Mechanistic study of nanoparticles deposition and release in porous media

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ABSTRACT

Physicochemical interaction between the nanoparticles and the pore walls can cause significant retention of nanoparticles in porous media. The objective here is to provide mechanistic model based on Extended DLVO theory to study the rate of deposition and release of nanoparticles in porous media at different temperature, ionic strength, and pH. Empirical equation has been derived to calculate zeta potential at different temperature, ionic strength, and pH. The interaction energy can be with/without energy barrier between the nanoparticles and the pore surface. The rate of deposition and release of nanoparticles in each case has been derived. Numerical model has been used to compare the theoretically calculated rates with several experimental data. Increasing the temperature decreases the energy barrier height and increases the rate of deposition. With increasing the ionic strength, the thickness of the electrostatic double layer decreases and hence the rate of deposition increases. The effect of pH on the rate of deposition depends on the location of environment pH with respect to the isoelectric point of the nanoparticles and rock. For the extreme values of pH, energy barrier exists and rate of deposition is low. However, when the pH of the solution is between the isoelectric points of the nanoparticles and rock, the energy barrier decreases and the rate of deposition increases. The rate of deposition is time dependent as it decreases with increasing the covered rock surface. The effect of surface roughness has been included in the model using the effective height and density of the surface roughness distribution. Finally, these theoretically calculated rate values are used in a numerical model of the advection-dispersion equation with source/sink term. Several experimental results have been perfectly matched that validate the theoretical calculations of the rate of deposition. The new mechanistic model for nanoparticles can be used to determine the fate of nanoparticles in porous media under different conditions of temperature, ionic strength, concentration, and pH. This model can help to understand the nanoparticles transport in porous media and effectively design nanoparticles fluid for injection into oil and gas reservoirs.

1. Introduction

In the past decade the applications of nanotechnology in the oil and gas industry have attracted many researchers (Mahmoud et al., 2016; Esfandyari Bayat et al., 2015; Abdelfatah et al., 2014; Hendraningrat and Torsæter, 2014; McElfresh et al., 2012; Caldelas et al., 2011; Ju and Fan, 2009; Binks et al., 2008; Huang et al., 2008). However, the injection of nanofluid into reservoir may cause formation damage by the retention of nanoparticles (NPs) in porous medium (Ju and Fan, 2009). Both experimental and modeling investigations were carried out to study the transport and retention of nanoparticle in reservoir rocks (Rahman et al., 2014; Yu et al., 2012; Zhang, 2012). The mechanism of nanoparticle retention at the pore scale is a complex phenomenon. McCarthy and Zachara (1989) introduced two main types of retention in saturated granular medium, deposition and straining. Deposition and release of

nanoparticles to the rock pore surface is mainly due to the physicochemical interactions, while straining is the entrapment of single or multiple nanoparticle plugging at pore throat which are too small to allow nanoparticles to pass. When the size of nanoparticle is several orders of magnitude smaller than the rock grains or the rock pore space, all retention of nanoparticles is contributed by deposition (Zhang, 2012; Yao et al., 1971). Derjaguin-Landau-Verwey-Overbeek (DLVO) theory can be used to evaluate the physicochemical interactions between the nanoparticles and rock pore surface, where van der Waals attraction and electrical double layer interaction are the two major interactions (Derjaguin and Landau, 1993; Verwey et al., 1948). DLVO theory has been successfully employed to analyze colloid stability in aqueous suspensions assuming the total DLVO interaction energy is the sum of van der Waals energy and electrostatic double layer energy (Adamczyk and Weroński, 1999). When the separation distance between two surfaces are less than a

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few nanometers, short-range repulsions such as Born repulsion and hydration repulsion present (Hoek and Agarwal, 2006). Adding these repulsions, which are called non-DLVO forces, into the classical DLVO theory more accurate total DLVO interaction energy is obtained (Ghosh, 2009). Particle size, separation distance, surface charge, ionic strength, pH, temperature and surface roughness of the rock are the main factors that control the total DLVO interaction energy (Yu et al., 2012). Rate of deposition of different nanoparticles (NPs) through different reservoir rocks varies widely and was found to be strongly dependent on nanoparticle and rock grain surface charge. Many researches indicated the significant effect of ionic strength on deposition of nanoparticles, because the electrical double layer interaction is highly dependent on ionic strength. Rahman et al. (2014) showed that alumina nanoparticle deposition increased with increasing ionic strength. Caldelas (2010) found a noticeable increase of surface-coated silica nanoparticles deposition on Boise sandstone at higher ionic strengths. Brant et al. (2005) indicated that zeta potential as a function of pH and ionic strength, affects the deposition rate. Reyes Bahena et al. (2002) showed zeta potential of alumina nanoparticle decreases as pH increases at constant ionic strength, and decreases as ionic strength increase at the same pH. Zeta potential of nanoparticles and rock grain surface controls the double layer interaction which governs the total DLVO interaction. Caldelas et al. (2011) studied the effect of temperature on deposition of silica nanoparticle through sandpack with crushed Boise sandstone. They found a slight increase of deposition when the temperature was raised from 55 °C to 80 °C. Besides, several experimental investigations on colloids transport through porous media suggested that rate of deposition is affected by the surface roughness of porous media. It is observed consistently that higher rate of deposition occurs on rougher surfaces, where the roughness is generally recognized by average height and density of protrusions (Shellenberger and Logan, 2002; Hoek et al., 2003).

The goal of this paper is to provide a mechanistic model for nanoparticle deposition in porous media. First, the modified equation for zeta potential is presented in section 2. This equation accounts for the effect of the environment variables i.e. pH, ionic strength, nanoparticle size, and temperature. In section 3, DLVO theory considering non-DLVO forces is used to analyze the interaction between nanoparticles and rock surface at different conditions. Equations for rate of deposition and release are presented based on the DLVO theory in section 4. Then, a numerical solution of the convection-diffusion equation with source/sink term accounting for nanoparticles retention in porous media is presented in section 5. This numerical model is used to validate the theoretical equations for rate of deposition and release, by comparing the model results with the data in literature (section 6.1). The numerical model is also used for sensitivity analysis of the different environmental conditions on nanoparticles interaction in porous media (section 6.2). In section 7, the summary and conclusion are presented.

2. Zeta potential

Zeta potential is the key parameter that controls the electrostatic interaction between dispersed nanoparticles and the rock surface. Zeta potential (ζ) cannot be measured directly but can be calculated from Henry's equation (Kim and Lawler, 2005). However, as long as the absolute value of Zeta potential is less than 40 mv in 1:1 electrolyte solution at room temperature, Henry's equation is the best approximation for zeta potential (Ohshima, 1994). Henry's equation can be rearranged to calculate the zeta potential as the following,

$$\zeta = \frac{3U_E\mu}{2\varepsilon f(\kappa a_p)} \tag{1}$$

U_E is electrophoretic mobility of a nanoparticle measured from electrokinetics experiment, ε is dielectric constant; μ is viscosity, kg.m^{-1}s^{-1}; κ is the inverse Debye length, m^{-1}; a_p is nanoparticle radius, m. $f(\kappa a_p)$ is the Henry's function. A simpler form of Henry's equation in which $f(\kappa a_p) = 1.5$ is known as the Smoluchowski equation (Kaszuba et al., 2010), and applies for large particle ($\kappa a_p \sim 100$) in high ionic strength with thin double layer. However, for small particle in low ionic strength with thick double layer another simplification can be used that $f(\kappa a_p) = 1$. The Debye length, κ^{-1} is characterized as the thickness of the electrical double layer of a particle in aqueous media (Eq. (2)).

$$\kappa^{-1} = \sqrt{\frac{\varepsilon k_B T}{2000 e^2 N_A I}} \tag{2}$$

$$I = \frac{1}{2}\sum_i z_i^2 M_i \tag{3}$$

where M_i is the molar concentration of the symmetric ($z : z$) electrolyte of ith ion, in the unit of $\frac{mole}{dm^3}$; I is ionic strength, M; N_A is the Avogadro number; k_B is the Boltzmann constant; T is the temperature, K; e is the elementary charge, C.

To analyze DLVO interaction energy at various conditions, an empirical correlation is modified to estimate zeta potential of nanoparticle and rock grain at different pH, ionic strength and temperature based on experimental measurements reported in literatures. The effect of ionic strength is corrected by Henry's function through the Debye length. Ohshima (1994) presented a simple approximate expression for Henry's function which is applicable for any value of κa_p and

$$f(\kappa a_p) = 1 + \frac{1}{2\left[1 + \frac{2.5}{\kappa a_p\left(1 + e^{-\kappa a_p}\right)}\right]} \tag{4}$$

Based on the treatment of double layer at a solid particle/electrolyte solution interface by Gouy–Chapman–Stern model, the electrical potential measured at the shear plane can be referred to as the zeta potential (Oldham, 2008). Fig. 1 shows potential (ψ_x) at a distance x from colloid
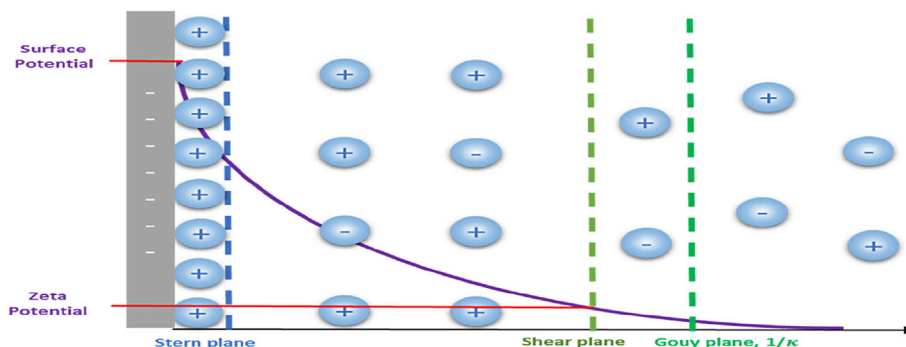

Fig. 1. Position of shear plane and corresponding zeta potential in electrical double layer.