



Microscale simulation of particle deposition in porous media



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ABSTRACT

In this work several geometries, each representing a different porous medium, are considered to perform detailed computational fluid dynamics simulation for fluid flow, particle transport and deposition. Only Brownian motions and steric interception are accounted for as deposition mechanisms. Firstly pressure drop in each porous medium is analyzed in order to determine an effective grain size, by fitting the results with the Ergun law. Then grid independence is assessed. Lastly, particle transport in the system is investigated via Eulerian steady-state simulations, where particle concentration is solved for, not following explicitly particles' trajectories, but solving the corresponding advection–diffusion equation. An assumption was made in considering favorable collector–particle interactions, resulting in a “perfect sink” boundary condition for the collectors. The gathered simulation data are used to calculate the deposition efficiency due to Brownian motions and steric interception. The original Levich law for one simple circular collector is verified; subsequently porous media constituted by a packing of collectors are scrutinized. Results show that the interactions between the different collectors result in behaviors which are not in line with the theory developed by Happel and co-workers, highlighting a different dependency of the deposition efficiency on the dimensionless groups involved in the relevant correlations.

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1. Introduction

The transport and deposition of colloidal particles in porous media are important phenomena involved in many environmental and engineering problems. Particle filtration [1], catalytic processes carried out through filter beds [2–4], chromatographic separation [5,6] and aquifer remediation [7], just to cite a few examples, all require the understanding of their fundamental mechanisms. Among the above cited applications, of particular interest is the injection of colloidal nanoscale zerovalent iron (NZVI) as a technology for remediation of contaminated aquifer systems [8–15]. In these applications, the possibility of employing reliable mathematical models for the simulation of colloidal particle transport and deposition in porous media is particularly interesting, and often needed. In order to describe large spatial domains the models have to ignore the micro-porous structure of the medium and must be derived from an homogenization procedure. The final macro-scale models result in different submodels for the each phenomenon involved and this work focuses on one of them: the rate of particle deposition on the surface of the grains constituting the porous medium. The commonly used theoretical framework for treating deposition of colloidal particles onto stationary collectors

is the classic colloid filtration theory (CFT) [16]. CFT describes fluid flow and particle deposition in porous media and is based on seminal work by Happel [17], Levich [18] and Kuwabara [19]. Some of these models have become very popular, as for example the Happel model, that has been used in many works [20–22] even in derivative forms, some of which developed upon the sphere-in-cell model while retaining many of its features [23,24], while others only use the simplicity of the spherical model as a starting point to develop more physical investigations [25,26]. Hydrodynamics and particle deposition for a number of different systems, namely the rotating disk, parallel-plate channel and for stagnation point flow have also been studied [27].

Deposition is seen as occurring in two steps. The first step is the transport of the colloidal particles from the bulk of the fluid to the collector surface by advection and diffusion, and is quantified by the collection efficiency, η_0 ; the second step is the physico-chemical attachment of the particles to the collector, quantified by the attachment efficiency, α , which represents the ratio of the number of particles sticking to the collector after collision to the number of particles colliding with the collector. The product of these two contributions is expressed by the total removal efficiency, η , which includes both the transport and the attachment of the particles. Among the different filtration theories, one which is very often referred to is the model by Yao et al. [1], used to understand particle deposition in packed beds [28]: its theoretical foundation

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will be explained later on. Another class of widely used models are the so called pore-network models, where the porous medium is described by a graph-like geometrical construct [29–33].

These models predict particle deposition, or in other words particle removal from the suspension, through the analytical solution for the fluid flow in simplified geometric models: Levich refers to diffusion to a single solid particle descending freely in an infinite medium at very low fluid and particle velocity (Stokes flow), whereas the Happel model represents the porous medium with a unit cell constituted by a spherical solid collector inside a fluid shell, with their volume ratio chosen so that the porosity of this single cell is equal to the porosity of the actual porous medium. Generally, these models are developed for a single collector, while the influence of the other grains of the porous medium on the flow around this collector is accounted for through geometry-based, often empirical, corrective parameters [17]. Moreover, these solutions are valid only for clean-bed filtration (before any significant deposition of particles on the collector occurs).

The difficulties in investigating these issues from the experimental point of view have prevented the development of accurate corrections to account for the presence of many grains (collectors) of irregular (i.e.: highly non-spherical) shapes and characterized by wide grain size distributions. Nowadays, the advancement of detailed mathematical models based on computational fluid dynamics (CFD) offers an interesting alternative to experimental investigation: some pore-scale simulations of physical packing of spheres [34] and uniformly-sized flattened half-spheres have recently been performed [35].

The objective of this work is therefore to improve the current understanding of particle transport and deposition in porous media, by means of more detailed CFD simulations. In the micro-scale simulations small but representative portions of several porous media are considered and the details of the porous structure included. Many different representations of grain packings are investigated, in order to explore the influence of porosity, grain size and shape values. Some of the geometries used in this work were also successfully used in a recent study of pore-scale flow of non-Newtonian fluids in porous media [36], and are similar to those employed by other authors in similar studies [37]. First fluid flow is described by solving the continuity and Navier–Stokes equations, since particles are assumed to follow the flow, and results are compared with theoretical predictions of flow in porous media. Then, under the hypothesis of clean-bed filtration, particle deposition is investigated with focus on Brownian and steric interception mechanisms. Particular attention is devoted to the quantification of the effect of the irregularity of the grains and of the presence of multiple grains (or collectors) in the packing.

2. Governing equations and theoretical background

Although the length-scales involved in the investigation of flow in the pores of porous media are very small (at the order of hundreds of μm), the continuum hypothesis for the fluids holds true. As a first step the fluid velocity field can be determined in a CFD simulation, by solving the continuity and Navier–Stokes equations, that in the case of incompressible fluids read as follows:

$$\frac{\partial U_i}{\partial x_i} = 0, \quad (1)$$

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 U_i}{\partial x_j^2}, \quad (2)$$

where U_i is the i th component of the fluid velocity, p is the fluid pressure, and ρ and ν are its density and kinematic viscosity, respectively. These equations are generally applied with non-slip

boundary conditions ($U_i = 0$) at the grain wall. The continuum approach can also be adopted for the particles, as long as their size is smaller than the size of the pores. Moreover, we assume the concentration of particles in the liquid to be low enough to describe the diffusive flux through Fick's law. Thus, in an Eulerian framework the transport of particles can be described by solving the well known convection–diffusion equation:

$$\frac{\partial C}{\partial t} + U_j \frac{\partial C}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\mathcal{D} \frac{\partial C}{\partial x_j} \right), \quad (3)$$

where C is the particle concentration and \mathcal{D} is the particle diffusion coefficient due to Brownian motion, generally estimated with the Einstein equation [38]:

$$\mathcal{D} = \frac{k_B T}{3\pi\mu d_p}, \quad (4)$$

where k_B is the Boltzmann constant, T is the temperature, $\mu = \rho\nu$ is the dynamic viscosity and d_p is the particle size. As mentioned it is assumed that particles follow the fluid: a condition typically verified for solid particles (of density of about 5000–10,000 kg m^{-3}) moving in water at room temperature with size equal to or smaller than 1 μm or, more properly, when the suspended particles' Stokes number, identifying the ratio between the characteristic relaxation time of the particle and that of the fluid is very small ($\ll 1$), as it is the case under all the operating conditions under scrutiny in this work.

On the other hand hydrodynamic interactions, namely the increase in viscous drag force on the particles in the vicinity of the collector, are also present. As a result, their velocity decreases due to the additional friction from the fluid and the wall. This hydrodynamic retardation phenomenon may cause a deviation of some significance in the particles' path from the streamlines of the undisturbed flow near the collector when the distance between the particle and the collector is of the order of 2 or 3 particle radii [39]. Moreover, the particles' mobility near the wall is also reduced, decreasing the particle diffusivity coefficient which is not constant anymore but depends on the distance to the wall. Corrective factors for both particle velocity and their diffusivity coefficient, accounting for these hydrodynamic interactions, have been obtained in a number of earlier studies [39–41]. In this work we will be considering the case where chemical conditions are favorable to particle attachment (as will be explained later on), thus accounting for the contribution of all near-wall, sub-particle size attractive and repulsive forces (e.g.: London attraction forces) in a single attachment efficiency parameter. In this framework, it would not be possible to include explicitly the effects of hydrodynamic interaction separate from the calculation of these forces as, in the absence of any attractive force, the particles would not be able to reach the collector lacking the means to overcome the viscous repulsion [22]. A useful approximation in this case is the Smoluchowski–Levich approximation, in which it is assumed that the hydrodynamic retardation experienced by the particle while approaching a solid wall is balanced by the attractive London forces [18,41]. In fact, Van der Waals, electrical double layer and hydrodynamic interactions are excluded from the calculations. Neglecting the effects of the latter makes it possible to assume that the particles move with velocity equal to the fluid (as seen earlier) and that the diffusion coefficient is independent of the particle's position in the domain. This approximation is only valid when the particle size is smaller than the thickness of the particle diffusion boundary layer, which sets an upper limit equal to, in the majority of cases, a few hundred nanometres of size [42,43]. This range covers a large part of the cases explored in this study, and an assessment of the possible deviations due to the use of this approximation in this work will be done in the results section.

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