles into the saturated porous media with an average porosity of 0.3 were investigated under different geological conditions, including assumed layered and heterogeneous cases. The fate of boron nanoparticles in a multi-dimensional subsurface would be simulated based on this newly developed simulator, while the fullerene nanoparticles transport was simulated using the simulator developed in our previous work (Bai and Li 2012). The study domain for nanoparticles transport would be targeted mainly in a rectangular region with length of 200 cm and depth of 54 cm. A steady-state flow condition was attained by imposing a hydraulic gradient of 0.02 along the x -direction, with a constant head boundary condition (Type I Dirichlet BC) applied on both the left and right boundaries and no-flow boundary condition (Type II Neumann BC) applied on the bottom boundary. Both the boron nanoparticles and fullerene nanoparticles were released through the left boundary with a constant concentration of 10 ppm for 2 d. The simulation domain was divided into 36 layers with uniform grid size of 1.5 cm in the z -direction. To obtain a detailed information about nanoparticles distribution around the source zone, the domain was unevenly discretised along the x -direction into 38 columns, with finer grid size around the source zone, as detailed in table 1. Six observation points, O1, O2, O3, O4, O5 and O6, were located at depths of 4.5, 13.5, 22.5, 31.5, 40.5 and 49.5 cm, respectively (27 cm to the left boundary for them).

Discretisation of the simulation domain was same for both the layered case and heterogeneous case, while the hydraulic conductivity distribution was different between these two cases. In the layered scenario, there were six layers with uniform thicknesses of 9 cm for each layer, and the corresponding hydraulic conductivity distribution from top to bottom layers was 129.6, 12.96, 129.6, 1.296, 12.96 and 129.6 m/d, respectively. In the heterogeneous scenario, the background hydraulic conductivity K equals 12.96 m/d, with four different slices arranged within the domain, as shown in figure 2. The hydraulic conductivity of the first slice was $K_1 = K/20$, which was located from 2 to 78.5 cm in the x -direction and 9 to 12 cm in the z -direction. The second slice's hydraulic conductivity was $K_2 = 20K$, located from 12 to 78.5 cm in the x -direction and 19.5 to 22.5 cm in the z -direction. The third slice's hydraulic conductivity was $K_3 = K/10$, located from 2 to 54 cm in the x -direction and 31.5 to 34.5 cm in the z -direction. The fourth slice's hydraulic conductivity was $K_4 = 50K$, located from 54 to 112 cm in the x -direction and 42 to 45 cm in the z -direction.

4. Results and discussion

4.1 Layered scenario

In a layered scenario, six observation points O1, O2, O3, O4, O5 and O6 were located at layers 1, 2, 3, 4, 5 and 6, respectively. The normalised aqueous-phase nanoparticles concentration (C/C_0) was obtained at these observation points. Specifically, the results show that C/C_0 concentration of boron nanoparticles at O2, O4 and O5 were smaller than 0.01, while at O1, O3 and O6 were 0.677, 0.638 and 0.651, respectively. The difference in C/C_0 at different points is mainly due to various soil permeabilities of layers. There are three groups of hydraulic conductivity distribution in the study domain, with the first group of layers 1, 3 and 6 has the highest hydraulic conductivity of 129.6 m/d, the second group of layers 2 and 5 has hydraulic conductivity of 12.96 m/d and the third group of layer 4 has the lowest hydraulic conductivity of 1.296 m/d. Higher hydraulic conductivity, higher soil permeability and higher velocity lead to higher normalised aqueous-phase nanoparticles concentration at the observation points for either

Figure 3. Breakthrough curves at observation points O1, O3 and O6 in layered case for (a) boron nanoparticles and (b) fullerene nanoparticles.

happens for both boron nanoparticles and fullerene nanoparticles, as shown in figure 3(a and b).

By comparison, boron nanoparticles have lower normalised concentration than the fullerene nanoparticles. At the end of the simulation, the normalised concentration for fullerene nanoparticles reached 0.999, 0.983 and 0.999 at points O1, O3 and O6, respectively. The main reason is that boron nanoparticles follow the CFT model (Liu *et al.* 2009), which is different from the mechanistic model of fullerene nanoparticles. Compared to fullerene nanoparticles, boron nanoparticles are kept to deposit on soil medium since there was no maximum retention capacity, which resulted in more boron nanoparticles on soil and less boron nanoparticles in aqueous phase. The less number of boron nanoparticles in the aqueous phase would in turn lead to a smaller value of C/C_0 at corresponding points. Figure 4 shows the

attached-phase concentration (S) distribution in the study domain for these two nanoparticles. For boron nanoparticles, S tends to accumulate at the inlet zone, as shown in figure 4(a). Specifically, there were two zones where boron nanoparticles were accumulated. One zone was the inlet of layer 2 with S concentration of 49–53 $\mu\text{g/g}$, and the other zone was the inlet of layer 5 with S concentration of 48–53 $\mu\text{g/g}$. The phenomenon that boron nanoparticles mainly accumulated at the inlet could be explained as that boron nanoparticles continuously attached to soil without a limit when the inlet portion's aqueous-phase boron concentration was highest. The combined effect of high aqueous-phase concentration (C) and high attachment coefficient (k_{att}) resulted in the high S at the inlet of layers 2 and 5. Here, even though the aqueous-phase boron concentration in layers 1, 3 and 6 was high, their attachment coefficient was low. Thus, most of the boron nanoparticles stay in the aqueous phase in layers 1, 3 and 6. Comparably, fullerene nanoparticles mainly accumulated at the interface of layers 3 and 4. The main reason is that fullerene nanoparticles follow maximum retention capacity model, and layer 4's retention capacity is the highest one, while the aqueous-phase fullerene concentration in layer 3 was high. Thus, a lot of fullerene nanoparticles accumulate at the interface of layers 3 and 4, with the highest S reached being 24 $\mu\text{g/g}$.

4.2 Heterogeneous scenario

To further investigate the impact of soil heterogeneity on the fate of boron nanoparticles in subsurface, this study simulated the transport and distribution of boron nanoparticles in a heterogeneous study domain. Figure 5 lists the aqueous-phase and attached-phase boron nanoparticles distribution after 2 d of release of 10 mg/l boron nanoparticles. Similar to the layered case, boron nanoparticles mainly accumulated at the inlet, with the maximum attached-phase boron nanoparticles concentration reaching 63 $\mu\text{g/g}$ at the inlet source zone near the second slice K_2 ($K_2 = 20K$) after 2 d of release. Due to the existence of low permeable zones K_1 and K_3 ($K_1 = K/20$ and $K_3 = K/10$), boron nanoparticles bypassed these two low permeable zones (K_1 and K_3). Thus, at these two zones of K_1 and K_3 , either the aqueous-phase or attached-phased boron nanoparticles concentration was very little, as shown in figure 5. However, some boron nanoparticles could reach K_2 zone after 2 d

Figure 4. Attached concentration distribution (unit: $\mu\text{g/g}$) in the 2D layered domain for (a) boron nanoparticles and (b) fullerene nanoparticles.

of release, which was higher permeable zone than K_1 and K_3 , and closer to the source zone compared to K_4 zone.

4.3 Effects of release concentration C_0

In this section, the effect of boron nanoparticles release concentration is investigated by varying the initial release concentration across two orders of magnitude. In this study, the release concentration of 1 and 100 ppm for boron nanoparticles is discussed and compared for each of the two scenarios. In general, the higher release concentration leads to a higher contamination level of boron nanoparticles, which happens for either layered or heterogeneous scenario. Figure 6 illustrates that the aqueous-phase boron nanoparticles concentration for C_0 equals 10 and 100 ppm, respectively. Obviously, the higher release concentration led to the higher concentration distribution in the whole domain. For the layered scenario, the release concentration of 100 ppm led to the observed concentration of 67.694, 63.824 and 65.138 ppm

at points of O1, O3 and O6, respectively. In comparison, an initial release concentration of 1 ppm only led to the concentration of 0.67656, 0.63785 and 0.65101 ppm at points of O1, O3 and O6, respectively. Besides, the higher release concentration caused standardised concentration (C/C_0) to increase slightly faster at the corresponding observation points, which could be explained as that soil medium was not so instant to attach all the released boron nanoparticles in the subsurface at a time. Also, the phenomenon of different layers' interaction happens for release concentration of 1 and 100 ppm. In other words, the standardised concentration at O1 was larger than that of O6, and then O3, even though layers 1, 3 and 6 have the same hydraulic conductivity. The higher release concentration also led to higher concentration of boron nanoparticles attached to the soil medium. When C_0 equals 100 ppm, the maximum attached-phase boron nanoparticles concentration was $530 \mu\text{g/g}$, while the maximum boron nanoparticles attached to soil was only $5.3 \mu\text{g/g}$ when C_0 was 1 ppm. Similarly,

Figure 5. Boron nanoparticles concentration distribution in the heterogeneous domain: (a) aqueous-phase concentration (unit: mg/l) and (b) attached-phase concentration (unit: $\mu\text{g/g}$).

there were two zones where boron nanoparticles accumulated. One zone was the inlet of layer 2 and the other zone was the inlet of layer 5. For the heterogeneous scenario, the higher release concentration also lead to higher level of boron nanoparticles contamination in the saturated porous media. Also, boron nanoparticles bypassed two low permeable zones of K_1 and K_3 , but reached high permeable zone of K_2 after 2 d of release. Most of the boron nanoparticles are attached to the soil medium around the source zone.

4.4 Effects of porosity

The porosity of soil depends on several factors, including packing density, cementing, etc. To explore the impact of soil porosity on the fate and transport of boron nanoparticles in saturated porous media, the sensitivity analysis was conducted for soil porosity of 0.2, 0.3 and 0.4 for both layered and heterogeneous scenarios. The result showed that the higher soil porosity increased

boron nanoparticles attachment rate and thus results in more retention and lower mobility of boron nanoparticles in saturated porous media. Figure 7 provides a comparison of the distribution of attached-phase boron nanoparticles across the study domain for porosity of 0.2 and 0.4 for a layered scenario. Specifically, the maximum attached-phase boron nanoparticles concentration reached 27 and 81 $\mu\text{g/g}$ for porosity of 0.2 and 0.4, respectively. After 2 d of release, the observed aqueous-phase concentration of boron nanoparticles was 8.302, 7.9714 and 8.0852 mg/l at observation points of O1, O3 and O6, respectively, when the soil porosity was 0.2. On the other hand, when the soil porosity was 0.4, the observed aqueous-phase concentration was 5.0846, 4.7326 and 4.8519 mg/l at O1, O3 and O6, respectively. Obviously, the higher the porosity, the tendency for boron nanoparticles to attach to soil is higher, which further results in more boron nanoparticles attached to the porous media and less boron nanoparticles remain in the aqueous phase. The influence of soil porosity

Figure 6. Aqueous-phase boron nanoparticles concentration (unit: mg/l) distribution in the layered domain: (a) $C_0 = 10$ ppm and (b) $C_0 = 100$ ppm.

was also examined for the heterogeneous scenario. Similarly, higher porosity results in higher attachment rate and more attached concentration and less aqueous-phase boron nanoparticles concentration. The maximum attached-phase concentration for boron nanoparticles in the study domain was 33, 63 and 97 $\mu\text{g/g}$ for porosities of 0.2, 0.3 and 0.4, respectively.

4.5 Effects of aggregate size d_p

To further investigate the impact of boron nanoparticles aggregate size, sensitivity analyses were conducted for particle size of 10, 100 and 1000 nm for both the layered and heterogeneous scenarios. In both scenarios, the larger the boron nanoparticles size was, the higher the mobility was. Figure 8 provided a comparison of boron nanoparticles concentration in the aqueous phase for diameters of 10 and 1000 nm in the heterogeneous scenario. Obviously, the larger nanoparticle

leads to higher mobility, and thus less attachment on soil. After 2 d of release, boron nanoparticles with a diameter of 1000 nm reached higher permeable zones of K_2 and even K_4 , while boron nanoparticles still bypassed low permeable zones of K_1 and K_3 . In addition, the maximum boron nanoparticles concentration in the aqueous phase was 5.9, 7.9 and 9.4 mg/l for diameters of 10, 100 and 1000 nm, respectively. The influence of d_p on the mobility of boron nanoparticles was also examined for the layered scenario. The smaller the particle diameter, the higher will be the attachment and thus lower mobility. The corresponding maximum attached-phase concentration was 120 and 27 $\mu\text{g/g}$ for diameters of 10 and 1000 nm. After 2 d's release, the observed aqueous-phase concentrations for particle diameter of 10 nm were 1.0748, 1.0110 and 1.0286 mg/l, at points of O1, O3 and O6, respectively. For particle diameter of 1000 nm, the concentrations were 8.9652, 8.6264 and 8.8028 mg/l at corresponding points

Figure 7. Attached-phase boron nanoparticles concentration (unit: $\mu\text{g/g}$) distribution in the layered domain: (a) porosity = 0.2 and (b) porosity = 0.4.

of O1, O3 and O6. The main reason is that the smaller nanoparticle size led to higher η_0 , and thus higher attachment rate (equation 3) and lower mobility.

5. Summary and conclusions

In this work, a multi-dimensional numerical simulator for the fate and transport of boron nanoparticles in saturated porous media was first developed and validated. Hypothetical scenarios for the release of boron nanoparticles into the 2D domain, including a layered domain and a heterogeneous domain, were explored. The results showed that nanoparticles tend to have high mobility in high permeable soil layers, which lead to higher normalised aqueous-phase concentration C/C_0 at corresponding observation points. In general, boron nanoparticles have lower normalised aqueous-phase concentration than fullerene nanoparticles, since boron nanoparticles continuously deposit on soil,

which in turn leads to less concentration in the aqueous phase and then smaller C/C_0 . For boron nanoparticles, even though the hydraulic conductivities for layers 1, 3 and 6 were same, their normalised aqueous-phase concentrations were different. Standardised concentration C/C_0 at layer 1 was larger than that of layer 6, and then layer 3. This phenomenon was interpreted as ‘interface interaction’ since the surrounding hydraulic conductivity of layer 3 was the smallest one. Different layers’ interface interaction was the reflection of the fact that layers with small K have lower C/C_0 . This phenomenon of different layers’ interface interaction happens for both boron nanoparticles and fullerene nanoparticles in the saturated porous media. Besides, boron nanoparticles tend to accumulate at the inlet zones, where the aqueous-phase boron nanoparticles concentration was high and they keep deposited onto soil. Comparably, fullerene nanoparticles mainly accumulate at the interface of layers 3 and 4, where the aqueous-phase concentration was high and the retention capacity

Figure 8. Aqueous-phase boron nanoparticles concentration (unit: mg/l) distribution in the heterogeneous domain: (a) $dp = 10$ nm and (b) $dp = 1000$ nm.

was also high. In the heterogeneous scenario, boron nanoparticles also accumulated at the inlet zones. Furthermore, boron nanoparticles bypassed the two low permeable zones (K_1 and K_3), but reached high permeable zone K_2 , which was comparably near the source than K_4 zone.

For the conditions investigated in this study, boron nanoparticles transport was sensitive to release concentration, soil porosity and boron nanoparticles aggregate size. The higher release concentration led to higher contamination of boron nanoparticles in the study domain. The higher soil porosity increased the attachment rate of boron nanoparticles on soil porous media, thus results in more retention and lower mobility. The smaller the nanoparticle size, the higher will be the attachment and thus lower mobility. The effects of release concentration, soil porosity and nanoparticles aggregate size on the transport of boron nanoparticles in saturated porous media were consistent for both scenarios. The mass balance discrepancies were

<0.1% for all the simulations discussed in this study.

Acknowledgements

The authors thank Dr Yusong Li at University of Nebraska-Lincoln for his helpful suggestions and discussions. This research was supported by the Project of the National Natural Science Foundation of China (51705078), Fuzhou University Research Funding Project (XRC-1546) and Fujian Provincial Department of Education Fund Project (JAT160050).

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