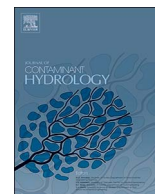




Contents lists available at ScienceDirect

Journal of Contaminant Hydrology

journal homepage: www.elsevier.com/locate/jconhyd

A robust upscaling of the effective particle deposition rate in porous media

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ARTICLE INFO

Keywords:

Deposition efficiency

Porous media

Colloid transport

Volume averaging

MSC:

76S05

35Q79

80A20

ABSTRACT

In the upscaling from pore to continuum (Darcy) scale, reaction and deposition phenomena at the solid–liquid interface of a porous medium have to be represented by macroscopic reaction source terms. The effective rates can be computed, in the case of periodic media, from three-dimensional microscopic simulations of the periodic cell. Several computational and semi-analytical models have been studied in the field of colloid filtration to describe this problem. They typically rely on effective deposition rates defined by complex fitting procedures, neglecting the advection-diffusion interplay, the pore-scale flow complexity, and assuming slow reactions (or large Péclet numbers). Therefore, when these rates are inserted into general macroscopic transport equations, they can lead to several conceptual inconsistencies and significant errors. To study more accurately the dependence of deposition on the flow parameters, in this work we advocate a clear distinction between the surface processes (that altogether defines the so-called attachment efficiency), and the pore-scale processes. With this approach, valid when colloidal particles are small enough, we study Brownian and gravity-driven deposition on a face-centred cubic (FCC) arrangement of spherical grains, and define a robust upscaling based on a linear effective reaction rate. The case of partial deposition, defined by an attachment probability, is studied and the limit of perfect sink is retrieved as a particular case. We introduce a novel upscaling approach and a particularly convenient computational setup that allows the direct computation of the asymptotic stationary value of effective rates. This allows to drastically reduce the computational domain down to the scale of the single repeating periodic unit. The savings are ever more noticeable in the case of higher Péclet numbers, when larger physical times are needed to reach the asymptotic regime and thus, equivalently, much larger computational domain and simulation time would be needed in a traditional setup. We show how this new definition of deposition rate is more robust and extendable to the whole range of Péclet numbers; it also is consistent with the classical heat and mass transfer literature.

1. Introduction

Particle transport and deposition are fundamental multi-scale phenomena behind several natural and engineered processes. One of the many examples of their importance is related to the ever greater attention attracted by the environmental issue of pollutants in groundwater systems and the development of correspondent remediations techniques, such as the injection of nanoscopic zero-valent iron particles, to cite a particular successful application (Krol et al., 2013; Vecchia et al., 2009; Velimirovic et al., 2016). More in general, the study of particle deposition is of central importance in filtration processes to enhance air and water quality (Huber et al., 2000; McDowell-Boyer et al., 1986; Tiraferri et al., 2011), chromatographic systems, catalytic cells and packed bed reactors (Bensaid et al., 2010; Dixon and Nijemeisland, 2001; Kolakaluri et al., 2015), enhanced oil

recovery techniques (Shi et al., 2013), and even drug delivery studies (Gordon et al., 2014; Pankhurst et al., 2003). All these processes rely on a detailed understanding of how transported solutes/particles flow through a porous matrix and interact with it. Despite the differences between solutes and nano-particles (or colloids), they are both affected by the upscaling challenges due to the pore-scale flow, and the simplified physical models of the latter can be conveniently reformulated, discretised and upscaled with similar techniques. Thus, in this introduction, we will give a brief overview of the theoretical framework typically used in the study of mass transport and particle deposition in porous media and, in particular, of the classical *colloid filtration theory*. Secondly, we will touch upon the issues that affect the correlations commonly used in macroscopic models and some inconsistencies in the process of upscaling the heterogeneous reaction at the pore-scale to a homogeneous reaction term in a macroscopic transport equation.

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Received 20 February 2017; Received in revised form 27 July 2017; Accepted 8 September 2017

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This will form the groundwork for the following sections, where a robust and mathematically sound methodology for the calculation and upscaling of deposition efficiency will be proposed, constituting the main contribution of this work. Results from micro-scale fluid dynamic simulations are then proposed in the last section.

1.1. Mass transfer and particle deposition

In the dimensional analysis of mass transfer phenomena, the most used dimensionless quantity is the Sherwood number, which describes the ratio between convective mass transfer and diffusive transport, and is the analogous of the Nusselt number used in heat transfer. It can be defined as:

$$N_{Sh} = \frac{hL}{\mathcal{D}_m}, \quad (1)$$

where L is a characteristic length (m), and \mathcal{D}_m is the molecular diffusion coefficient ($\text{m}^2 \text{s}^{-1}$); h (m s^{-1}) is the mass transfer coefficient commonly used in the mass transfer equation:

$$I = h \Delta C \mathcal{S}, \quad (2)$$

where I is the molar flux (mol s^{-1}), \mathcal{S} the effective mass transfer surface (m^2), and ΔC the concentration driving force (mol m^{-3}). In most mass transfer applications in porous media, the characteristic length is taken to be equal to the effective grain diameter d_g . As such, the mass transfer is then characterised as

$$N_{Sh} = Id_g/(\mathcal{D}_m \Delta C \mathcal{S}).$$

We will make use of these definitions in our work, where we will consider the case of solute deposition (or, equivalently, filtration). A wide bibliography is available on this topic, and the approach most commonly employed in order to determine a single parameter describing the filter effectiveness from its features and the operating conditions under investigation, is to define a *collector efficiency* η (Logan et al., 1995; Yao, 1968; Yao et al., 1971). This *total efficiency coefficient* is expressed as the contribution of two terms: $\eta = \alpha\eta_0$. The first, α , is the attachment efficiency, describing the probability of a particle colliding with the solid grain being adsorbed, with $0 < \alpha < 1$ depending on the specific physico-chemical features of the system. The second term, η_0 , describes the migration of particles from the bulk of the fluid to the surface of the grains, and is usually thought of as a contribution of different mechanisms, namely Brownian diffusion, sterical interception and inertial (and gravitational) effects. Furthermore, it is typically assumed that these contributions are additive¹(Prieve and Ruckenstein, 1974; Yao et al., 1971):

$$\eta_0 = \eta_B + \eta_I + \eta_G. \quad (3)$$

Many efforts in colloid filtration theory have been devoted to the precise quantification of the efficiency η in specific micro-scale models, and to formulate its expression as a function of macro-scale parameters. The earliest studies, by Levich (1962), dealing with diffusion on a solid sphere immersed in an infinite flow field moving with creeping flow, resulted in the evaluation of the molar flux towards the grains as:

$$I = 7.98C_\infty \mathcal{D}_m^{\frac{2}{3}} U^{\frac{1}{3}} a^{\frac{4}{3}}, \quad (4)$$

where a is the solid grain radius (m), C_∞ is the upstream solute concentration (mol m^{-3}), and U is the fluid upstream approach velocity (m s^{-1}). Defining the deposition efficiency as the ratio between the molar flux to the grains and the advective molar flux leads to ² (for the sole Brownian mechanism):

$$\eta_B = \frac{I}{\pi d_g^2 U C_\infty} = 4.04 N_{Pe}^{-\frac{2}{3}}, \quad (5)$$

where N_{Pe} is the Péclet number.

One issue with this model, aside from the clear impossibility of representing a randomly packed bed as a collection of isolate spheres, lies in the particular boundary condition employed by Levich (1962), where the solute concentration on the surface of the grain at the impinging point is set equal to the upstream concentration. This comes from the assumption of advection being dominant over diffusion, which limits the usefulness of this expression (and others, built on this same simplification) to $N_{Pe} \gtrsim 70$.

In order to account for the packed bed topology and, most importantly, for the effect that neighbouring grains have on the filtration efficiency of a single collector, Pfeffer (1964) and Pfeffer and Happel (1964) obtained the following relation:

$$N_{Sh} = As^{\frac{1}{3}} N_{Pe}^{\frac{1}{3}},$$

where As is a porosity-dependent parameter equal to $As = \frac{2(1-\gamma^5)}{2-3\gamma+3\gamma^5-2\gamma^6}$, where $\gamma = (1-\epsilon^{1/3})$ and ϵ is the porous medium porosity. Considering the As parameter and putting the last few expressions together, an expression for η similar to Levich's relation can be obtained, i.e.:

$$\eta_B = 4As^{\frac{1}{3}} N_{Pe}^{-\frac{2}{3}}. \quad (6)$$

A great deal of work has been done over the years, based on the colloid filtration theory, to refine the understanding of solute fate and transport by improving these single collector models (Johnson and Hilpert, 2013; Long and Hilpert, 2009; Rajagopalan and Tien, 1976; Tufenkji and Elimelech, 2004), and then building a connection between the single collector efficiency η calculated at the microscopic scale, and an upscaled reaction rate employable in a macroscopic transport equation, K_d .

In the next section, we will detail some of the issues with these studies, especially with regards to the assumptions considered in the derivation of the micro-scale models, and their impact on a successful upscaling. For the sake of clarity, we will limit the following exposition to the case of Brownian deposition and gravity, but the same approach can be extended to other physical mechanisms that have been subject of a considerable amount of work such as the effects of particle inertia, Van der Waals interactions and other chemical–physical interaction phenomena: the reader is referred to the extensive literature on the wider topic of colloid deposition.

1.2. Upscaling particle deposition: the role of η and K_d

As it has been mentioned, the most widely used approach in the colloid deposition literature has been to study in detail simplified models representing a single collector, followed by a heuristic step providing the link between solute transport in the vicinity of one collector and the evolution of the phenomenon at the macro-scale. The construction of the simplified model itself is of critical importance in order to avoid gross misrepresentations of the structure of the porous medium under consideration. In the preceding section we have mentioned that the early models of the colloid filtration theory described the porous matrix as an assemblage of isolated spheres (Levich, 1962; Yao et al., 1971); Rajagopalan and Tien (1976) then combined the results from Yao with the conceptualization of Happel's sphere in cell model, which inherently carries the information about the packing porosity and takes into account the effect of neighbouring grains on the transport around one collector.

In turn, a relatively modern description improved on Happel's model by substituting the single sphere with two touching hemispheres (Ma et al., 2009): this seemingly simple change does correct for the glaring missing piece in Happel's models, via the introduction of contact

¹ As we will demonstrate later on, this is not true for η .

² It has to be noted that the approximated numerical coefficients in this and preceding equation are not coming from empirical estimations, but result from the analytical evaluation of volume integrals in Levich's axisymmetric single sphere model development. For the breakdown of all the steps, refer to Levich (1962) (Section 14, "Diffusion to a free-falling solid particle").

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