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# General correlation equations for predicting filtration efficiency under unfavorable surface interactions

# You-IM Chang\*, Wei-You Cheng, Keng-Yi Liao

Department of Chemical Engineering, Tunghai University, 40704 Taichung, Taiwan

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## 1. Introduction

In deep bed filtration used in water and wastewater treatment, a thorough understanding of the transport and deposition behavior of colloidal particles in porous media is essential to the design and operation of filtration systems. Accurate predictions of the dynamic filtration behavior of colloidal particles can be obtained by using the method of trajectory analysis [1] or solving the convective diffusion equation [2,3]. Results of such rigorous approach reveal that the aspect ratio, the influent flow rate, the gravitational force and the parameters determining the magnitudes of interaction energy barriers according to DLVO theory [4], all play important roles in describing the filtration behavior of colloidal particles. When written in the dimensionless forms, the initial collection efficiency  $\eta_0$  of colloidal particles can be expressed as

$$\eta_0 = \eta_0(N_R, N_{Pe}, N_G, N_A, N_{Lo}, N_{DL}, N_{E1}, N_{E2})$$
(1)

where  $N_R$  is the aspect ratio,  $N_{Pe}$  is the Peclet number,  $N_G$  is the gravitational number,  $N_A$  is the attraction number,  $N_{Lo}$  is the van der Waals number,  $N_{DL}$  is the electric double layer number (*i.e.*  $N_{DL} > > 1.0$  means  $a_{pi} > > \kappa^{-1}$ ),  $N_{E1}$  and  $N_{E2}$  are the first and the second electrokinetic numbers of the DLVO theory, respectively. The definitions of these dimensionless numbers are provided in Table 1. Theoretical analysis of general correlation equations to predict  $\eta_0$  in porous media abound in the literatures. A thorough review of these studies can be found in Tien and Ramarao [5]. Some of the important correlation equations are briefly introduced below.

\* Corresponding author.

E-mail address: yichang@thu.edu.tw (Y.-I. Chang).

## ABSTRACT

General correlations were developed in this work for predicting the initial collection efficiency and the filter coefficient ratio under the unfavorable surface condition when electrostatic repulsive force prevents colloidal particles from reaching the filter grain surfaces. Simulation was done by using the Brownian dynamics method and experimental data was used for verifying the general correlations developed. It was found that the theoretical and experimental results fit the predicted filter coefficient ratio best by using algebraic averaged correlations.

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Generally speaking, those correlation equations for predicting  $\eta_0$  could not explain the experimental results satisfactorily under unfavorable surface interactions. When the combined surface interaction forces between filter grains and colloidal particles of the DLVO theory (including the electric double layer repulsive force and the van der Waals attractive force) is repulsive, colloidal deposition becomes unfavorable. This problem was not solved until an empirical equation established by Bai and Tien [6] was found to describe those experimental results reasonably well. By adopting the concept of Vaidyanathan and Tien [7], they found that those available colloidal filtration data under the unfavorable deposition conditions at various ionic strengths of suspension can be well described by using a filter coefficient ratio  $\alpha$ , which is defined as the ratio of the initial collection efficiency  $\eta_0$  to its value in the absence of the electrostatic repulsive force of DLVO theory  $\eta_{0S}$  (Curves D shown in Figs. 2 and 4) as

$$\alpha = \frac{\eta_0}{\eta_{0S}} \tag{2}$$

This filter coefficient  $\alpha$  was found to be a function of those parameters used in describing the magnitudes of van der Waals attractive and electrostatic repulsive energies of DLVO theory. Note that this filter coefficient  $\alpha$  represents the fractional reduction in the deposition rates of colloidal particles caused by the presence of the repulsive energy barrier of DLVO theory.

Since the accurate prediction of the effects of unfavorable surface interactions on filtration for filter coefficient is important when establishing the guidelines for making colloidal suspensions more amenable to the filtration process, an investigation on the general correlation equations for predicting  $\alpha$  is given in this work.

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Table 1

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Sur	nmarv	of	dimensionless	parameters	presented	in	the	general	correlation	equations

Parameter	Definition	Physical interpretation
As	$\frac{2(1-\gamma^5)}{2-3\nu+3\nu^5-2\nu^6}$	Porosity-dependent parameter
N <sub>A</sub>	$\frac{A}{12\pi \mu a_{nl}^2 U}$	Attraction number
N <sub>DL</sub>	кa <sub>pi</sub>	Electric double-layer force parameter
N <sub>E1</sub>	$va_{pi}(\xi_p^2 + \xi_g^2)/4k_BT$	First electrokinetic parameter
N <sub>E2</sub>	$2\left(\frac{\xi_p}{\xi_g}\right)/[1+\left(\frac{\xi_p}{\xi_g}\right)^2]$	Second electrokinetic parameter
$N_G$	$\frac{2}{9} \frac{a_{Pi}^2(\rho_{Pi} - \rho_f)g}{\mu U}$	Gravity number; ratio of the Stokes particle setting velocity to the approach velocity of the fluid
N <sub>Pe</sub>	$\frac{Ud_g}{D_{\infty}}$	Peclet number characterizing ratio of the convective transport to the diffusive transport
N <sub>R</sub>	$\frac{d_p}{d_p}$	Aspect ratio
Nr.	-sA	London force parameter

The parameters in the various dimensionless groups are as follows:  $d_g$  is the collector diameter,  $d_p$  is the particle diameter, U is the inlet fluid velocity,  $D_{\infty}$  is the bulk diffusion coefficient (describe by Stokes-Einstein equation), A is the Hamaker constant,  $k_B$  is the Boltzmann constant, T is the fluid absolute temperature,  $a_{pi}$  is the *i*th particle radius,  $\rho_{pi}$  is the *i*th particle density,  $\rho_f$  is the fluid density, g is the gravitational acceleration,  $\kappa$  is the reciprocal of the electric double layer thickness,  $\nu$  is the dielectric constant of the fluid (=89x 10<sup>-19</sup>coulombs/volt/cm),  $\xi_p$  and  $\xi_g$  are the surface (zeta) potentials (in mV) of particle and collector, respectively, and  $\gamma = (1 - \varepsilon)^{1/3}$ .



Fig. 1. The schematic diagram for simulating the deposition of colloidal particles in a SCT constricted tube model.

#### Table 2

Summary of parameter values adopted in the present simulations.

Parameter	Range			
Particle radius, $a_{pi}$	0.1–1.0 $\mu$ m			
Collector (grain) Diameter, $d_g$	$100\mu m$			
Inlet fluid velocity, U	0.1–3.0 cm/s			
Inlet particle concentration, $C_{in}$	1000 particles/cm <sup>3</sup>			
Hamaker constant, A	$1.0 \times 10^{-20}$ J			
Fluid absolute temperature, T	293.2 K			
Porosity, $\varepsilon$	0.4			
Absolute fluid viscosity, $\mu$	1.0 cP			
Particle density, $ ho_{pi}$	1.00-1.10 g/cm <sup>3</sup>			

## 2. Correlation equations for predicting $\eta_0$

Assuming that the filter coefficient due to three deposition mechanisms, namely diffusion  $\eta_D$ , interception  $\eta_I$  and gravitational force  $\eta_G$  are additive, Yao's model [8] is the first water filtration model that successfully predicts the initial collection efficiency  $\eta_0$  by numerically solving a simplified convective diffusion around a spherical collector for the various sizes of colloidal particles.

$$\eta_0 = \eta_D + \eta_I + \eta_G \tag{3}$$

with 
$$\eta_D = 4.04 A_S^{1/3} N_{Pe}^{-2/3}$$
  
 $\eta_I = \frac{3}{2} A_S N_R^2$   
 $\eta_G = \frac{(\rho_p - \rho)}{18 \mu U} g d_p^2$ 

Here, by using Happel's sphere-in-cell model [9],  $A_S$  is a porosity-dependent parameter defined as

$$A_{S} = \frac{2(1-\gamma^{5})}{2-3\gamma+3\gamma^{5}-2\gamma^{6}}$$
(4)

where  $\gamma = (1 - \varepsilon)^{1/3}$ , and  $\varepsilon$  is the porosity of the filter. However, the effects of the hydrodynamic interactions and the interaction energy barriers of DLVO theory were not considered in this classic filtration equation.

A more rigorous approach that includes hydrodynamic retardation corrections for the favorable surface interactions was developed by Rajagopalan and Tien [10]. Based on numerical solutions of the trajectory analyses made with a sphere-in-cell porous media model under various physical conditions, a correlation equation was obtained

$$\eta_0 = (1-\varepsilon)^{2/3} A_s N_{Lo}^{1/8} N_R^{15/8} + (3.375 \ x \ 10^{-3}) (1-\varepsilon)^{2/3} A_s N_G^{1.2} N_R^{-0.4} + 4(1-\varepsilon)^{2/3} A_s^{1/3} N_{Pe}^{-2/3}$$
(5)

Eq. (5) was found to be accurate enough in the interception range as well as the diffusion dominated region. Later on, by solving the convective diffusion equation with a perfect sink boundary condition, Tufenkij and Elimelech [11] obtained a modified correlation equation for describing the initial collection efficiency of colloidal particles onto a single spherical collector as

$$\eta_0 = \eta_D + \eta_I + \eta_G = 2.4A_S^{1/3} N_R^{-0.081} N_{Pe}^{-0.715} N_{Lo}^{0.052} + 0.55A_S N_R^{1.675} N_A^{0.125} + 0.22N_R^{-0.24} N_G^{1.11} N_{Lo}^{0.053}$$
(6)

The authors proved that their modified correlation equation showed remarkable agreement with those experimental results where electrostatic double layer interactions were negligible. Unfortunately, all the above correlation equations were inadequate

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