A Normalized and Extended Correlation Equation for Predicting Single-Collector Efficiency in Physicochemical Filtration in Saturated Porous Media

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ABSTRACT

The colloidal transport and deposition are phenomena involved in different engineering problems. In the environmental engineering field the use of micro- and nano-scale zerovalent iron (M-NZVI) is one of the most promising technologies for groundwater remediation. Colloid deposition is normally studied from a micro scale point of view and the results are then implemented in macro scale models that are used to design field-scale applications.

The single collector efficiency concept predicts particles deposition onto a single grain of a complex porous medium in terms of probability that an approaching particle would be retained on the solid grain. Different approaches and models are available in literature to predict it, but most of them fail in some particular conditions (e.g. low fluid velocity and/or very small or very big particle dimension) because they predict efficiency values exceeding unity.

By analysing particle fluxes and deposition mechanisms and performing a mass balance on the entire domain, the traditional definition of efficiency was reformulated and a novel total flux normalized correlation equation is proposed for predicting single-collector efficiency under a broad range of parameters. The new equation has been formulated starting from a combination of Eulerian and Lagrangian numerical COMSOL Multiphysics® simulations, performed under Smoluchowski-Levich conditions in a geometry which consists of a sphere enveloped by a cylindrical control volume (Figure 1). The normalization of the deposited flux is performed accounting for all of the particles entering into the control volume through all transport mechanisms (not just the upstream convective flux as conventionally done) to provide efficiency values lower than one under any possible combination of transport mechanisms. The particle fluxes onto the collector and through the control volume have been described mathematically as a summation of terms. In order to guarantee the independence of each term, the correlation equation is derived through a rigorous hierarchical parameter estimation process, accounting for single and mutual interacting transport mechanisms.

The new correlation equation provides efficiency values lower than one over a wide range of parameters (Figure 2) and it is valid both for point and finite-size particles. Moreover the correlation equation is extended to include porosity dependence and reduced forms are also proposed by elimination of the less relevant terms without losing the main features of the full equation.

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GRAPHICS

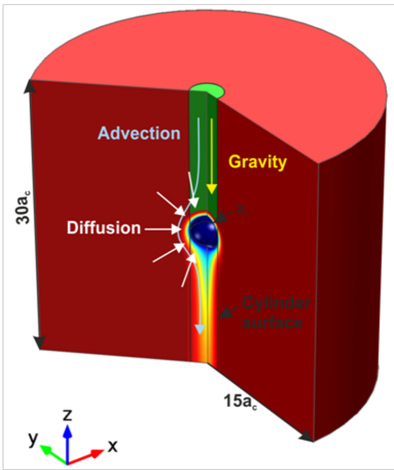

Figure 1: Geometry analyzed, sphere enveloped by a cylindrical control volume

Graphic1

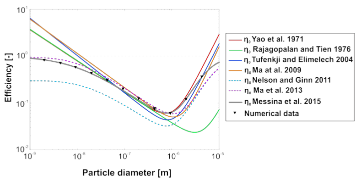

Figure 2: Comparison of the proposed equation with existing models for a typical range of particle size. Parameter values: porosity n=1, fluid density ρ_f =998 kg/m³, particle density ρ_p =1050 kg/m³, temperature T=288 K, fluid viscosity μ =9.8·10-4 Pa·s, collector radius a_c=250 μm, fluid approach velocity U=1·10⁻⁶ m/s.

Graphic2

$$\eta_N^R = \frac{1.5062 A_S N_R^{1.9834} + 7.5609 N_{Pe}^{-1} + N_G + 2.9352 A_S^{0.366} N_{Pe}^{-0.6338}\left(1 + 0.93621 N_R^{0.3737}\right) + 0.9461 N_G^{0.6550} N_{Pe}^{-0.3450}}{\left(1 + 6.0098 N_R^{1.9834}\right) + 7.5609 N_{Pe}^{-1} + N_G + 2.9352 A_S^{0.366} N_{Pe}^{-0.6338}\left(1 + 0.93621 N_R^{0.3737}\right) + 2.7972 N_G^{0.6550} N_{Pe}^{-0.3450}}$$

Graphic3