Temperature dependency of virus and nanoparticle transport and retention in saturated porous media

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ABSTRACT

The influence of temperature on virus (PRD1 and ΦX174) and carboxyl-modified latex nanoparticle (50 and 100 nm) attachment was examined in sand-packed columns under various physiochemical conditions. When the solution ionic strength (IS) equaled 10 and 30 mM, the attachment rate coefficient (k_{att}) increased up to 109% ($p < 0.0002$) and the percentage of the sand surface area that contributed to attachment (S_f) increased up to 160% ($p < 0.002$) when the temperature was increased from 4 to 20 °C. Temperature effects at IS = 10 and 30 mM were also dependent on the system hydrodynamics; i.e., enhanced retention at a lower pore water velocity (0.1 m/day). Conversely, this same temperature increase had a negligible influence on k_{att} and S_f values when IS was 1 mM or >50 mM. An explanation for these observations was obtained from extended interaction energy calculations that considered nanoscale roughness and chemical heterogeneity on the sand surface. Inter-action energy calculations demonstrated that the energy barrier to attachment in the primary minimum ($\Delta\Phi_a$) decreased with increasing IS, chemical heterogeneity, and temperature, especially in the presence of small amounts of nanoscale roughness (e.g., roughness fraction of 0.05 and height of 20 nm in the zone of influence). Temperature had a negligible effect on k_{att} and S_f when the IS = 1 mM because of the large energy barrier, and at IS = 50 mM because of the absence of an energy barrier. Conversely, temperature had a large influence on k_{att} and S_f when the IS was 10 and 30 mM because of the presence of a small $\Delta\Phi_a$ on sand with nanoscale roughness and a chemical (positive zeta potential) heterogeneity. This has large implications for setting parameters for the accu-rate modeling and transport prediction of virus and nanoparticle contaminants in ground water systems.

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1. Introduction

Groundwater may become contaminated with enteric pathogenic viruses from contaminated recharge water sources, such as infiltration beneath septic tanks, leaking sewer pipes, and managed aquifer re-charge with treated wastewater and urban stormwater (Da Silva et al., 2011; Torkzaban et al., 2006; You et al., 2005). Additionally, the increas-ing use of nanotechnology in a wide range of applications and products will inevitably result in the release of engineered nanoparticles into the subsurface environment (Torkzaban et al., 2013; Wiesner et al., 2006). An understanding and ability to predict the fate and transport of viruses and nanoparticles (NPs) in soils and aquifers are therefore very

important for protection of human and environmental health. During passage through porous media, various physicochemical and biological factors influence the attachment of viruses and NPs to solid surfaces, which in turn affects their transport in the subsurface environment. Some of these factors include flow velocity (Hijnen et al., 2005), type of virus or NP (Chu et al., 2001; Fang et al., 2013), temperature (Bradford et al., 2006; Castro and Tufenkji, 2007; Chrysikopoulos and Aravantinou, 2014; Gallardo-Moreno et al., 2003; García-García et al., 2006; Kim and Walker, 2009; McCaulou et al., 1995), solution chemistry (e.g., ionic strength, pH, ion type) (Gutierrez et al., 2010; Kim et al., 2009), solid surface roughness (Bradford and Torkzaban, 2013; Torkzaban and Bradford, 2016) and chemical heterogeneities (Johnson et al., 1996). A few studies observed an increased adsorption for micro-latex colloids, bacteria, and viruses to several adsorbents with tempera-ture and attributed to factors such as an increase in viscosity of the me-dium, enhanced bacterial polymer formation, viral protein folding, protein attachment, and virus hydrophobicity, and higher inactivation of bacteria/virus at a higher temperature (Bales et al., 1991; Bellamy et al., 1985; Fletcher, 1977; Hendricks et al., 1979; McCaulou et al., 1995;

Nomenclature

k_{att}	attachment rate coefficient (day^{-1})
S_f	percentage of the sand surface area that contributed to attachment (%)
S_{fT}	theoretical values of S_f
S_{max}	maximum solid phase concentrations of attached latex NPs on site 1 + 2 (N kg^{-1})
C_0	input concentration (N mL^{-1})
C	effluent concentration (N mL^{-1})
C/C_0	relative effluent concentrations
v	pore water velocity (m day^{-1})
A_z	zone of influence on the solid-water-interface (nm^2)
f_r	nanoscale roughness fraction
h_r	roughness height (nm)
f_+	positive zeta potential fraction
ζ_+	positive zeta potential (mV)

Greek symbols

η	single-collector efficiency
α	attachment efficiency
α_T	theoretical values of α
$\Phi_1{}^0{}_{min}$	depth of the primary energy minimum
Φ_{max}	height of the energy barrier
$\Delta\Phi_a$	energy barrier to attachment in the primary minimum
$\Phi_2{}^0{}_{min}$	depth of secondary energy minimum

Zhang et al., 2012). While temperature has been noted to affect transport, little research attention has been given to understanding how the temperature influences the attachment process of viruses and NPs (Chrysikopoulos and Aravantinou, 2014).

Attachment of viruses and NPs to solid surfaces of porous media under saturated conditions is commonly described using colloid filtration theory (CFT). According to this theory, the attachment rate is dependent on the mass transfer rate of particles from the bulk solution to the collector surface (quantified by the single-collector efficiency, η) and subsequent particle-surface interaction (quantified by the attachment sticking efficiency, α) (Schijven and Hassanizadeh, 2000; Tufenkji and Elimelech, 2004). Correlation equations have been developed for calculating η as a function of parameters such as flow velocity, viscosity, temperature, diffusion, and particle size. It is predicted that the value of η, and consequently the attachment rate coefficient (k_{att}), increases with temperature due to an increase in the diffusion coefficient (Schijven and Hassanizadeh, 2000; Tufenkji and Elimelech, 2004; Yao et al., 1971). For example, the value of η increases by about 37% with an increase in temperature from 4 to 20 °C. However, several studies have reported that the value of k_{att} increased with temperature to a much greater extent than η (Kim and Walker, 2009; McCaulou et al., 1995). For example, Kim and Walker (2009) observed that k_{att} for latex microspheres at 25 °C was 173% greater than that at 10 °C. It is, therefore, reasonable to expect that the value of α should also increase with temperature.

The value of α strongly depends on the interaction energy between a particle (e.g., virus and NP) and collector (e.g., sand grain) surface (Shen et al., 2010; Tufenkji and Elimelech, 2004). Extended Derjaguin-Landau-Verwey-Overbeek (XDLVO) theory predicts that the total interaction energy consists of electrostatic double layer (EDL) and van der Waals (vdW) interactions (Derjaguin, 1941; Verwey, 1947), as well as poorly characterized short-range interactions such as Born, Lewis acid-base, and hydration interactions (Van Oss, 1993; Yoon et al., 1997). The depth of secondary energy minimum ($\Phi_2{}^0{}_{min}$) is very small for NPs (Bhattacharjee et al., 1998). Consequently, the value of α for NPs is mainly controlled by the energy barrier to attachment in the primary minimum ($\Delta\Phi_a$) and the depth of the primary energy minimum ($\Phi_1{}^0{}_{min}$); the value of $\Delta\Phi_a = \Phi_{max} - \Phi_2{}^0{}_{min}$ where Φ_{max} is the height of the energy barrier. The attractive vdW energy is expected to increase with temperature, due to an increase in the Hamaker constant with temperature (Yan et al., 2015). The magnitude of the repulsive EDL energy is predicted to slightly decrease with increasing temperature due to the decrease in the dielectric constant of the solution, surface potentials of the particle and solid surfaces, and the inverse Debye length (Adamczyk, 2006; Galisteo et al., 1990; Yan et al., 2015). Consequently, an increase in temperature may enhance particle attachment in the primary minimum by lowering $\Delta\Phi_a$ to levels that allow a nanoparticle to diffuse over the energy barrier. However, XDLVO theory for homogeneous interacting surfaces commonly predicts the existence of a sizable energy barrier against attachment in the primary minimum (e.g., >7 kT, where k is the Boltzmann constant and T is the absolute temperature) under unfavorable chemical conditions typical of fresh groundwater (e.g., ionic strength <10 mM) (Bradford and Kim, 2012; Bradford and Torkzaban, 2013; USGS, 2013). Note that the thermal energy of diffusing particles is considerably less than a few kT with an average of 1.5 kT (Shen et al., 2007). Hence, the energy barrier approach (Bhattacharjee et al., 2000) predicts that a small reduction of $\Delta\Phi_a$ with temperature is unlikely to produce enhanced attachment in the primary minimum when $\Delta\Phi_a$ is large (Bradford et al., 2004). In contrast, a substantial increase in the rate and extent of particle attachment has been experimentally observed when the temperature of the solution was increased by 10 or 20 degrees (Kim and Walker, 2009).

Nanoscale roughness and chemical heterogeneities on grain surfaces have been shown to substantially reduce or eliminate $\Delta\Phi_a$ at some localized locations under a net-unfavorable condition (Bhattacharjee et al., 1998; Shen et al., 2012; Suresh and Walz, 1997; Torkzaban and Bradford, 2016). For example, under low ionic strength (<10 mM) conditions, particle attachment may occur on some localized "favorable" sites that exhibit no repulsion or a shallow energy barrier (a few kT) to attachment in the primary energy minimum (Huang et al., 2009). Therefore, the value of α is proportional to the fraction of the solid surface that is "favorable" for attachment. Indeed, numerous studies have shown that only a small percentage of the surface area of a porous medium is favorable for particle attachment (S_f) under a given chemical condition (Argent et al., 2015; Magal et al., 2011; Sasidharan et al., 2014; Treumann et al., 2014). Therefore, we hypothesize that nanoscale surface roughness and chemical heterogeneity play the main role in enhancing the influence of temperature on NP attachment. An increase in temperature further reduces the magnitude of a shallow $\Delta\Phi_a$ created by nanoscale roughness and chemical heterogeneity, which enables more particles to realize a $\Phi_1{}^0{}_{min}$ attachment at higher temperature. Thus, it is reasonable to expect that the value of α and thereby, the value of S_f would increase with temperature. However, no systematic theoretical and experimental studies have been conducted to investigate the effect of temperature on the value of S_f.

The objective of this study was to experimentally and theoretically investigate the influence of water temperature, coupled with solution chemistry and flow velocity, on the extent and kinetics of virus and NP attachment in a porous medium. For this purpose, two different biotic (PRD1 and ΦX174 viruses) and abiotic (50 and 100 nm carboxyl-modified latex NPs) nanoparticles were employed in this study. The transport experiments were performed at 4 and 20 °C at various solution ionic strength (IS) and pore water velocities. Values of k_{att} and S_f were determined by parameter fitting to the observed breakthrough concentrations of the NPs. XDLVO calculations between a chemically and physically heterogeneous collector and homogeneous particle were conducted to explain the observed enhanced attachment of the viruses and latex NPs at the higher temperature. Specific solution chemistry conditions were identified when temperature-dependent particle transport is expected. Results from this work provide insight into the underlying mechanisms that control the influence of temperature on particle attachment in porous media and have important implications