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Regular Article

# An extended and total flux normalized correlation equation for predicting single-collector efficiency

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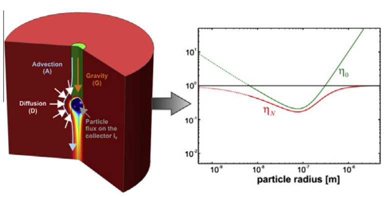
## GRAPHICAL ABSTRACT

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## ABSTRACT

In this study a novel total flux normalized correlation equation is proposed for predicting single-collector efficiency under a broad range of parameters. The correlation equation does not exploit the additivity approach introduced by Yao et al. (1971), but includes mixed terms that account for the mutual interaction of concomitant transport mechanisms (i.e., advection, gravity and Brownian motion) and of finite size of the particles (steric effect). The correlation equation is based on a combination of Eulerian and Lagrangian simulations performed, under Smoluchowski–Levich conditions, in a geometry which consists of a sphere enveloped by a cylindrical control volume. 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 over a wide range of parameters. 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 correlation equation, valid both for point and finite-size particles, is extended to include porosity dependency and it is compared with previous models. Reduced forms are proposed by elimination of the less relevant terms.



## 1. Introduction

Particle transport and deposition in saturated porous media are important processes occurring in natural and engineered systems. Colloidal filtration is a phenomenon of pivotal importance in numerous fields, including the propagation of contaminants and of microorganisms in aquifer systems [1–8], and the clogging of depth filters and wells [9,10]. Other applications involving particle transport and deposition are: the design of remediation interventions by using nanoparticles as reagents [11–15], the delivery of agents for contrast [16] or for thermo-radiotherapy in medicine [17,18], enhanced oil recovery or imaging in reservoir engineering [19] and several others [20,21].

In order to master and control all these applications, a deep understanding of the phenomena involved in particle transport and deposition in saturated porous media is necessary. In this context porous media are described as an ensemble of "collectors" or grains on which the transported particles are collected or

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deposited. In turn, deposition of particles from a suspension to a collector surface may be viewed as a two-step process: (1) the transport of the particles from the bulk of the suspension to the proximity of the collector and (2) the particle adhesion to the collector/grain surface, which depends on the nature of particle-collector interactions [22]. The first step is usually quantified by $\eta_0$, the single collector contact efficiency, that expresses the number of particles that reach the collector divided by the advective rate entering through the projection of the collector (Eq. (3)); the second step is commonly quantified by the attachment efficiency $\alpha$, which is the fraction of the particles coming into contact with the collector that actually attaches onto it. The product of these two values gives, as a result, the single collector removal efficiency $\eta$, which accounts for both the transport and attachment steps [23,24].

According to previous studies, the mechanisms responsible for particle transport are mainly three: Brownian motion, gravity and interception [25] (respectively the blue trajectory *AD* in Fig. 1b, the magenta trajectory *G* in Fig. 1a and the red trajectory *AS* in Fig. 1a). Taking advantage of the additivity concept, Yao et al. [25] firstly proposed in 1971 a correlation equation for the single collector contact efficiency, that is the summation of three partial efficiencies due to Brownian motion $\eta_D$, due to gravity $\eta_G$, and due to interception $\eta_I$. This approach, that neglects the full set of mutual interactions between the different transport mechanisms, reads as follows:

$$\eta_{0\ \mathrm{Yao}} = \eta_D + \eta_G + \eta_I = 4.04 N_{Pe}^{-2/3} + N_G + \frac{3}{2} N_R^2 \quad (1)$$

where $N_{Pe}$ is the Peclet number, $N_G$ is the gravity number and $N_R$ was defined as the interception number, but in this study for the sake of generalization it will be referred to as steric number or aspect ratio. A detailed definition of these dimensionless numbers is reported in Table 1. It is important to remind here that the additivity is clearly a simplification hypothesis, as the different mechanisms, which are inherently non-linear, operate jointly and therefore neglecting their interactions may lead to large errors.

The first term at the right side of Eq. (1) was derived analytically at high Peclet numbers ($N_{Pe} > 70$) from the results of Levich [26], and takes into account the mutual influence of advection and Brownian motion (or Brownian diffusion). The gravity and interception terms, were analytically calculated by Yao [27], and account respectively for the deposition rate due to gravity and to advection (in this last case for finite-size particles).

Many other more sophisticated correlation equations based on different geometries, such as Happel's and Hemisphere-in-cell, derived by using different numerical approaches (i.e., Lagrangian versus Eulerian) and including more interaction mechanisms (i.e., Van der Waals forces and others) were proposed afterward. Most of them were fully or partially derived starting from the above-mentioned additivity assumption.

Rajagopalan and Tien [28] (RT in the figures) extended heuristically the correlation equation presented by Yao et al. [25] by performing a numerical trajectory analysis of non-Brownian particles in the presence of the Van der Waals force and of the hydrodynamic retardation in the Happel's sphere-in-cell model [29]. In 2004 Tufenkji and Elimelech [30] (TE) developed a correlation equation by performing Eulerian simulations in the Happel's geometry and accounting for the simultaneous presence of the transport mechanisms and the effects of the Van der Waals force and of the hydrodynamic retardation [31]. In 2005 Nelson and Ginn [32] adopted a Lagrangian approach in the Happel's geometry, simulating the simultaneous presence of all the forces acting on the particles (i.e., fluid drag, gravity, Van der Waals, electric-double layer, Brownian diffusion and hydrodynamic retardation). Ma et al. [33] (MPFJ) introduced the hemispheres-in-cell model geometry which allows the effect of grain-to-grain contact points to be taken into account. Recently Boccardo et al. [34] solved the full Navier Stokes flow field by exploiting a Eulerian approach and then proposing an extension of the correlation equation for higher Reynolds numbers. As already discussed, all the above mentioned models are based on the simplification hypothesis of additivity of the three partial efficiencies ($\eta_D$, $\eta_G$ and $\eta_I$), as reported in Eq. (1), accounting for two single acting transport mechanisms (gravity and advection) and one mixed term due to the interaction of Brownian diffusion and advection.

As already pointed out by Song end Elimelech [35], Nelson and Ginn [31] and Ma et al. [36], the other main drawback of most of

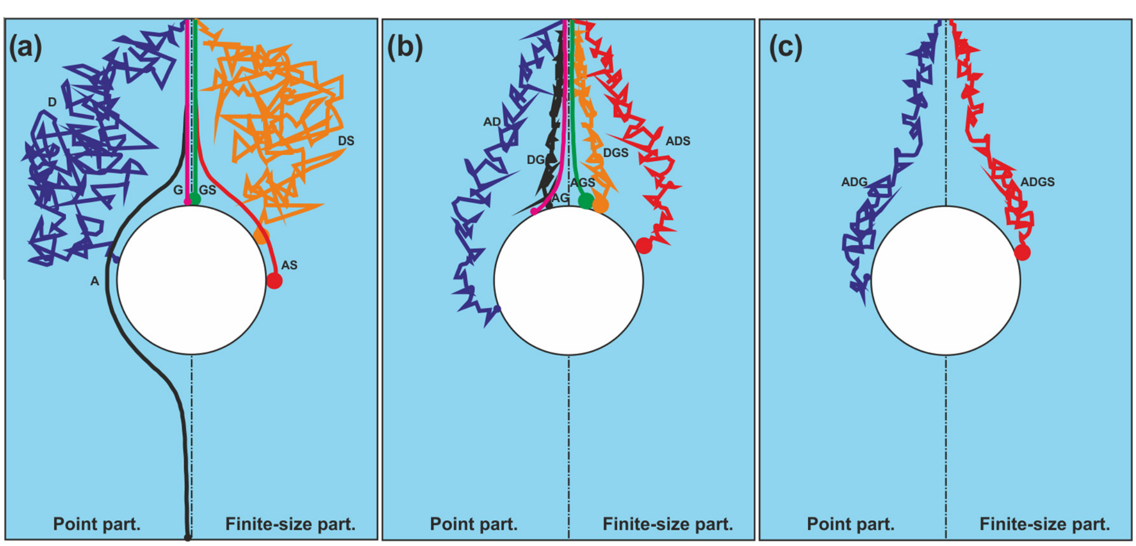


**Fig. 1.** Main mechanisms of particle transport and deposition. (a) Single transport mechanism: diffusion *D* (blue line), advection *A* (black line), gravity *G* (magenta line), diffusion and steric effect *DS* (orange line), advection and steric effect *AS* (red line), gravity and steric effect *GS* (green line); (b) Two active transport mechanisms: diffusion and advection *AD* (blue line), gravity and diffusion *DG* (black line), advection and gravity *AG* (magenta line), diffusion–advection and steric effect *ADS* (red line), gravity–diffusion and steric effect *DGS* (orange line), advection–gravity and steric effect *AGS* (green line); (c) Three transport mechanisms acting together: advection–diffusion and gravity *ADG* (blue line), advection–diffusion–gravity and steric effect *ADGS* (red line). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)