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Proposal for initial collection efficiency models for direct granular upflow filtration

Alexandre Botari[1*], Luiz Di Bernardo[2] and Angela Di Bernardo Dantas[3]

[1]*Departamento de Tecnologia, Universidade Estadual de Maringá, Avenida Ângelo Moreira da Fonseca, 1800, Zona VII, 87506-370, Umuarama, Paraná, Brazil.* [2]*Departamento de Hidráulica e Saneamento, Escola de Engenharia de São Carlos, Universidade de São Paulo, São Carlos, São Paulo, Brazil.* [3]*Universidade de Ribeirão Preto, Ribeirão Preto, São Paulo, Brazil. *Author for correspondence. E-mail: abotari@uem.br*

ABSTRACT. Mathematical models of the filtration process are based on the mass balance in the filter bed. Models of the filtration phenomenon describe the mass balance in bed filtration in terms of particle removal mechanisms, and allow for the determination of global particle removal efficiencies. This phenomenon is defined in terms of the geometry and the characteristic elements of granule collectors, particles and fluid, and the composition of the balance of forces that act in the particle collector system. This type of resolution is well known as the trajectory analysis theory. Particle trajectory analysis by mathematical correlation of the dimensionless numbers that represent fluid and particle characteristics is considered the main approach for mathematically modeling the initial collection efficiency of particle removal in water filtration. The existing initial collection efficiency models are designed for downflow filtration. This study analyzes initial collection efficiency models, and proposes an adaptation of these models to direct upflow filtration in a granular bed of coarse sand and gravel, taking into account the contribution of the gravitational factor of the settling removal efficiency in the proposal of initial collection efficiency models.

Keywords: mathematical modeling, trajectory analysis, mass balance, drinking water.

Proposta de modelos para o cálculo da eficiência inicial de remoção de partículas na filtração granular direta ascendente

RESUMO. Modelos matemáticos para a descrição do processo de filtração são baseados no balanço de massa em um dado volume de controle no meio filtrante e que permite determinar a eficiência global de remoção de partículas. Neste processo, são definidas as características físicas do fluido, dos grãos coletores e das partículas, tais como sua geometria e forma, e a composição das forças atuantes no sistema partícula-grão coletor. Este tipo de abordagem, conhecida como teoria pela análise da trajetória, é descrita pela correlação matemática de números adimensionais e constitui a principal abordagem na modelação matemática da eficiência inicial de remoção de partículas na filtração de água. Os modelos de eficiência inicial de remoção de partículas encontrados na literatura foram concebidos para a filtração descendente. Este trabalho analisa tais modelos e propõe novos para a filtração ascendente em meio granular de areia e pedregulho, alterando-se a contribuição da força gravitacional na parcela de eficiência de remoção pela sedimentação nos modelos de eficiência inicial global de remoção de partículas.

Palavras-chave: modelação matemática, análise da trajetória, balanço de massa, tratamento de água.

Introduction

Current models for calculating initial collection efficiency were conceived for downflow filtration (NGO et al., 1995) (TUFENKJI; ELIMELECH, 2004) (MAYS; HUNT, 2005) (NELSON; GINN, 2005). This paper proposes the adaptation of these models for application to direct upflow filtration in granular material, considering the primary importance of the gravitational factor in reaching the initial collection efficiency value. This proposition and analysis are based on experimental direct upflow and downflow filtration data from bench scale facilities.

The filtration medium may be considered a set of collectors in a given control volume. It is therefore possible to determine the removal efficiency of a single collector and then, assuming a geometric cell structure, add the contribution of the other collectors to complete the filtration medium (TUFENKJI; ELIMELECH, 2004).

The conception of the collector removal model required the definition of the following elements (BOTARI; DI BERNARDO, 2012):

- a geometric model of the collector and of the cellular arrangement (or set) of collectors and the respective conditions of the surrounding fluid;

- forces acting in the removal of particles;
- conditions for the solution of the trajectory or convective-diffusive equation.

For the non-Brownian particles, the convective-diffusive equation can be written as equation (1) (BOTARI; DI BERNARDO, 2012):

$$\frac{\partial C}{\partial t} + \vec{U} \times gra\vec{d}C = div\left(D \cdot gra\vec{d}C + m_o\ C\ gra\vec{d}\Phi\right) \quad (1)$$

where:
m_o represents particle mobility (s kg^{-1});
Φ is the interaction colloidal energy (*J*);
D is the diffusion constant ($m^2 s^{-1}$);
C is the particle concentration in the liquid phase (kg m^{-1});
and U is the fluid's superficial velocity (m s^{-1}).

The resolution of equation (1) requires extensive calculations and powerful computational tools; however, a more practical approach is based on the correlation of dimensionless numbers. This approach simplifies the trajectory analysis by correlating the dimensionless numbers of the mass balance in the control volume and the removal efficiency.

Initial collection efficiency models

Yao-Habibian's modified or Happel's modified model (YH)

Yao-Habibian's modified or Happel's modified model (YH) introduces a modification in the Yao-Habibian model, while retaining the other properties of the original model. This modification consists of the incorporation of Happel's (As) constant not only in the diffusive phenomenon but also in the convective and interception phenomena in the initial collection efficiency equation, according to equation (2) (see Table 1) (YAO et al., 1971):

$$\eta = 4\ A_S^{1/3}\ N_{Pe}^{-2/3} + \frac{3}{2}\ A_S\ N_R^2 + N_G \quad (2)$$

It is interesting to note that this model is appropriate not only for particles smaller than 1 μm, as observed in the earliest models, but also for larger particles (DHARMAPPA et al., 1992). See Table1.

The parameters of the dimensionless are: d_p is the particle diameter (m); d_c is the grain collector diameter (m); ρ_p is the specific particle mass (kg m^{-3}); ρ_f is the specific fluid mass (kg m^{-3}); g is the gravity acceleration (m s^{-2}); μ is the dynamic viscid of the fluid (N m^{-2} s^1); U is the fluid superficial velocity (m s^{-1}); H is the Hamaker constant (*J*)*;* K is the Boltzmann constant (*J* K^{-1}); T is the absolute temperature in Kelvin (*K*); f is the filtration bed porosity (dimensionless) and D is the diffusivity coefficient from Stokes-Einstein equation (m^2 s^{-1}).

Table 1. Physical Interpretation and Mathematical Definition of the dimensionless.

Physical Interpretation	Dimensionless	Mathematical Definition
Stokes particle sedimentation velocity in relation to fluid velocity	N_G: Gravitational Number	$N_G = \frac{d_p^2(\rho_p - \rho_f)g}{18\mu\ U}$
Interaction between London and van der Waals forces and the fluid velocity in the particle deposition in the grain.	N_{Lo}: London Number	$N_{Lo} = \frac{4H}{(9\pi d_p^2 \mu U)}$
Combination between van der Waals attraction force and London force influences and fluid velocity (interception)	N_A: Attraction Number	$N_A = \frac{H}{(3\pi d_p^2 \mu U)}$
Rate of energy interaction of van der Waals force and particle thermal energy	N_{vdW}: van der Waals Number	$N_{vdW} = \frac{H}{K\,T}$
Coefficient dependent of the porosity from Happel's model (sphere in cell)	A_s: Happel coefficient	$A_S = \frac{2(1-\gamma^5)}{2 - 3\gamma + 3\gamma^5 - 2\gamma^6}$ where: $\gamma = \sqrt[3]{(1-f)}$
Coefficients dependents of the porosity from Lee-Gieske model for superficial velocity correction	K_W e *p:* Lee-Gieske coefficients	$K_W = 1 - 1.8\alpha_f^{1/3} + \alpha_f - 0.2\alpha_f^2$ where: $\alpha_f = 1 - f$ and $p = \frac{(1 + 2\alpha_f)}{3 - 3\alpha_f}$
Relations of sizes: particle and grain collector	N_R: Interception Number	$N_R = \frac{d_p}{d_c}$
Relation forces: inertial and viscid forces	N_{Re}: Reynolds Number	$N_{Re} = \frac{\rho_f U d_c}{\mu}$
Relation between convective and diffusive transport	N_{Pe}: Peclet Number	$N_{Pe} = \frac{U d_c}{D}$ where: $D = \frac{KT}{(3\pi \mu d_p)}$

Lee-Gieske's modified model (LG)

The Lee-Gieske modified model (LG) is also based on spheres present in the geometric cell model similar to Happel´s Model. As in the Yao-Habibian modified or Happel modified model (YH), the LG model introduces a correction factor in the velocity of the collisions of the particles with the collector (TUFENKJI; ELIMELECH, 2004).

The factor correction coefficient (K_W) is incorporated in the initial collection efficiency model, as indicated in equation (3) (see Table 1):

$$\eta = 3.54\left(\frac{f}{K_W}\right)^{1/3} N_{Pe}^{-2/3} + \frac{3}{2}\frac{f \cdot N_R^2}{K_W\left(1+N_R\right)^p} + N_G \qquad (3)$$

In the LG model, the Lee-Gieske coefficient (K_W) also influences the diffusive and convective terms of the initial collection efficiency equation (DHARMAPPA et al., 1992). Another parameter introduced into the LG model is the coefficient (p), which considers the influence of porosity on the correction of particle velocity in the collector, as indicated in Table 1. These parameters influence the Brownian term (or portion) and the convective term (or portion) through the interception number (N_R) (see Table 1). This fact is repeated in the Rajagopalan-Tien (RT) and Tufenkji- Elimelech (TE) models. The LG model is also suitable for particles smaller and larger than 1 μm.

The Rajagopalan-Tien model (RT)

The Rajagopalan-Tien model (RT) is more complete than earlier models because it considers not only terms for the interception, sedimentation (gravity settling) and diffusion mechanisms of particle removal but also includes the effects of the reduction in the number of collisions due to the resistance of the incompressible fluid caused by the collision of two particles. This phenomenon is called the hydrodynamic restraining effect. The RT model also considers the effects of the London-van der Waals (LvdW or DLVO) forces of attraction and the electric interactions on the surface of particles or the Electric Double Layer Force (EDL). Today, this model is the most commonly used to calculate the initial collection efficiency in the filtration of drinking water (PETOSA et al., 2010; NELSON; GINN, 2005). The RT regression model is represented by equation (4) (see Table 1) (LOGAN et al., 1995):

$$\eta = 4A_S^{1/3} N_{Pe}^{-2/3} + A_S N_{Lo}^{1/8} N_R^{15/8} + 0.00338 A_S N_G^{1/2} N_R^{-2/5} \qquad (4)$$

The fluid velocity used for obtaining equation (4) was superficial velocity. Equation (4) shows the new dimensionless parameter called the London Number (N_{Lo}), which incorporates the London-van der Waals forces of attraction and the electric interaction charges on the surfaces (EDL), see Table 1. This equation was obtained by extensive computational efforts and resulted in a solution that combines the aforementioned particularities of the other models into an extensive range of values of the dimensionless numbers representative of the initial collection efficiency model (AMIRTARAJAH, 1988). The RT model also uses Happel's geometric model for the collector set. It is important to emphasize that the RT model is only valid for N_R of less than 0.18 (Table 1) (LOGAN et al., 1995).

Tufenkji-Elimelech's model (TE)

Tufenkji and Elimelech (2004) developed a new equation to calculate the initial collection efficiency based on Happel's geometric model. According to the authors, the model includes the hydrodynamic interactions and mechanical and electrical surface interactions. Equation (5) presents the two new dimensionless numbers (see Table 1):

$$\eta = 2.4 A_S^{1/3} N_{Pe}^{-0.715} N_R^{-0.081} N_{vdW}^{-0.052} + 0.55 A_S N_A^{0.125} N_R^{1.675} + 0.22 N_G^{1.11} N_R^{-0.24} N_{vdW}^{0.053} \qquad (5)$$

The TE model introduces the dimensionless numbers which consider the van der Waals forces of attraction in the interaction with particle thermal energy – the van der Waals Number (NvdW) – and the relation between the van der Waals forces of attraction and the fluid velocity in the interception of particle collision – Attraction Number (N_A) (see Table 1).

Unlike the RT model, the TE model does not present restrictions for low approach velocities or a Brownian regime. The TE model also considers hydrodynamics and van der Waals interactions in this regime (TUFENKJI; ELIMELECH, 2004) (JACOBS et al. 2007) (HOEK; AGARWAL, 2006).

Table 1 lists the physical interpretation and the mathematical definition of the dimensionless numbers used in the models presented in this study and listed in Table 2. Table 2 shows the four models of initial collector efficiency for downflow filtration used presented here. All the initial collection efficiency models in this section were developed for downflow filtration and are composed of the sum of the three transport mechanisms ($\eta = \eta_D = \eta_I = \eta_G$), diffusive transport ($\eta_D$); interception ($\eta_I$) and gravitational settling (η_G).

Table 2. Summary of the initial efficiency collector models equations for downflow filtration.

Model	Efficiency equation
Yao-Habibian Modify (YH)	$\eta = 4 A_S^{1/3} N_{Pe}^{-2/3} + \frac{3}{2} A_S N_R^2 + N_G$
Lee-Gieske (LG)	$\eta = 3.54\left(\frac{f}{K_W}\right)^{1/3} N_{Pe}^{-2/3} + \frac{3}{2}\frac{f \cdot N_R^2}{K_W (1+N_R)^p} + N_G$
Rajagopalan and Tien (RT)	$\eta = 4A_S^{1/3} N_{Pe}^{-2/3} + A_S N_{Lo}^{1/8} N_R^{15/8} + 0.00338\, A_S N_G^{1/2} N_R^{-2/5}$
Tufenkji and Elimelech (TE)	$\eta = 2.4 A_S^{1/3} N_{Pe}^{-0.715} N_R^{-0.081} N_{vdW}^{-o.052} + 0.55 A_S N_A^{0.125} N_R^{1,675} + 0.22\, N_G^{-0.24} N_R^{1.11} N_{vdW}^{-0.053}$

Upflow concept

For upflow filtration, Tien and Ramarao (2007) recommended the use of the initial collection efficiency models conceived for downflow filtration; however, the generalized application of these models in upflow filtration is not completely correct. Filtration experiments in sand bed using aerosol fluids with monodispersed particles of 1 μm in both directions (downflow and upflow) showed differences in the initial particle removal efficiency. According to Thomas et al. (1971), this difference is due to the gravitational effect in the flow direction. In upflow filtration, the direction of the gravity acceleration vector is opposite to that of the fluid velocity vector (fluid + particles), while in downflow filtration both vectors are in the same direction. In this case, the particle removal mechanism that is modified by the flow direction (gravitational effect) is gravitational settling (η_G).

The deeper penetration of the particles into the filtration medium in the upflow process explains the variation in global particle collection efficiency in deep bed filtration (THOMAS et al., 1971). Other authors (PARETSKY et al., 1971; GEBHART et al., 1973) proposed an upflow concept considering the change of the gravitational factor in the direction of the flow, using aerosols. This concept and the proposition of this study are also discussed herein.

Gebhart et al.'s concept

Gebhart et al. (1973) showed the differences between gravitational sedimentation in upflow and downflow aerosol filtration in terms of the hydrodynamic behavior of the particle's trajectory in streamline flows. The authors found the following relations, expressed through equations (6) and (7):

$$\frac{C\downarrow}{C_0} = \exp -\left(k + a\frac{V_s^b}{U^c}\right) L \qquad (6)$$

$$\frac{C\uparrow}{C_0} = \exp -\left(k - a\frac{V_s^b}{U^c}\right) L \qquad (7)$$

where:
C and C_0 are, respectively, the particle concentration or remaining particles (# L^{-1}) and the initial particle concentration (# L^{-1});
k represents the sum of all collection efficiency mechanisms that do not depend on the flow direction (dimensionless);
V_s is the settling velocity (cm s^{-1});
U is the fluid approach velocity (cm s^{-1});
L is the length of the filtering medium (cm);
a is the empirical factor and b, c are empirical exponents.

Dividing equations (6) and (7), one has:

$$\frac{C\uparrow}{C\downarrow} = \exp\ 2\ a\frac{V_S^b}{U^c} L \qquad (8)$$

Or, in the form of a Napierian logarithm,

$$\ln\left(\frac{C\uparrow}{C\downarrow}\right) = 2\ a\ V_S^b \left(\frac{1}{U}\right)^c L \qquad (9)$$

Gebhart et al. (1973) constructed two graphics on a bilogarithmic scale for V_S and 1 U^{-1}, obtaining straight lines with the following angular coefficients: $b = 0.69$ and $c = 0.90$. As indicated in Figures 1a and 1b, these values can be obtained, respectively, from the sum of constants d_1 and d_2 through the linearization equations (10) and (11) below:

$$\lg\left\langle \ln\left(\frac{C\uparrow}{C\downarrow}\right)\right\rangle = b \lg V_S + d_1 \qquad (10)$$

$$\lg\left\langle \ln\left(\frac{C\uparrow}{C\downarrow}\right)\right\rangle = c \lg\left(\frac{1}{U}\right) + d_2 \qquad (11)$$

From equation (12), the value of a is given by:

$$\log\left(2\ a\ L\right) = d_1 + d_2 \qquad (12)$$

Coefficients d_1 and d_2 of equation (12) are obtained from the graphics presented in Figures 1a and 1b. Gebhart et al. (1973) adopted an L value of 41 cm, which leads to an a value of approximately 0.02. The portion of the total initial collection efficiency provided by gravity settling is given by equation (13):

$$\eta_G = -0.02\,\frac{V_s^{0.69}}{U^{0.9}} \tag{13}$$

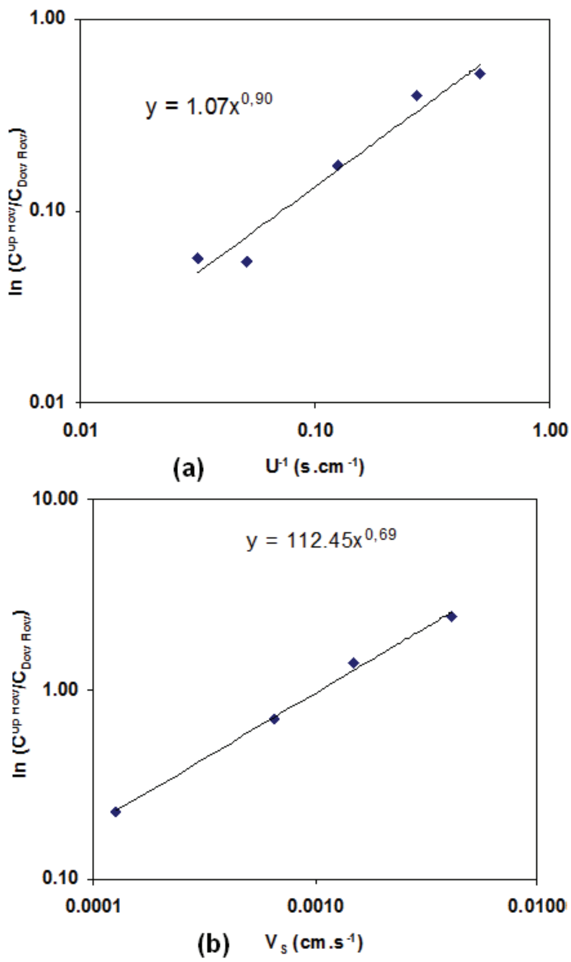

Figure 1. Graphics of mathematical regression to obtain the coefficients of Gebhart equation: d1 (Figure 1a) and d2 (Figure 1b). Source: Adapted from Gebhart et al. (1973).

Paretsky et al.'s concept

Paretsky et al. (1971) also observed experimental flows in both directions (up and down) in aerosol filtration as well as in horizontal sand filtration. These authors studied the mechanisms of diffusion, inertial interception and settling in deep bed filtration, and concluded that the collection efficiency due to gravity sedimentation (settling) at low velocities (less than 0.01 m s^{-1}) are independent of bed granule size, even without taking into account the influence of particle size variations (polystyrene particles of 1.1 μm).

Thomas el al. (1971) described the equations considering the flow direction in the collector's initial efficiency by the gravity settling removal mechanism for the downflow (equation 14) and upflow (equation 15) directions:

$$\eta_G\downarrow = (1+N_R)\,G \tag{14}$$

$$\eta_G\uparrow = -(1+N_R)\,G \tag{15}$$

where:
$\eta_G\uparrow$ and $\eta_G\downarrow$ are, respectively, the collection efficiency due to gravity sedimentation in the upflow and downflow directions;
N_R is the interception number ($d_p\ d_c^{-1}$); G is $V_s\ U^{-1}$ (V_s): particle settling velocity; and U is the approach velocity or filtration rate.

Therefore, the total initial collection efficiency for upflow and downflow filtration is given, respectively, by equations (16) and (17),

$$\eta\uparrow = \eta^* + \eta_G\uparrow \tag{16}$$

$$\eta\downarrow = \eta^* + \eta_G\downarrow \tag{17}$$

where:
η is the total initial particle collection efficiency of the collector and η^* is the initial particle collection efficiency due to all the mechanisms except gravity settling.

Combining equations (16) and (17) one obtains equation (18) that shows the effect of gravity on the equation of collection efficiency by the settling mechanism, comparing the total efficiency in both upflow and downflow filtration directions:

$$\eta\downarrow - \eta\uparrow = 2\,\eta_G\downarrow \tag{18}$$

Based on mathematical regressions, Paretsky et al. (1971) presented the following equations for upflow and downflow filtration efficiencies, respectively:

$$\eta_G\uparrow = 0.0375\ N_G^{1/2} \tag{19}$$

$$\eta_G\downarrow = \eta_G\uparrow + 0.21\ N_G^{0,78} \tag{20}$$

It is interesting to note that, according to Tien and Ramarao (2007), from a practical standpoint there is no difference between the two correlation equations (19) and (20).

Material and methods

Proposition of initial collection efficiency models for upflow

In the Yao-Habibian and Lee-Gieske models, the initial collection efficiency is a function of the following dimensionless parameters: the Péclet number (N_{Pe}), the interception number (N_R) and the gravitation number (N_G). The difference between the models is that the porosity is expressed in the former by Happel's parameter (A_S) and in the latter by Lee-Gieske's parameter (K_W e p).

In the RT model, the initial collection efficiency is a function of the dimensionless parameters presented in equation (21), while in the TE model this efficiency is a function of the dimensionless parameters shown in equation (22), both in the $\eta = \eta_D = \eta_I = \eta_G$ forms (DARBY et al., 1992):

$$\eta = F\left(A_{S,} N_{Pe}, N_{Lo}, N_R, N_G\right) \qquad (21)$$

$$\eta = F\left(A_S, N_{Pe}, N_R, N_{vdW}, N_A, N_G\right) \qquad (22)$$

Table 3 presents the models for calculating the initial collection efficiency in downflow filtration, which are modified and adapted to upflow filtration in the models proposed here. The modified term is gravity sedimentation (gravitational settling) η_G, based on the direction of the flow, i.e., upflow or downflow. The equations shown in Table 3 present the following coefficients: a_n, b_n (n = 1, 2, and 3), c_n (n = 1 and 2) and d_n (n = 3) in the efficiency term related to gravity sedimentation (gravitational settling) (η_G).

Using the equations below (23) for down and upflow filtration, respectively, one can obtain the values of $(\eta_0\ \alpha_0)_{\text{Dow Flow}}$ and $(\eta_0\ \alpha_0)_{\text{Upflow}}$ from experimental data, allowing for the isolation of the adhesion coefficient (adhesion between particles and collector granules) (α_0):

$$(\eta_0 \alpha_0)_{\text{Dow Flow}} = -\frac{2}{3}\left[\frac{1}{(1-f_0)}\right]\frac{d_c}{L}\ln\left(\frac{C}{C_0}\right)_{t=0} \text{ and } \qquad (23)$$
$$(\eta_0 \alpha_0)_{\text{Up Flow}} = -\frac{2}{3}\left[\frac{1}{(1-f_0)}\right]\frac{d_c}{L}\ln\left(\frac{C}{C_0}\right)_{t=0}$$

The above equations (23) for both down and upflow show the same adhesion coefficient values because this parameter does not depend on the distance between the particle and the collector, but solely on the chemical aspects involved in the capture of the particle by the collector. The adhesion coefficient (α_0) has probabilistic characteristics due to the complex mechanisms of the adhesion between particle and collector. The adhesion coefficient (α_0) is given by equation (24) (DARBY et al., 1992):

$$\alpha_0 = \frac{\textit{rate of particles attached to the collector}}{\textit{rate of particles coliding the collector}} \qquad (24)$$

The removal efficiency (η) is a transport characteristic and depends essentially on suspension characteristics and operational conditions of bed filtration, particularly on the hydrodynamic conditions. Thus, the distance between the particle and collector is a very important factor. The removal efficiency (η), which also has probabilistic characteristics, is given by (DARBY et al., 1992):

$$\eta = \frac{\textit{rate of particles coliding the collector}}{\textit{rate of particles approaching the collector}} \qquad (25)$$

Isolating the adhesion coefficient (α_0) from $(\eta_0\ \alpha_0)_{\text{Dow Flow}}$ and $(\eta_0\ \alpha_0)_{\text{Upflow}}$ allows one to calculate the coefficients listed in Table 3 by a mathematical correlation with convergence to a minimum value for the sum of the modules' differences between the $(\eta_0\ \alpha_0)_{\text{Calculated}}$ and $(\eta_0\ \alpha_0)_{\text{Experimental}}$ values of upflow filtration. In this case, only the gravitational settling term (η_G) is modified in the initial collection efficiency equation models (see Table 3).

Table 3. Summary of the initial efficiency collector models equations for downflow to be adapted to the upflow filtration.

Model	Efficiency equation
Yao-Habibian Modify (YH)	$\eta = 4A_S^{1/3}N_{Pe}^{-2/3} + \frac{3}{2}A_S N_R^2 + a_1\ N_G^{b_1}$
Lee-Gieske (LG)	$\eta = 3.54\left(\frac{f}{K_W}\right)^{1/3} N_{Pe}^{-2/3} + \frac{3}{2}\frac{f \cdot N_R^2}{K_W(1+N_R)^p} + a_1\ N_G^{b_1}$
Rajagopalan and Tien (RT)	$\eta = 4A_S^{1/3}N_{Pe}^{-2/3} + A_S N_{Lo}^{1/8} N_R^{15/8} + a_2\ A_S N_G^{b_2} N_R^{c_2}$
Tufenkji and Elimelech (TE)	$\eta = 2.4A_S^{1/3}N_{Pe}^{-0.715}N_R^{-0.081}N_{vdW}^{-o.052} + 0.55A_S N_A^{0.125}N_R^{1.675} + a_3 N_G^{b_3} N_R^{c_3} N_{vdW}^{d_3}$

The values of the equations of the initial collection efficiency model for direct upflow filtration were obtained through a mathematical regression implemented in the *Excel* routine for the gravitational settling term (η_G) of the four models listed in Table 2. The purpose of the routine was to minimize the difference between the values of $(\eta_0\ \alpha_0)_{Experimental}$ and $(\eta_0\ \alpha_0)_{Calculated}$, obtained through iterative resolution of the nonlinear equation method of steepest gradient available in the *solver* program (a *Microsoft Excel 2010* tool). Restrictions involving superficial velocity parameters and particle diameters were considered in the mathematical regression convergence goal. This restriction is aimed at minimizing differences in the efficiency of the gravitational settling term (η_G) for upflows and downflows at low settling velocities and at maximizing the difference between particle diameters in upflows and downflows, based on the experimental observations of Gebhart et al., (1973).

Experimental data

The experimental work, which was conducted in bench-scale laboratory facilities, aimed to compare the particle collection efficiency of direct downflow and upflow filtration according to the conditions listed in Table 4 (BOTARI; DI BERNARDO, 2012).

These efficiency data were used to determine the initial collection efficiency using model equations proposed in this study for upflow filtration. Glass microspheres ranging in size from 430 to 600 µm, with a specific mass of 2.5 g cm^{-3}, were used as the filtration medium. Two types of particles were added to the water: hydrophobic particles of polystyrene latex microspheres with the sulfate group (PGS) and hydrophilic particles of polystyrene latex microspheres with the carboxylate modify group (CML). The particles in both groups had an average diameter of 2.9 µm and a specific mass of 1.055 g cm^{-3}. For more details see Botari and Di Bernardo (2012).

Table 4. Main Characteristics of same examples of experimental data used in modeling to obtain initial efficiency collector models for upflow direct filtration (BOTARI; DI BERNARDO, 2012).

$\eta_0\ \alpha_0$	Particles	Coagulant	Flow Direction	Total Concentration Particles (# mL^{-1})	Bed length (cm)	Filtration rate (m h^{-1})
3.3214E-03	Sulfate Latex	Calcium Chloride 5 g L^{-1}	Upflow	4.50 E+5 (Turbidity: 12 uT)		5
4.0980E-03			Downflow			
1.3326E-03		Aluminum Sulfate 1 mg L^{-1}	Upflow	1.40 E+6 (Turbidity: 40 uT)		
2.7065E-03			Downflow			
1.6219E-03	Carboxylate Latex Modify (CLM)	Calcium Chloride 5 g L^{-1}	Downflow	4.50 E+5 (Turbidity: 12 uT)		
2.2656E-03						

Results and discussion

Table 5 shows the equations for four initial collection efficiency models adapted for direct upflow filtration models by the concept proposed in this study. Tables 6 and 7 present the same models modified by concepts adapted from Gebhart et al. (1973) and Paretsky et al. (1971).

Table 5. Summary of initial efficiency collector models for upflow filtration – Concept of these authors.

Model	Efficiency equation
Yao-Habibian Modify	$\eta = 4 A_S^{1/3} N_{Pe}^{-2/3} + \frac{3}{2} A_S N_R^2 + 0.36452\ N_G^{0.930}$
Lee-Gieske (LG)	$\eta = 3.54\left(\frac{1-f}{K_W}\right)^{1/3} N_{Pe}^{-2/3} + \frac{3}{2}\frac{f \cdot N_R^2}{K_W (1+N_R)^p} + 0.36452\ N_G^{0.930}$
Rajagopalan and Tien (RT)	$\eta = 4 A_S^{1/3} N_{Pe}^{-2/3} + A_S N_{Lo}^{1/8} N_R^{15/8} + 0.00270\ A_S N_G^{0.469} N_R^{-0.203}$
Tufenkji and Elimelech (TE)	$\eta = 2.4 A_S^{1/3} N_{Pe}^{-0.715} N_R^{-0.081} N_{vdW}^{-ο.052} + 0.55 A_S N_A^{0.125} N_R^{1.675} + 0.13044\ N_G^{1.050} N_R^{-0.165} N_{vdW}^{0.129}$

Table 6. Summary of initial efficiency collector models for upflow filtration – Concept adapted from the model of Gebhart et al. (1973).

Model	Efficiency equation
Yao-Habibian Modify	$\eta = 4 A_S^{1/3} N_{Pe}^{-2/3} + \frac{3}{2} A_S N_R^2 - 0.02\ \frac{N_G^{0.69}}{U^{0.21}}$
Lee-Gieske (LG)	$\eta = 3.54\left(\frac{1-f}{K_W}\right)^{1/3} N_{Pe}^{-2/3} + \frac{3}{2}\frac{f \cdot N_R^2}{K_W (1+N_R)^p} - 0.02\ \frac{N_G^{0.69}}{U^{0.21}}$
Rajagopalan and Tien (RT)	$\eta = 4 A_S^{1/3} N_{Pe}^{-2/3} + A_S N_{Lo}^{1/8} N_R^{15/8} - 6.76.10^{-5} A_S \frac{N_G^{0.345}}{U^{0.105}} N_R^{-2/5}$
Tufenkji and Elimelech (TE)	$\eta = 2.4 A_S^{1/3} N_{Pe}^{-0.715} N_R^{-0.081} N_{vdW}^{-ο.052} + 0.55 A_S N_A^{0.125} N_R^{1.675} - 4.40.10^{-3} \frac{N_G^{0.766}}{U^{0.233}} N_R^{-0.24} N_{vdW}^{0.053}$

Table 7. Summary of initial efficiency collector models for upflow filtration – Concept adapted from the model of Paretsky et al. (1971).

Model	Efficiency equation
Yao-Habibian Modify	$\eta = 4A_S^{1/3}N_{Pe}^{-2/3} + \frac{3}{2}A_S N_R^2 + 0.0375\ N_G^{1/2}$
Lee-Gieske (LG)	$\eta = 3.54\left(\frac{1-f}{K_W}\right)^{1/3} N_{Pe}^{-2/3} + \frac{3}{2}\frac{f \cdot N_R^2}{K_W(1+N_R)^p} + 0.0375\,N_G^{1/2}$
Rajagopalan and Tien (RT)	$\eta = 4A_S^{1/3}N_{Pe}^{-2/3} + A_S N_{Lo}^{1/8} N_R^{15/8} + 1.2675.10^{-4} A_S N_G^{1/4} N_R^{-2/5}$
Tufenkji and Elimelech (TE)	$\eta = 2.4A_S^{1/3}N_{Pe}^{-0.715}N_R^{-0.081}N_{vdW}^{-o.052} + 0.55A_S N_A^{0.125}N_R^{1.675} - 4.40.10^{-3}\frac{N_G^{0.766}}{U^{0.233}}N_R^{-0.24}N_{vdW}^{0.053}$

The RT model, which is the one most frequently used in filtration research, was the model that presented the maximum difference between the $(\eta_0\,\alpha_0)_{Calculated}$ and $(\eta_0\,\alpha_0)_{Experimental}$ values.

In all the models adapted from Gebhart et al.'s concept (1973), even in the case where the gravitational settling (η_G) efficiency was considered solely proportional to the gravitational number (N_G) – the Yao-Habibian modified model (YH) and the Lee-Gieske (LG) model, the mathematical regressions presented negative values of global initial collection efficiency for direct upflow filtration, as indicated in Table 6. The same behavior was not observed in the initial collection efficiency models for direct upflow filtration based on our concept nor in the adapted Paretsky et al.'s concept (1971), as indicated in Tables 5 and 7.

Figures 2, 3 and 4 depict bilog graphics of the gravitational settling term (η_G) efficiency as a function of the variation of the gravitational number (N_G). These graphs illustrate the results of the equations that express the three concepts described herein, according to Tables 5, 6 and 7, respectively, and the respective original models for downflow filtration with respect to equations (2) to (5) presented earlier.

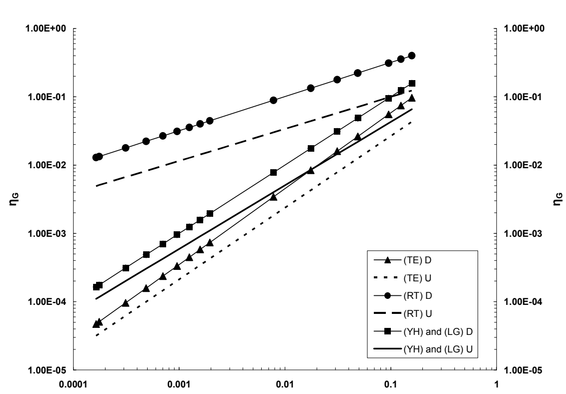

Figure 2. Gravitational settling efficiency (η_G) in function of the variation of the Gravitational number (N_G) for Up and Down Flow (The letters *U* and *D* in the legends of the figures indicate Upflow and Downflow initial collection efficiency models) – Table 5 – Concept of these authors.

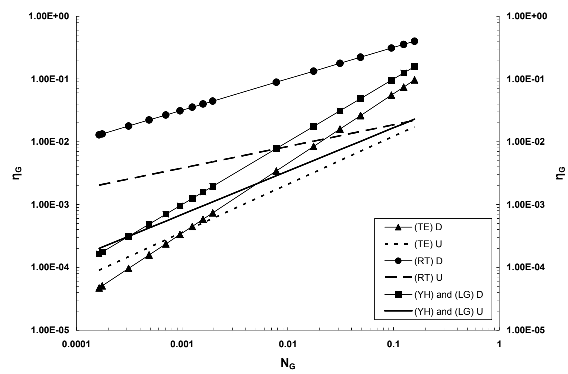

Figure 3. Gravitational settling efficiency (η_G) in function of the variation of the Gravitational number (N_G) for Up and Down Flow (The letters *U* and *D* in the legends of the figures indicate Upflow and Downflow initial collection efficiency models) – Table 6 – Concept adapted from Gebhart et al. (1973).

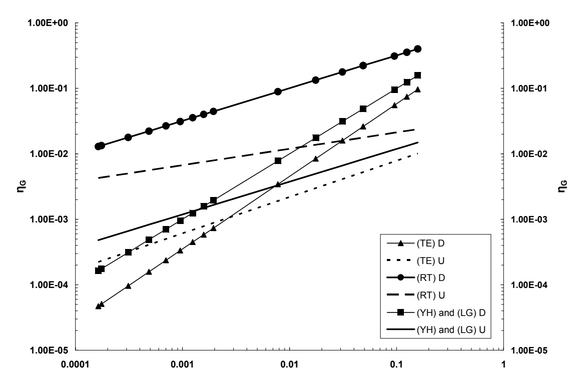

Figure 4. Gravitational settling efficiency (η_G) in function of the variation of the Gravitational number (N_G) for Up and Down Flow (The letters *U* and *D* in the legends of the figures indicate Upflow and Downflow initial collection efficiency models) – Table 7 – Concept adapted from Paretsky et al. (1971).

It is important to notice that the graphics in Figures 2, 3 and 4 present a wide range of values for the gravitational number (N_G), similar to those normally found in water filtration in porous media. Note that the gravitational settling efficiencies of the upflow filtration models in Figure 2 were not lower than those of their counterpart downflow models, according to the concepts adapted from Gebhart et al. (1973) and Paretsky et al. (1971) (Figures 3 and 4). This lack of discrepancy is incompatible with our experimental data for that range of N_G.

However, the models constructed according to our proposition preserve each model's main inherent characteristics, as indicated by the slight differences between the angular coefficients of the downflow models and the respective upflow models. The reason is that the only difference between the models is the gravitational factor in the gravitational settling efficiency term. All the values of the gravitational settling efficiency (η_G) of the models based on the concept adapted from Gebhart et al. (1973), which consider that the gravitational settling efficiency term is negative in the total initial collection efficiency, were considered in modulus in Figure 3.

In this figure, the RT model of the concept adapted from Gebhart et al. (1973) presents much lower η_G values for upflow filtration than does the respective downflow model. The other upflow filtration models, however, present slightly lower overall values and even higher η_G values than their respective downflow models, as indicated in Figure 3. This finding also applies to the Paretsky et al. (1971) concept adapted to the same models. In both cases, this behavior, which may occur in a wide range of N_G values commonly found in water filtration through porous media, is usually inconsistent with experimental data and theoretical fundaments.

Similarly, the RT model in Figure 4 presents lower η_G values for upflow filtration than for downflow filtration in the entire range of N_G values. However, the YH, LG and TE models showed an inversion of this relation for N_G of less than 0.003. Therefore, the three concepts for initial collection efficiency models are based on a decrease of the influence of gravitational settling efficiency (η_G) in the calculation of the total initial collection efficiency in upflow filtration. This is also observed in the initial collection efficiencies in experimental filtration data.

Table 8 gives a summarized example of the calculation of initial collection efficiency using the YH, LG, RT and TE upflow filtration models in Tables 5 to 7 compared with downflow models, based on equations (2) to (5) and on experimental data from an essay conducted in a pilot plant for direct upflow filtration.

The values of the initial collection efficiency models for upflow filtration in Table 8 are about 42% lower than those calculated by the initial collection efficiency models for downflow filtration. It should be noted that the standard deviation is about 18% of the average value.

Table 8. Summary of the essay parameters of an application example and results for initial efficiency collector models for up- and down- filtration.

Experimental media value of η_0 for up flow filtration			
$6.712.10^{-3}$			
Values of η_0 for down filtration models (Table 2):			
YH	LG	RT	TE
$1.930.10^{-3}$	$1.920.10^{-3}$	$7.071.10^{-2}$	$1.159.10^{-3}$
Values of η_0 for up filtration models (Table 5) Concept of these authors			
YH	LG	RT	TE
$1.268.10^{-3}$	$1.258.10^{-3}$	$1.968.10^{-2}$	$8.462.10^{-4}$
Percentage of reduction in relation to the downflow models (%)			
34.30	34.48	72.17	26.99
Values of η_0 for up filtration models (Table 6) Concept adapted from Gebhart:			
YH	LG	RT	TE
$7.717.10^{-5}$	$6.692.10^{-5}$	$(- 4.076.10^{-3})$	$4.466.10^{-5}$
Percentage of reduction in relation to the downflow models (%)			
96.00	96.51	–	96.15
Values of η_0 for up filtration models (Table 7) Concept adapted from Paretsky:			
YH	LG	RT	TE
$1.856.10^{-3}$	$1.845.10^{-3}$	$1.362.10^{-2}$	$1.479.10^{-3}$
Percentage of reduction in relation to the downflow models (%)			
3.83	3.91	80.74	-27.61 (largest)

Porous media data and Operations conditions: Length bed (L) = 0.14 m; U = 16.67 cm min.-1; dc (media) = 1.3 mm; dp = 2.1 μm; ρp = 2,600,00 kg m-3; f = 0.39; ρf = 997.048 kg m-3; H = 4.7.10-20 J; k = 1.3805.10-23 J K-1; g = 9.81 m s-2; μ T298 K = 8.94.10-4 kg m-1 s-1; T = 298 K; α0 = 1.

The models adapted from Gebhart et al.'s (1973) upflow filtration concept can lead to very high and, in this particular case, inconsistent initial collection efficiency values (as well as negative values).

The models adapted from Paretsky et al.'s (1971) upflow filtration concept can yield widely varying values for initial collection efficiency. In this case, incoherent values were obtained for the initial collection efficiency in upflow filtration. For example, the TE model yielded an increase instead of a reduction in the initial collection efficiency of upflow filtration in relation to downflow filtration.

The models based on the concept proposed by the authors of this paper lead to initial collection efficiencies in upflow filtration that are about 14% lower than the experimental value (average value). Using the concept adapted from Gebhart et al. (1973), the initial collection efficiency for upflow filtration was about 100% lower than the average experimental values, while the concept adapted from Paretsky et al. (1971) led to a 30% lower initial collection efficiency than the average experimental values in upflow filtration.

In general, the concept proposed differs from the concepts adapted from Gebhart et al. (1973) and Paretsky et al. (1971) in the following aspects:
- It does not consider that the determination of the gravity settling term efficiency in upflow filtration is dependent solely on the gravitational number (N_G);
- It does not consider solely the hydrodynamic characteristics to obtain initial collection efficiency models in upflow filtration;

- It does not subtract the gravity settling efficiency term (η_G) from the total (global) initial collection efficiency model in upflow filtration, but reduces its value;
- It considers that the value of the gravity settling efficiency term (η_G) in upflow filtration shows a consistent and coherent reduction within a wide range of values of the gravitational number (N_G) in relation to the initial collection efficiency models for downflow filtration;
- It considers that the gravity settling efficiency term (η_G) in upflow filtration preserves the inherent particularities of the initial collection efficiency models originally conceived for downflow filtration, and it changes only the direction of the gravity vector in this term for a wide range of N_G values.

Conclusion

In general, the concept proposed herein presents the same particularities as the concepts adapted from Gebhart et al. (1973) and Paretsky et al. (1971) concerning the hydrodynamic characteristics in the variation of flow direction to build the initial collection efficiency models and also lead to a reduction in removal efficiency values. However, the concept presented by the authors of this paper proved to be a coherent and consistent option for calculating initial collection efficiency models for direct upflow filtration.

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