Science of the Total Environment 596–597 (2017) 222–229

Contents lists available at ScienceDirect

Science of the Total Environment

journal homepage: www.elsevier.com/locate/scitotenv

Modeling of retention and re-entrainment of mono- and poly-disperse particles: Effects of hydrodynamics, particle size and interplay of different-sized particles retention

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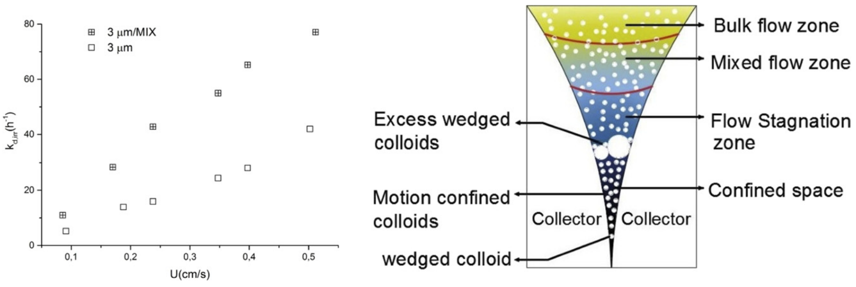
HIGHLIGHTS

- Numerical model of transport, retention and re-entrainment in porous media
- Particle retention and re-entrainment dynamics under different hydrodynamic conditions
- Wedged particles drastically restrain the re-entrainment of the smallest.
- Strained and wedged larger particles supply excess retention sites for the smallest.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 16 December 2016
Received in revised form 27 March 2017
Accepted 28 March 2017
Available online xxxx

Editor: Kevin V. Thomas

Keywords:
Transport
Deposition
Numerical modeling
Straining and wedging
BTC

ABSTRACT

In this paper, numerical simulations of experimental data were performed with kinetic rate coefficients to characterize the retention and re-entrainment dynamics under different hydrodynamic conditions for monodisperse and polydisperse latex particles (3, 10, 16 μm and the mixture). The results show that drastic increase in fluid velocity provokes hardly any remarkable decrease in retention in the presence of large energy barriers (>2000 kT). Systematical increases in deposition and re-entrainment dynamic rates were observed with fluid velocity and/or particle size. Increased irreversible deposition rate indicates straining and wedging dominate deposition in this study. Excess retention of 3 μm particle in the polydisperse particle suspension was observed. The origins are reckoned that deposited larger particles may hinder the re-entrainment of smaller particles near the grain-to-grain contact and can provide additional sites of attachment.

1. Introduction

For more than recent four decades, the colloid filtration theory (CFT) stemming from Yao et al. (1971) has been supplying the basis for a functioning theory to predict particle transport and removal in homogeneous porous media without particle-grain repulsion. However in aquifers, both particles and porous medium grain typically are found to be negatively charged and the subsurface water generally has a low ionic strength and neutral pH (Bradford et al., 2006a). Under these conditions, the electrical double layer interaction is repulsive, yielding an energy barrier for attachment (so-called unfavorable conditions). Nearly no particle deposition is predicted by existing models derived from CFT in the presence of energy barriers (see Fig. 1) because these models are constructed on the basis of the hypothesis of totally equivalent surface characteristics (e.g. zeta potentials and surface topography) across the whole surfaces. However significant deviations were often found between the predictions with mean-filed approaches and experimental

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http://dx.doi.org/10.1016/j.scitotenv.2017.03.254

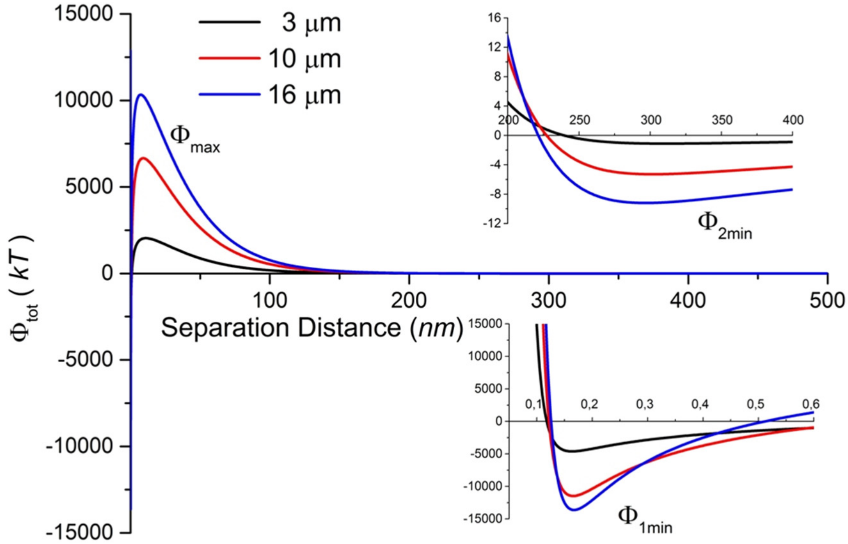

Fig. 1. Extended-DLVO Interaction energy profiles for all tested particles as functions of the separation distance between the particle and grain: (Φ_{min}) is the interaction energy associated with the primary minimum (Φ_{1min}) or the second minimum (Φ_{2min}), (Φ_{max}) is the interaction energy associated with the energy barrier.

results under unfavorable conditions for both biological and nonbiological particles. (Bolster et al., 1999; Bradford et al., 2002; Li et al., 2004; Redman et al., 2001; Tufenkji, 2007; Yang et al., 2015). A variety of explanations for the observed retention in the presence of strong energy barriers have been proposed and corroborated in the literature over the last decade. According to these studies, retention mechanisms can be broadly classified into two types: straining and non-straining. As to non-straining mechanisms, three main mechanisms were considered: retention at physically and chemically heterogeneous bulk surface, wedging at grain-to-grain contacts and retention via secondary energy minimum (see Fig. 1) association. Since 2002, straining has been argued to be the main mechanism dominating the particle retention under unfavorable conditions over a threshold particle:collector ratio of only 0.002 to 0.005 (Bradford et al., 2003, 2006a; Xu et al., 2006) rather than 0.154 (Herzig et al., 1970). However, Johnson et al. (2007b, 2010); Johnson and Hilpert (2013) argued that the so-called straining with such a small particle:collector ratio might just be the removal of particles at grain-to-grain contacts, or wedging. Straining and wedging are the mechanisms engendered by pore space geometry, like pore throats and grain-to-grain contacts, which are not considered in the single collector model. As for the retention on bulk surface, nano to micro scale discrete roughness and chemical heterogeneity have been reported to contribute to particle retention, both in the presence of energy barriers (Assemi et al., 2006; Bradford and Torkzaban, 2012, 2013; Bradford et al., 2013; Duffadar et al., 2009; Pazmino et al., 2014a, 2014b; Torkzaban and Bradford, 2016) and in absence of energy barriers (Jin et al., 2015a, 2015b; Jin et al., 2016).

Furthermore, the fluid flow is much weaker near collector surface and grain-to-grain contact, or flow stagnation zones relative to bulk fluid domain. Thence particle transport and removal at separation distance corresponding to secondary energy minimum has been proved to have an important influence in particle retention. The retained particles in secondary energy minimum are very sensible to hydrodynamic and chemical conditions and easy to be released back to the bulk fluid or to translate along the collector surface (Li et al., 2005; Tong and Johnson, 2006; Johnson et al., 2007a; Torkzaban et al., 2015). Such retention is called reversible retention, which would dramatically increase the particle residence times and yield extended tailing observed during the elution phase in the column experiment.

Most previous literature concerns the monodisperse particle, but however natural particles in underground water are often polydisperse or continuously distributed. Blocking and ripening are found to result in time- and concentration-dependent attachment behavior. Under unfavorable conditions, the reduction of attachment resulting from blocking is significant due to very few attachment sites relative to favorable conditions. The tangential flow along a deposited particle may create a shadow zone behind the particle, and blocking effects are therefore significantly enhanced. The hydrodynamic shadow effects were observed to be increased with increasing particle size and fluid velocity, thus resulting in a higher blocking rate (Ko and Elimelech, 2000). For the polydisperse particle, surface retained large particles would enhance the effects of blocking on the attachment of small ones. The ripening was observed to be negligible on the smooth surface in the presence of energy barriers but increase with the number and length of grain-to-grain contacts (Tong et al., 2008). Wedging and straining of large particles would supply excess number of contacts with collector surface, thus enhancing the ripening of small particles. Some researchers (Ahfir et al., 2016; Bradford et al., 2006b; Yoon et al., 2006) conducted sand-packed column experiments of size continuously distributed particles. To identify the retention mechanisms of particles with continuous size distribution, the particle cumulative size distribution were measured in influent and effluent. Furthermore, to exhibit the characteristics of retained particles more clearly, the particle size distribution of retained particles at different positions was also measured in Ahfir et al. (2016) and Abbar et al. (2017). However, the interplay of different-sized particles retention cannot be elaborated clearly in such experiments. Xu and Saiers (2009) utilized bidisperse particles (3.1 and 5.1 μm) as injected particle and observed that the larger particle could enhance the retention of the smaller particle. The shortcoming of the experiment is that the studied particle sizes are so close that the retention mechanisms might be similar.

The objectives of this work are to use a numerical method to investigate the effects of fluid velocity and the particle size (3 μm, 10 μm and 16 μm) as well as the interplay of greatly different-sized particles retention by the mixed particles injection. The model of irreversible and reversible retention is utilized to simulate the particle transport and fate, by which can be reproduced the extended tailings of the breakthrough curves (BTCs). The coefficients of retention and re-entrainment kinetics are exhibited as functions of fluid velocity and particle size. The irreversible deposition rate coefficient ($k_{d,irr}$) of every size particle in the tridisperse particles is calculated by the effluent mass recovery of every particle in the effluent at different fluid velocities. Then it is compared with the $k_{d,irr}$ of every size monodisperse particle to figure out the effects of particle size non-uniformity. Based upon different results of pore scale simulations in the previous literature, the particle behavior in the fluid stagnation zone are elaborated distinctly. The