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Short Communication

Motion of particle breakthrough curve and permeability reduction in Voronoi and triangular networks

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ABSTRACT

This paper employs the Brownian dynamics simulation method to compare the particle breakthrough history and permeability reduction of porous media between Voronoi and regular triangular networks of the same coordination number. For the case of transporting Brownian particles through these two networks, it is found that their breakthrough concentrations are of the same value, but have different breakthrough moments and permeability reduction rates under either favorable or unfavorable deposition conditions. Same results are also obtained for the non-Brownian particles.

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1. Introduction

In the study of colloidal transport phenomena through porous media, to understand how the permeability reduction depends on the pore structure of granular media is an important topic [1]. For example, the migration of fine clay particles in the porous media of the oil reservoir always causes a several-fold reduction in the permeability of the reservoir [2]. The permeability reduction rate in the porous media is dependent on several system parameters which are: the fluid superficial velocity and the grain and particle sizes, the geometry of collector, the interaction forces between particles and collector surfaces and the pore structure [1]. Among which, to find an efficient approach of properly describing the pore structure of a porous medium became the subject of numerous studies in last two decades [3–7]. One popular approach is the regular network model, in which the pore space is represented as a graph of connected sites. In this regular network model, the topology of porous media can be defined by using the coordination number Z defined by the number of bonds connected to a node site in the network structure [8]; for example, $Z = 3$ stands for a regular honeycomb network, $Z = 4$ stands for a simple square network and $Z = 6$ stands for a normal triangular network in the two-dimensional coordinates (i.e. abbreviated as 2-D below). In our previous papers [9,10], we adopted the Brownian dynamic simulation method of solving Langevin type equations [11], and assumed that the porous media of the filter bed is unconsolidated, we had successfully tracked the motion of individual particles with Brownian motion behavior as they move through the filter bed, by using the 2-D models of the modified square network and the triangular network, respectively. Through this process, the temporal variations of the permeability reduction and the effluent concentration of particles, caused either by the straining or by the direct deposition of particles on the pore walls, were determined. We found that the distribution of pore size has more profound effect on the reducing of the permeability ratio than that of the particle size distribution, especially at the initial period of filtration.

In principle, the regular network model replicates both the geometry and topology of porous media. However, the direct replication has proven unrealistic because the distribution of pore space in real porous media is complicated and has a topologically disordered network; i.e. the number of bonds connected to the same node site varies according to a distribution. If the granular collector in the porous media is unconsolidated (not overlapping), then we can adopt the Voronoi type network to represent this disordered network; a two-dimensional example of which is shown in Fig. 1 below [12]. The Voronoi type network have been used for many applications, such as the displacement process that occurred in the tertiary oil recovery process [13] and the modeling of fluid transport in disordered fibrous materials [14]. Since the averaged coordination number of the Voronoi network is the same as that of the triangular regular network ($Z = 6$), Jerauld et al. [15] verified by means of the Monte Carlo simulation method that the effective conductivity of these two models are similar (i.e. the ease with which fluid can flow through the pore spaces of these two models are the same with each other). When the transient phenomena of diffusion and conduction in heterogeneous media represented by the Voronoi network were studied, Sahimi and Tsotsis [2] had also

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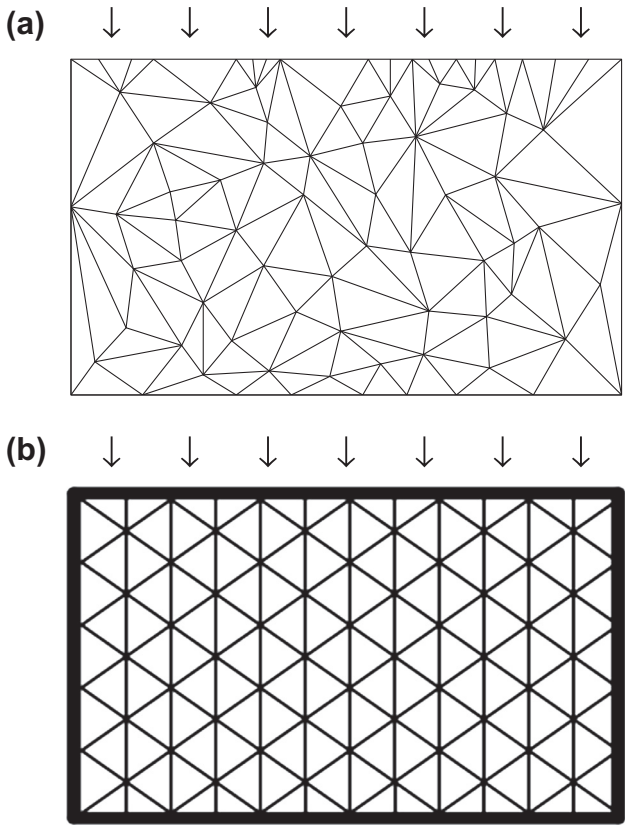

Fig. 1. The 2-D networks adopted in the present simulations, (a) The Voronoi network. (b) The regular triangular network.

verified that the EMA predictions [4] are in agreement with the Monte Carlo results. Since there is still no analysis of the comparisons of the particle effluent concentration and the permeability reduction between the Voronoi network and the regular triangular network of the same coordination number, we seek herein to amend this deficiency by conducting a case study by using the Brownian dynamic simulation method of solving Langevin type equations. The effect of the particle's Brownian motion behavior on its breakthrough concentration and the permeability reduction of these two network models will also be investigated.

2. Theoretical formulas

2.1. Network model

In the present study, we use the 2-D Voronoi and regular triangular networks of the same size (as shown in Fig. 1a and b) to represent the porous media, and adopt the Brownian dynamic simulation method to track the individual particles as they move through the network. The Voronoi network is mapped by setting (x = rand (1, 10); y = rand (1, 10); plot (x, y, 'diamond')) with the application of MATHLAB software [16]. The averaged coordination number of the present Voronoi network is found to be $Z = 5.8$, which is close to the value of regular triangular network $Z = 6$. In Fig. 1a and b, all bonds in the network are assumed to have the Raleigh form pore size distribution [4].

As particles of a given size distribution transport through the bonds of the network shown in Fig. 1a and b, they will arrive at a node where the fluid will be separated by two or more paths that flow further into the network. In the present study, we adopt the method of flow biased probability to determine which path the particles will flow through. This biased method is based on the principle that the movement of the particle will be toward a path with a greater flow rate. Usually, the greater the flow rate, the greater the probability of the particle choosing that path. Details of this method can be found elsewhere [5].

2.2. Constricted tube cell

Because of its superiority in describing voids of porous media as a collection of pore spaces connected by constrictions, the parabolic geometric structure (PCT as parabolic constricted tube) used by Tien et al. [3] is considered for the constricted tube model in the present study. The flow field equations established by Chow and Soda [17] and modified by Chiang and Tien [18] are adopted.

2.3. Brownian dynamics simulation

Similar to our previous papers [9,10], with the consideration of the Brownian diffusion force in determining particle trajectories, the method of Brownian dynamics simulation is adopted in the present study. Assume that the distribution of the initial position (r_{in}, θ_{in}) of each particle is assigned by the random number generator in the flow field simulation (see Fig. 2). With consideration of the inertia term in the force balance equation and of the specification of the flow fluid through the pore of PCT (i.e. one PCT is represented by one bond length in the present network), the particle trajectory can be determined by integrating the Langevin type equation as shown below. In this simulation method, the new position of the particle in the network model can be obtained by the integration of a Langevin type equation with a sufficient short time interval (i.e. 10^{-6} s) as follows:

$$m_p \frac{dV}{dt} = -m_p\beta(V-u) + F_{DLVO} + m_pA(t) \tag{1}$$

where m_p is the mass of the particle, V and u are the particle and fluid velocity vectors, β is the friction coefficient per unit mass of the particle, F_{DLVO} is the external DLVO forces (which is the sum of the van der Waals and electrostatic forces) and $A(t)$ represents the Brownian diffusion forces per unit mass of the particle caused by random collisions of the fluid molecules. When the particle's Brownian motion behavior is not considered, termed as non-Brownian particle in the present paper, this Brownian diffusion force is excluded in Eq. (1).

From those trajectories of influent particles in the network, the permeability reduction ratio K/K_0 in a percolation history can be determined by the method outlined in our previous papers [9,10]. In order to express the extent of permeability reduction as percolation proceeds, we use the permeability ratio K/K_0 as the function of the pore volumes of fluid injected into the filter bed. Here, the pore volume ($p.v.$) of the injection fluid is defined as:

$$p.v. = \frac{U_{in}t}{\varepsilon_0 L} \tag{2}$$

where U_{in} is the influent flow rate and C_{in} is the influent concentration of particles.

3. The interaction energy curve of DLVO theory

In the present paper, the effects of two type interaction energy curves of DLVO theory [19] on the effluent concentration of particles, and permeability ratio will be investigated for these two network models.

According to the DLVO theory, the total interaction energy between the approaching colloidal particles and collector surfaces is the algebraic sum of the van der Waals and double-layer electrostatic potentials as follows:

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