Macroscopic modeling of colloids adsorption in porous media

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1. Introduction

Natural porous media such as soils or aquifers, contain colloidal particles. Depending on geochemical and hydrodynamic conditions, they can be transported by water, developing high reactivity and mobility. They may therefore act as vectors of pollutants and viruses dissemination in soils and groundwater. Some colloidal particles like bacteria are also likely to present a risk to the environment and health. However, adsorption of colloids on the solid matrix may severely limit their mobility in porous media, consequently, their fate depends on physico-chemical and hydrodynamic conditions.

Previous experimental studies [1] highlighted the role of ionic strength and Peclet number on both adsorption and release of particles. The objective of this work is to propose a macroscopic model (Darcy scale) that accurately describes the transport of colloids in the presence of adsorption process observed experimentally.

2. Experimental conditions

Artificial sintered porous media (diameter $= 5\,cm$; length $= 5\,or\,15cm$) were used in experiments. Colloidal suspensions of latex particles ($2a_p = 780\,nm$) were continuously injected. Breakthrough curves (BTC's) were obtained for different values of ionic strength $I \in [3; 12]\,mM$ at constant Peclet number, and for different values of $Pe \in [1.12; 75.]$ at a given value of I.

3. Macroscopic model

The transport of colloidal particles including adsorption on solid matrix of porous media is here described by a 1D advection-dispersion equation (Eq.1) [2, 6]:

$$\frac{\partial}{\partial t}\left(C + \frac{\rho_b}{\phi}\left(S_{par} + S_{ad}\right)\right) = D\frac{\partial^2 C}{\partial x^2} - V\frac{\partial C}{\partial x} \tag{1}$$

Where C represents the number of mobile colloids per unit volume of the aqueous phase. ρ_b, ϕ, D and V are respectively bulk density of solid matrix, porosity, dispersion coefficient and interstitial velocity. S_{ad} represents the fraction of colloidal particles that are irreversibly removed from flowing suspension. It is assumed to depend on C according to a first order reaction: $\frac{\rho_b}{\phi}\frac{\partial S_{ad}}{\partial t} = K_d C$. The adsorption coefficient K_d is given by $K_d = \frac{3}{4}\frac{1-\phi}{d_g}\alpha\eta U$ [5, 4], where α and η are respectively collision and collector efficiencies and d_g the grain diameter.

In (Eq.1) S_{par} represents the fraction of colloids that are attached to the solid matrix in an equilibrium state with a partition coefficient K_p such as $S_{par} = K_p C$. (Eq.1) can then be written as :

$$(1 + R)\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - V\frac{\partial C}{\partial x} - K_d C \tag{2}$$

Where R is the retardation factor; $R = \frac{\rho_b}{\phi}K_p = \frac{\rho_b}{\phi}\frac{S_{par}}{C}$; that governs the delay in breakthrough curves while K_d determines the BTC's final plateau value.

4. Results and discussion

Numerical simulations are performed using the commercial software COMSOL ®.
On (Fig.1a) and (Fig.1b) are shown the simulated BTC's as experimental data when varying I and Pe respectively.

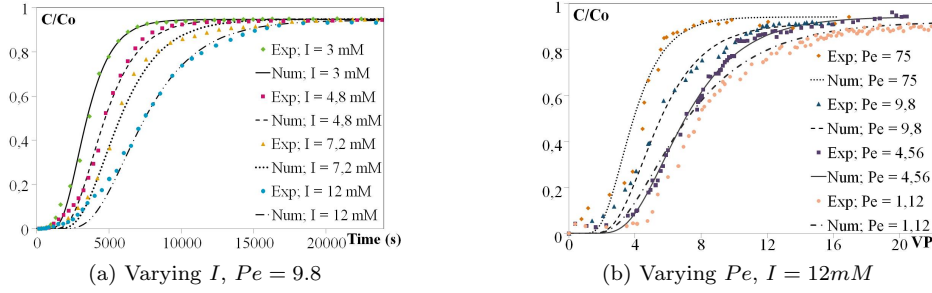(a) Varying I, $Pe = 9.8$

(b) Varying Pe, $I = 12mM$

Figure 1: Numerical and experimental breakthrough curves

Doing so, and knowing the experimentally determined values of K_d, R values corresponding to the best fit were obtained for each experiments (Fig.2).

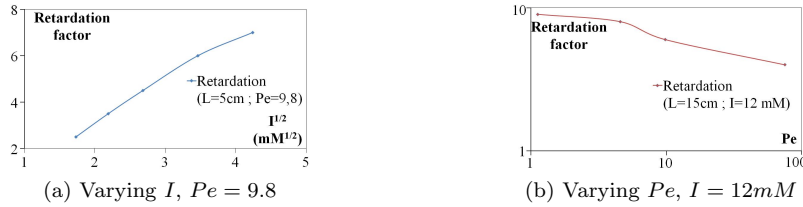(a) Varying I, $Pe = 9.8$

(b) Varying Pe, $I = 12mM$

Figure 2: Evolution of Retardation Factor

Following Tien [3], $\frac{S_{par}}{S_0} = \frac{C}{C_0}$, where C_0 and S_0 represent respectively injected concentration and the number of particles adsorbed at the inlet of the medium per unit of solid mass and are assumed to be constant at given experimental conditions. As S_0 should be proportional to the inverse of excluded area (area on which particles cannot be adsorbed), $\pi \left(a_p + \kappa^{-1}\right)^2$, where κ^{-1} is the Debye length, R is expected to follow a power law of I: $R \propto I^{\frac{1}{2}}$. (Fig.2a) shows that R effectively depends on I in the same way and is influenced by the electrostatic interactions through the excluded area of deposited particles at given hydrodynamic conditions. Moreover, even if it is difficult to predict the exact dependance of excluded area on Peclet number, it is however expected to increase with Pe due to hydrodynamic shadowing in the rear region of deposited particles. Nevertheless, this phenomenon becomes only important in the convection dominant regime. Whereas, very weak Pe influence should be observed in the diffusion regime. These asymptotic behaviors can be observed in (Fig.2b) even if the number of data is limited. For more quantitative predictive law, further experiments are necessary.

5. Conclusions

A macroscopic model with a retardation factor, R, and an adsorption coefficient, K_d, has been used to describe experimental data. The dependence of the retardation factor on both ionic strength (electrostatic interactions) and Peclet number (Hydrodynamics) has also been highlighted. Moreover, a non-dependence on medium length for same values of Pe and I has been underlined.

6. Bibliography

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