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Simulation: the deposition behavior of Brownian particles in porous media by using the triangular network model

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Abstract

The individual Brownian particles movement through the filter bed, and the effect of different interaction energy curves of DLVO theory, on the permeability reduction in a filter bed is investigated by applying the triangular network model using the Brownian dynamics simulation method. When energy barrier exists and both the particle and the pore size distributions are of the Raleigh type, it is found that particles with Brownian motion behavior are easier to get straining at small pores, and resulted in higher permeability reduction than those without considering the Brownian motion behavior. It is found that the present model shows fair agreement between the theory and the permeability reduction and the filter coefficient experimental results when the direct deposition mechanism is dominant.

Keywords: Network model; Deposition; Brownian particles; Porous media

1. Introduction

The deposition behavior of Brownian particles in suspension onto the granular collectors is an important topic in the study of the transport phenomena of porous media [1]. For example, the migration of fine clay particles in the porous media of oil reservoir is always triggered by the formation of an incompatible brine solution, which in turn will cause a several-fold reduction in the permeability of the reservoir [2]. The permeability reduction rate along the porous media is dependent on several system parameters which have been the subjects of numerous studies, those parameters are: the fluid superficial velocity, the grain and the particle sizes [3–5], the geometry of the collector [6], the interaction forces between the particles and the collector surfaces [7,8], and the pore size distribution [2,9–11].

Generally, there are two theoretical approaches to calculate the deposition rates of colloidal particles onto the collector surfaces, namely the Eulerian method and the Lagrangian method [12]. The Eulerian method considered the deposition rates of colloidal particles onto the collector surfaces are governed by the convective diffusion equation established by Prieve and Ruckenstein [13], and Spielman and Friedlander [14]. Two important conclusions were obtained from their works: (1) in order to take the contribution of the motion behavior of small particles into account, the hydrodynamic retardation factors shall be included when calculating the particle's diffusivity; (2) the surface interaction forces is considered as a first order chemical reaction at the collector surfaces, which can be imposed on the boundary condition of the convective diffusion equation. The paper published by Elimelech [15] provides the detailed numerical technique to solve this convective diffusion equation. Contrary to the Eulerian approach, the Lagrangian approach can determine the trajectory of a particle by calculating the force balance and the torque balance on the particle [1]. Hence, by assuming the types of forces acting on the particle and the hydrodynamic flow field around the collector surfaces, for example, one can describe the particle's path near a collector surface by using the constricted tube model established by Payatakes et al. [16]. Then, by applying the concept of the limiting trajectory [17],

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the deposition rates of particles can be determined. However, since the Brownian motion of particles is stochastic in nature, hence the random motion behavior of Brownian particles cannot be described by this deterministic trajectory equation. The inclusion of these random forces in the Lagrangian type trajectory equation leads to a Langevin type equation, which was solved successfully by Kanaoka et al. [18] and Gupta and Peters [19]. As described in Rajagopalan's dissertation [20], when the inertia term in the force balanced equation is ignored, there is a direct relationship between the Langevin equation and the convective diffusion equation via the Fokker–Planck–Kolmogov equation, and the equivalent Ito form of the Stratonovich differential equation. By utilizing Langevin type equation and by adopting the concept of the control window [21,22], a stochastic simulation method describing the deposition behavior of Brownian particles was established by Ramarao et al. [23], and this method is adopted in the present paper.

In order to describe the effect of pore size distribution on the particle deposition behavior along the filter bed, the network model has been applied extensively to simulate the deposit formation in the porous media [24]. For example, by applying the theory of the effective medium approximation (EMA) [25], Sharma and Yortsos [2] had successfully established a set of population balance equations, and calculated the temporal variations of the filter coefficient caused by the particle deposition in a filter bed. Both straining and direct deposition mechanisms were considered in a capillary tube model. The permeability reductions resulting from particle's deposition were then calculated by using the EMA method, where the fluid velocity is assumed to be the same in all pore throats of a given size in the network. Then, by applying the principle of flow biased probability and the concept of wave front movement, both Rege and Fogler [9] and Imdakm and Sahimi [10] were able to predict the permeability and the effluent concentration of particles, and were in good agreement with the available experimental data. Later on, by considering the void space of porous media as a constricted tube unit bed element (UBE), Burganos et al. [26] developed a three-dimensional network simulator to calculate the filter coefficient, at which the deposition rate of particles is determined by using the method of trajectory analysis. They found that the filter coefficients predicted by using 2D network model are lower than those valued predicted by using the 3D network model. However, the Brownian diffusion force of particles was not considered.

Recently, with the adoption of the Brownian dynamic simulation method mentioned above, we had successfully applied the two-dimensional modified square network model to track the individual particles with Brownian motion behavior as they move through the porous media of a filter bed [27]. From which, the temporal variations of the permeability reduction, pressure drop and the effluent concentration of particles, either caused by the straining or by the direct deposition of particles on the pore walls, can be determined. In the present paper, instead of using the modified square network model, we will use the triangular network model to investigate the deposition behavior of Brownian particles in porous media. The sinusoidal constricted tube (SCT) will be adopted [1]. In addition, the effects of the total interaction energy curve of DLVO theory with various shapes [28] are also investigated. The permeability reduction predicated by the present triangular network model shows good agreement with the available experimental data of Soo and Radke [29,30]. The experimental results of Elimelech and O'Melia [31] and Bai and Tien [32] on the filter coefficients of colloidal particles at different ionic strengths can also be predicted by this work.

2. Network model

In the present study, we use the modified two-dimensional triangular network (as shown in Fig. 1) to represent the porous media of the filter, and adopt the Brownian dynamic simulation method to track the individual particles as they move through the network. In Fig. 1, all bonds in the network are assumed to have the same length, but with a Raleigh form pore size distribution [2]:

$$f_{\mathrm{p}}(r') = 2r' \exp(-r'^2) \tag{1}$$

where f_{p} and r' are the dimensionless distribution density and the dimensionless radius of pores, respectively. Eq. (1) satisfies the following equation:

$$\int_0^\infty 2r' \exp(-r'^2)\,\mathrm{d}r' = 1 \tag{2}$$

This distribution can then be assigned randomly to the bonds in the network as follows:

$$\int_0^{r'_1} 2r' \exp(-r'^2)\,\mathrm{d}r' = 1 - \exp(-r'^2_1) \tag{3}$$

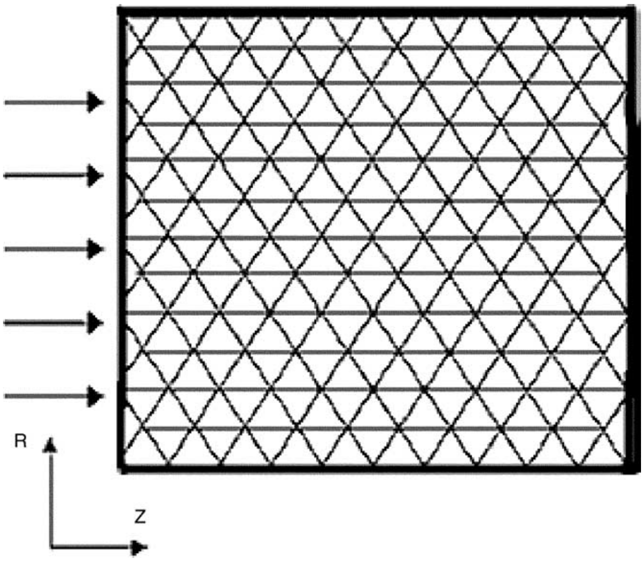

Fig. 1. The two-dimensional triangular network model.