



Hydrodynamic analysis of particle collection efficiency: comparing downflow and upflow filtration

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ABSTRACT. 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. These models are defined in terms of the geometry and characteristic elements of granule collectors, particles and fluid, and also the composition of the balance of forces that act in the particle collector system. This work analyzes particles collection efficiency comparing downflow and upflow direct filtration, taking into account the contribution of the gravitational factor of the settling removal efficiency in future proposal of initial collection efficiency models for upflow filtration. A qualitative analysis is also made of the proposal for the collection efficiency models for particle removal in direct downflow and upflow filtration using a Computational Fluid Dynamics (CFD) tool. This analysis showed a strong influence of gravitational factor in initial collection efficiency ($t = 0$) of particles, as well as the reasons of their values to be smaller for upflow filtration in comparison with the downflow filtration.

Keywords: mathematical modeling, CFD analysis, particle collection efficiency, direct filtration.

Análise hidrodinâmica da eficiência de remoção de partículas: comparando filtração descendente e ascendente

RESUMO. Modelos de filtração descrevem o balanço de massa no meio filtrante em termos de mecanismos de remoção de partículas e permitem a determinação da eficiência global da remoção de partículas. Tais modelos são definidos pela geometria e pelas características dos grãos coletores, bem como, pela composição de forças que agem no sistema partícula-coletor. O presente trabalho analisa a eficiência de remoção de partículas, comparando a filtração direta descendente e ascendente. Para tal, considerou-se o efeito da contribuição do fator gravitacional na eficiência de remoção por sedimentação da partícula no grão coletor, visando futuras propostas de modelos de cálculo da eficiência inicial de remoção de partículas na filtração ascendente. O trabalho apresenta, ainda, a análise qualitativa de proposta de modelos de remoção inicial de partículas na filtração direta descendente e ascendente a partir de uma ferramenta de Fluidodinâmica Computacional (CFD). A análise demonstrou significativa influência do fator gravitacional na eficiência inicial de remoção ($t = 0$) de partículas, bem como os motivos de seus valores serem menores para a filtração ascendente em comparação com a filtração em escoamento descendente.

Palavras-chave: modelagem matemática, CFD, remoção de partículas, filtração direta.

Introduction

The mathematical model allows the prediction of the control and operation conditions which lead to an improvement of the filtration process when producing drinking water. The mathematical models describe filtration process through particles removal mechanisms which take place in the granular bed filtration. This work analyzes the conditions of initial efficiency collector for upflow direct filtration in comparison with initial efficiency collection downflow filtration in saturated porous media.

The trajectory particles analysis through mathematical correlation by the dimensionless numbers representatives of fluid and particles characteristics are considered to be the main approach for mathematical modeling of initial efficiency collector of particles removal in water filtration context (TUFENKJI; ELIMELECH, 2004).

The filtration phenomenon is based on mass balance in granular bed filtration and permits the determination of global particles efficiency removal. The filtration phenomenon is defined in terms of geometry and characteristic elements of grain collectors (bed components), particles and fluid and also the

forces composition balance which act in the particle-collector system. This type of resolution is well known as the trajectory analysis theory (TUFENKJI; ELIMELECH, 2004). This work makes a qualitative analysis to the initial efficiency collector particles removal comparing downflow and upflow direct filtration through the use of Computational Fluid Dynamics (CFD) tool. And also, shows the influence of the flow direction in pilot-plant filtration experiments, comparing upflow and downflow direct filtration runs.

The filtration medium can 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.

The conception of the collector removal model required the definition of the following elements (TIEN, 1989):

- 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) (TIEN, 1989):

$$\frac{\partial C}{\partial t} + \vec{U} \times \text{grad} C = \text{div} (D \cdot \text{grad} C + m_o C \text{grad} \Phi) \quad (1)$$

where:

m_o represents particle mobility (s kg^{-1}); $\vec{\Phi}$ is the interaction colloidal energy (J); D is the diffusion constant ($\text{m}^2 \text{s}^{-1}$); C is the particle concentration in the liquid phase (kg m^{-3}); and U is the fluid's superficial velocity (m s^{-1}).

The resolution of equation (1) requires extensive calculations and powerful computational tools, but a more practical approach is based on the correlation of dimensionless numbers (TUFENKJI; ELIMELECH, 2004). This approach simplifies the trajectory analysis by correlating the power functions by dimensionless numbers that represent fluid and particle characteristics of the mass balance in the control volume and the removal efficiency.

Material and methods

Qualitative analysis of flow filtration direction

Representative flow equations and particle-tracking equations

In this section it is presented a Computational Fluid Dynamics (CFD) modeling for a qualitative

analysis intending to show the main influence of the gravity vector in quantifying initial efficiency collection by settling mechanism. Further, is presented the experimental data of efficiency collection for upflow and downflow direct filtration.

Considering the continuity hypothesis for a Newtonian fluid, there are equations associated to conservation principles (CFX, 2004).

Continuity Equation

$$\underbrace{\frac{\partial \rho}{\partial t}}_{\text{Mass Variation Rate in the Control Volume}} + \underbrace{\nabla \cdot (\rho \mathbf{u})}_{\text{Mass Flow through the Surface of the Control Volume}} = 0 \quad (2)$$

where:

u is the velocity vector and ρ is the fluid's density.

Momentum Equations (Navier-Stokes Equations)

$$m\mathbf{a} = F_{\text{surface}} + F_{\text{body}} \quad (3)$$

where:

F is force, m is mass, and $\mathbf{a} = \frac{D\mathbf{u}}{Dt} = \frac{\partial(\mathbf{u})}{\partial t} + (\mathbf{u} \cdot \nabla)(\mathbf{u})$, which is acceleration.

Considering the incompressible flow and constant physical properties hypothesis, one can obtain:

$$\underbrace{\frac{\partial \mathbf{u}}{\partial t}}_{\text{Momentum Variation Rate}} + \underbrace{(\mathbf{u} \cdot \nabla) \mathbf{u}}_{\text{Convective Flow of the Momentum}} = \underbrace{-\frac{1}{\rho} \nabla p}_{\text{Pressure Gradient Force}} + \underbrace{\nu \nabla^2 \mathbf{u}}_{\text{Diffusive Flow of the Momentum or Dissipation Kinetic Energy}} \quad (4)$$

where:

p is pressure and ν is kinematic viscosity.

The convective flow term of the momentum also expresses the nonlinear interactions within the typical spectrum of energy of the flow.

Energy Equation

$$\underbrace{\frac{\partial T}{\partial t}}_{\text{Energy Variation Rate}} + \underbrace{(\mathbf{u} \cdot \nabla) T}_{\text{Energy Convective Flow}} = \underbrace{\alpha \nabla^2 T}_{\text{Energy Diffusive Flow}} + \underbrace{S_E}_{\text{Energy Source}} \quad (5)$$

where:

T is temperature; α is thermal conductivity; and S_E is the energy source.

For a discrete particle in a continuous flow, the forces acting upon this particle and affecting its acceleration are due to the differences of velocity between fluid and particle and the mass fluid displaced by the particle's path. According CFX (2004), the particle-tracking equation was described by Basset, Boussinesq and Oseen for rotational references:

$$\begin{aligned}
 m_p \frac{dv_p}{dt} = & \underbrace{\frac{1}{8} \pi d^2 C_d |v_f - v_p| (v_f - v_p)}_{\text{Resulting Force on the Particle}} + \underbrace{\frac{\pi d^3 \rho_f}{6} \frac{dv_f}{dt}}_{\text{Viscous Dragging Force (Stokes Law)}} + \underbrace{\frac{\pi d^3 \rho_f}{12} \left(\frac{dv_f}{dt} - \frac{dv_p}{dt} \right)}_{\text{Force from Pressure Gradient}} + \underbrace{\frac{1}{6} \pi d^3 (\rho_p - \rho_f) g}_{\text{Gravity Force}} + \\
 & \underbrace{\frac{3}{2} d^2 \sqrt{\pi \rho_f \mu} \int_{t_0}^t \left(\frac{dv_f}{dt'} - \frac{dv_p}{dt'} \right) (t - t')^{-0.5} dt'}_{\text{Forces Basset Term}} - \underbrace{\frac{1}{6} \pi d^3 (\rho_p - \rho_f) \omega \times (\omega \times R)}_{\text{Centripetal Force}} - \underbrace{\frac{\pi d^3 \rho_p}{3} \omega \times v_p}_{\text{Coriolis Force}} + \underbrace{F_U}_{\text{Setting External Force}}
 \end{aligned} \quad (6)$$

where:

m_p : particle mass, d : particle diameter, v : velocity, ρ : specific mass, μ : fluid dynamic viscosity, g is the gravity acceleration ($m \cdot s^{-2}$), C_d : drag coefficient, ω : rotational velocity, R : rotation axis vector; and F_U : external force (set by the user). The variable t_0 is used for the initial time, while the subscript "f" refers to the fluid and "p" to the particle.

The qualitative analysis of the hydrodynamic behavior of a single particle in an upflow or downflow was conceived for the laminar regime and is as known as the Forchheimer flow regime ($N_{Re} < 50$ – grain Reynolds number), according to the type of flow that takes place in granular bed filtration.

Experimental data – filtration runs for upflow and downflow

The experimental work, which was conducted in pilot-plant facilities, aimed to compare the initial particle collection efficiency ($\eta_0 \alpha_0$ – initial efficiency collector) of direct downflow and upflow filtration according to the conditions

listed in Table 1, the influent characteristics is presented in Table 2 and the schemes illustrated in Figures 1 and 2. The examples results of filtration runs for upflow and downflow are presented in Figures 3 and 4.

As can be observe in Table 1, the initial efficiency collection ($\eta_0 \alpha_0$) presents different values according different particles (Sulfate or CML Latex) and coagulants ($CaCl_2$ or $Al_2(SO_4)_3 \cdot 18 H_2O$) are used in the experiments. It is important to consider the conditions of particles related with affinity to water sample solution: hydrophobic or hydrophilic. The electrical superficial charge, hydrophobicity or not, and other superficial contact forces can be modify the adhesion conditions to the grain collector and, therefore, conditioning the attachment or detachment of the particle in the grain collector (BERGENDAHL; GRASSO, 1999).

Table 1. Characteristics of the experimental runs used to obtain initial efficiency collection data to conceived equation models for upflow direct filtration.

Essay	$\eta_0 \alpha_0$ value	Particles	Coagulant	Flow Direction	Total Concentration Particles (#. mL^{-1})	Bed length (cm)	Filtration rate ($m \cdot h^{-1}$)
1	3,3214E-03	Sulfate Latex	Calcium Chloride 5g L^{-1}	Up	4.50 E+5 (Turbidity: 12 NTU)	5	5
2	4,0980E-03			Down	4.50 E+5 (Turbidity: 12 NTU)		
3	1,3326E-03		Aluminum Sulfate 1mg L^{-1}	Up	1.40 E+6 (Turbidity: 40 NTU)		
4	2,7065E-03			Down	1.40 E+6 (Turbidity: 40 NTU)		
5	1,6219E-03	Carboxylate Latex Modify (CLM)	Calcium Chloride 5g L^{-1}	Up	4.50 E+5 (Turbidity: 12 NTU)		
6	2,2656E-03			Down	4.50 E+5 (Turbidity: 12 NTU)		

Table 2. Influent Characteristics of the filtration experimental runs summarized in Table 1.

Essays	Particle	Coagulant Dose	Influent Zeta Potential (mV)	Influent pH	Influent Temperature ($^{\circ}C$)
1	Sulfate Latex	$CaCl_2$ 5 g L^{-1}	-	6.99	25
2	Sulfate Latex	$CaCl_2$ 5 g L^{-1}	-1.26	7.00	25
3	Sulfate Latex	$Al_2(SO_4)_3 \cdot 18 H_2O$ 1.0 mg L^{-1}	-3.12	7.14	25
4	Sulfate Latex	$Al_2(SO_4)_3 \cdot 18 H_2O$ 1.0 mg L^{-1}	-3.10	7.20	25
5	CML Latex	$CaCl_2$ 5 g L^{-1}	+1.55	6.94	25
6	CML Latex	$CaCl_2$ 5 g L^{-1}	-0.88	6.91	25

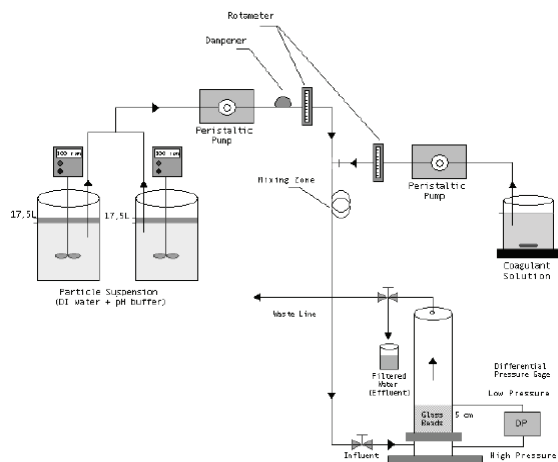


Figure 1. Schematic of upflow direct filtration pilot plant used in essays indicated in Table 1.

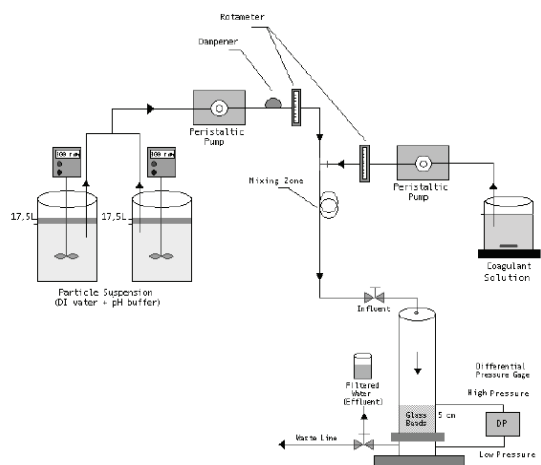


Figure 2. Schematic of downflow direct filtration pilot plant used in essays indicated in Table 1.

The particle suspension were placed in two 20-liter plastic reservoirs where they were maintained in suspension by a rotating shaft mixer. A peristaltic pump was used to pump the particle in suspension at a fixed flow rate through a pulsation dampener and a rotameter. The Calcium Chloride and Aluminum Sulfate solutions were prepared in a 4 L beaker and pumped into a main line through a T-connection. A series of expansions and contractions were provided to allow mixing of the two streams before the influent (Particles + CaCl_2 or alum) enters the filtration column. The column is made of 3.81 cm inner diameter plexiglass tube and is 35 cm high.

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 $2.9 \mu\text{m}$ and a specific mass of 1.055 g cm^{-3} .

The main idea in varying the types of particles (hydrophobic and hydrophilic) was to allowed the large range to particles (primary particles) interaction in the filtration such real conditions and therefore to obtain the generalized model of initial efficiency collector in this aspect and considerer the gravitational settling influence in fluid flow direction.

The effluent turbidity and the total particle concentrations were consistently higher for upflow experiments, confirming the importance of the gravity effect on the filtration efficiency. According the Figures 3 and 4, for the two types of particles 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), were obtained the similarity results for filtration with both coagulants: Calcium Chloride or aluminum sulfate. Nevertheless, in micro scale, the colloidal surfaces interaction point of view, is important to considerer such influence in the particle-collector interactions. To the other hand, the scale of gravity effect force and your influence in determination of the global initial efficiency collection is much higher to any kind of colloidal surfaces interaction forces (TUFENKJI; ELIMELECH, 2004).

Results and discussion

Experimental filtration runs results

The Computational Fluid Dynamics tool used here was developed with ANSYS CFX[®] 10.0 - AEA Technology – Engineering Software. This tool consists of three modules: CFX[®]-Pre, CFX[®]-Solver and CFX[®]-Post. Each module is responsible for one stage of the mathematical modeling.

Table 3 summarizes the general characteristics of the domain and the simulations performed to analyze the particle's trajectory in an upflow and a downflow. Figure 5 presents the grid of the domain and a detail of the grid surrounding the granule (collector) used in the simulations to analyze the particle's trajectory using the CFD tool.

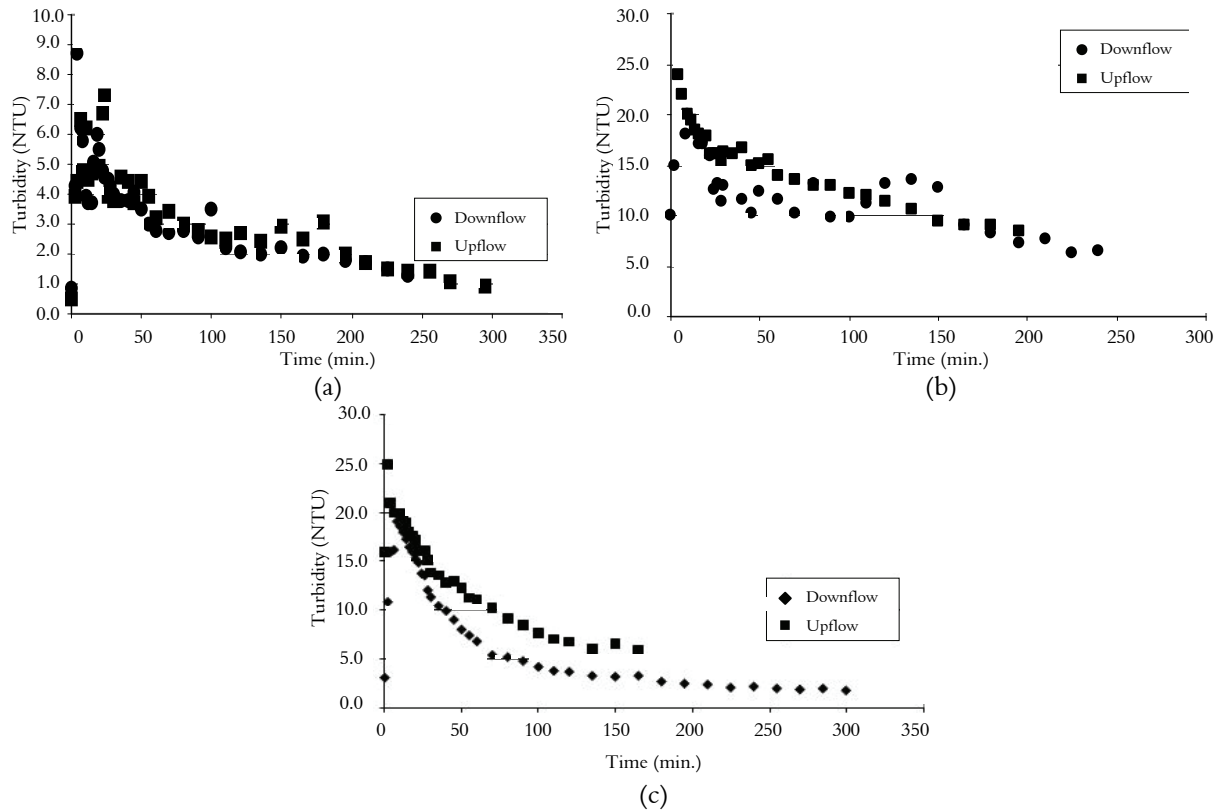


Figure 3. Examples of Filtration runs indicated in Table 1. Comparison between Upflow and Downflow–Turbidity.

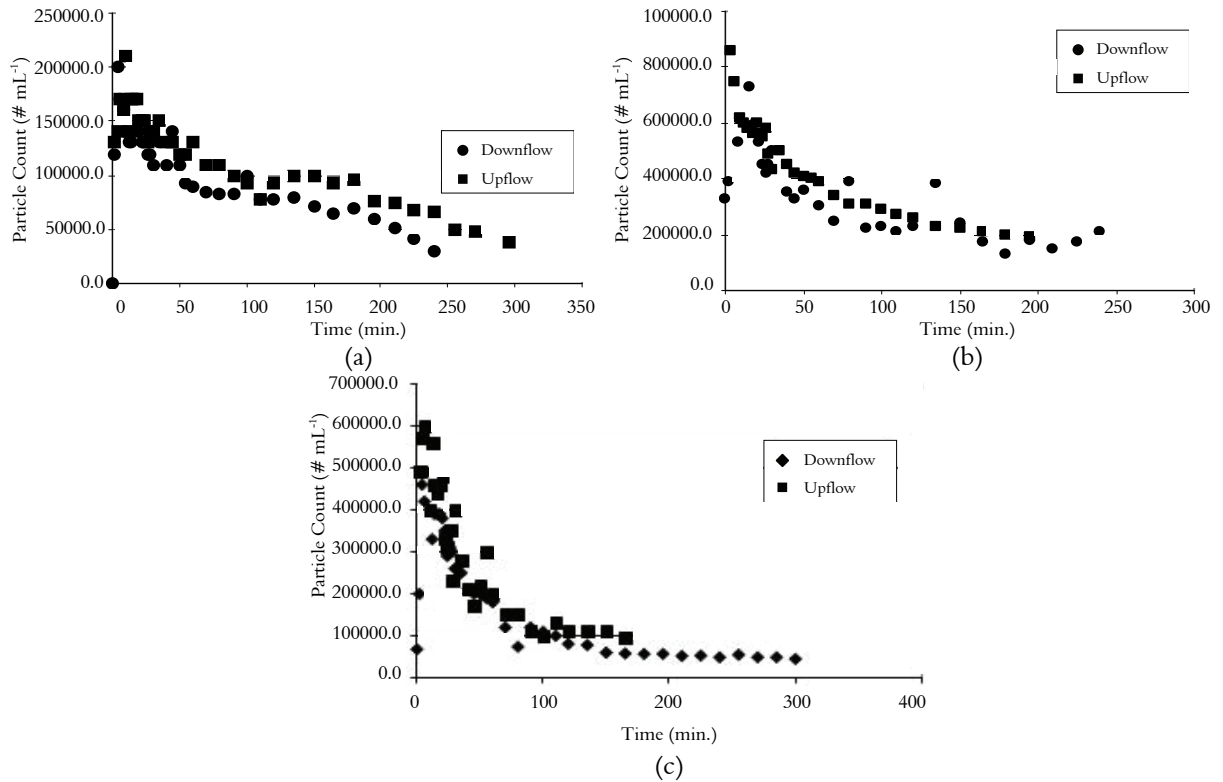


Figure 4. Examples of Filtration runs indicated in Table 1. Comparison between Upflow and Downflow–Particles number. CFD studies results.

As can be observed in Table 3 and Figure 5, the dimensions of filter bed is different to the pilot plant experimental facilities, because the collector (Sphere) adopted in this simulation indented to show particle tracking and the trajectory surround, therefore its size as well as diameter of the cylinder was increased to minimize the “wall effect” and maximize the view of particles trajectories.

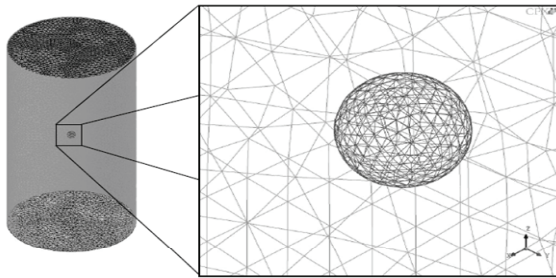


Figure 5. Mash domains and a detail of the grain contour mesh used in the simulations of particle tracking for a trajectory analysis by CFD tool.

Figure 6 shows CFD simulations for 2.1 μm diameter particles in downflow (Figure 6a) and upflow (Figure 6c). This figure also shows a 25-fold magnified view of the particle's path through the

streamlines around the collector granules in downflow (Figure 6b) and upflow (Figure 6d) directions, respectively. Figure 7 shows CFD simulations for 21.0 μm diameter particles in downflow (Figure 7a) and upflow (Figure 7c). A 25-fold magnification of the particle's path through the streamlines around the collector granules in downflow is depicted in Figure 7b, and a 2.5-fold magnification of the upflow is shown in Figure 7d.

The detail in Figure 6b shows that in the downflow, the particle's path is tangential to the streamline, but does not cross it. In contrast, the magnified view of the simulated upflow in Figure 6d reveals that the distance between particle and collector is also greater than in downflow and that the particle's path crosses the streamline.

This same behavior is illustrated clearly in Figure 7a and b, which show the downflow path, with the particle tracking across the streamline towards the collector. In the upflow, the particle trajectory crosses two consecutive streamline flows, moving away from the collector, according to the detail magnified in Figure 7c and Figure 7d, for a 21 μm diameter particle.

Table 3. Summary of the general characteristics of the domain and the simulations of CFD tool for particle tracking and trajectory analysis in upflow and downflow.

Domain			
Cylinder Dimensions	Diameter = 15.0 cm; High = 30.0 cm.		
Sphere Dimension	Diameter = 1.0 cm		
Nodes number	78,898		
Tetrahedral Elements number	425,725		
Prismatic Elements number	3,340		
Faces number	16,692		
Fluid and Particles			
Water		Particles	
Temperature	25 °C	Temperature	25°C
Dynamic Viscosity	$8,899.10^{-4} \text{ kg m}^{-1} \text{ s}^{-1}$	Specific Mass	$2,600 \text{ kg m}^{-3}$
Specific Mass	998 kg m^{-3}	Particles Diameters	2.1 and 21.0 μm
Reynolds number	≈ 50	Restitution Coefficient	1
Simulations			
Time step	0.2 s		
Timing Simulation	20.0 s		
Processing Characteristics	Processors Opteron 64bits 3 GHz (Cluster)		
Timing Particles Trajectories	100 s		
CPU Timing processing	$1.121.10^4 \text{ s}$		
Initial and Boundary Conditions			
Sides	Walls		
Superior	Opening (Upflow); Inlet (Downflow)		
Inferior	Opening (Downflow); Inlet (Upflow)		
Gravity acceleration (z)	-9.806 m s^{-2} (Upflow); 9.806 m s^{-2} (Downflow)		
Inlet conditions	$u(\text{Water}) = 0$; $u(\text{Particles}) = 0$; $v(\text{Water}) = 0$; $v(\text{Particles}) = 0$; $w(\text{Water}) = 4.4628.10^{-3} \text{ m s}^{-1}$; $w(\text{Particles}) = 4.4628.10^{-3} \text{ m s}^{-1}$; $P(\text{Water}) = 0$.		
Outlet Conditions	$du/dz(\text{Water}) = 0$; $du/dz(\text{Particles}) = 0$; $dv/dz(\text{Water}) = 0$; $dv/dz(\text{Particles}) = 0$; $dw/dz(\text{Water}) = 0$; $dw/dz(\text{Particles}) = 0$; $P(\text{Water}) = 0$.		
Initial Conditions	$u(\text{Water}) = 0 \text{ m s}^{-1}$; $u(\text{Particles}) = 0$; $v(\text{Water}) = 0$; $v(\text{Particles}) = 0$; $w(\text{Water}) = 0$; $w(\text{Particles}) = 0$; $P(\text{Water}) = 0$.		

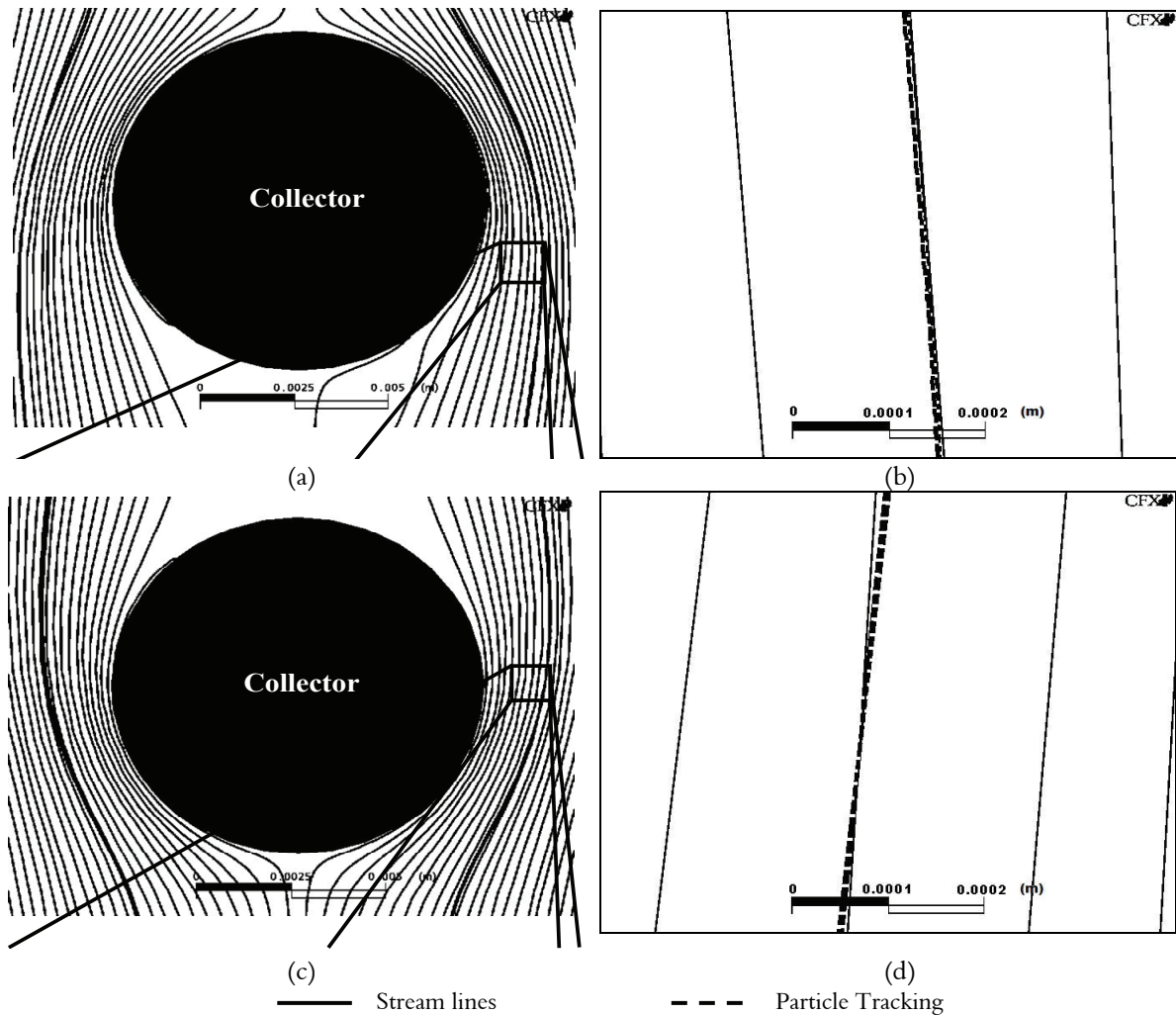


Figure 6. (a) Particle hydrodynamic behavior related to the stream lines in CFD modeling. Particle diameter $2.1 \mu\text{m}$. (b) Detail amplified 25-fold magnification – Downflow; (c) Particle hydrodynamic behavior related to the stream lines. Particle diameter $2.1 \mu\text{m}$; (d) Detail amplified 25-fold magnification – Upflow.

The CFD simulations corroborate the observations of Gebhart et al. (1973), Paretzky et al. (1971) and Thomas et al. (1971) about the initial collection efficiency equations for upflow filtration, in which the collection efficiency appears to be smaller.

However, the hydrodynamic characteristics of fluid and particle mass are not the only parameters that characterize the equations of initial collection efficiency models. Evidently, the hydrodynamic characteristics of the fluid and the particle mass are important aspects in the determination of efficiency. However, these aspects cause other physicochemical characteristics to diverge, especially the surface interaction forces. These characteristics are

components of the efficiency collector equation and are related to the gravitational settling term in the total initial collection efficiency equation for particle removal.

Particle mass is obviously the main factor responsible for the augmented influence of the trajectory. However, it is the direction of the flow, i.e., upflow or downflow, which determines whether the trajectory is towards the collector or away from it. The pressure and velocity vectors for the opposite directions do not present any difference between upflow or downflow in terms of intensity. Figures 8a and b illustrate the symmetry between velocity vectors, while Figures 8c and d also show the symmetry of pressure for up and downflow, respectively.

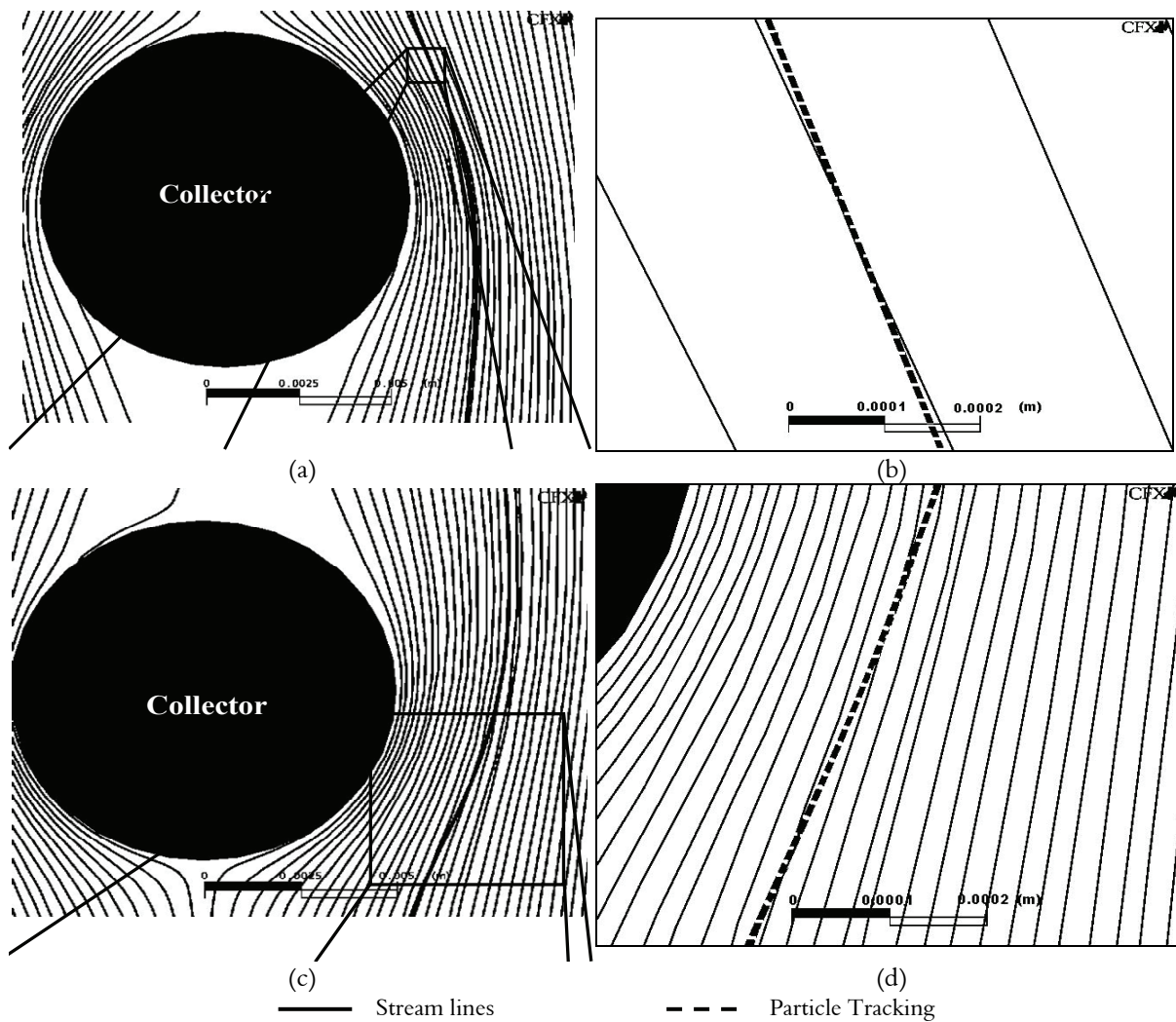


Figure 7. (a) Particle hydrodynamic behavior related to the stream lines in CFD modeling. Particle diameter 21 μm ; (b) Detail amplified 25-fold magnification – Downflow; (c) Particle hydrodynamic behavior related to the stream lines. Particle diameter 21 μm ; (d) Detail amplified 2.5-fold magnification – Upflow.

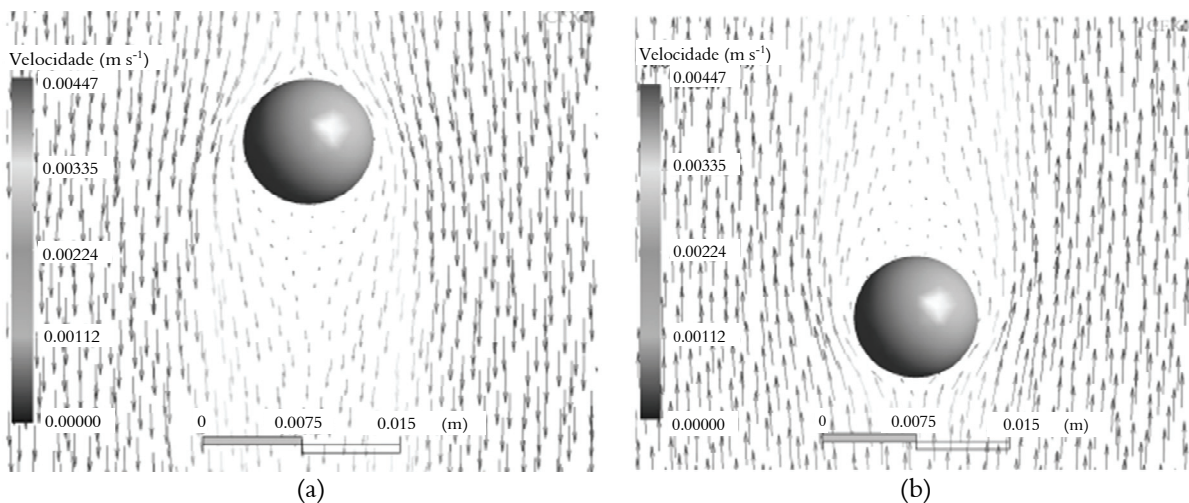


Figure 8. CFD modeling results: Velocity vectors (m s^{-1}) for (a) Downflow and (b) Upflow; Total Pressure Field (Pa) for (c) Downflow and (d) Upflow.

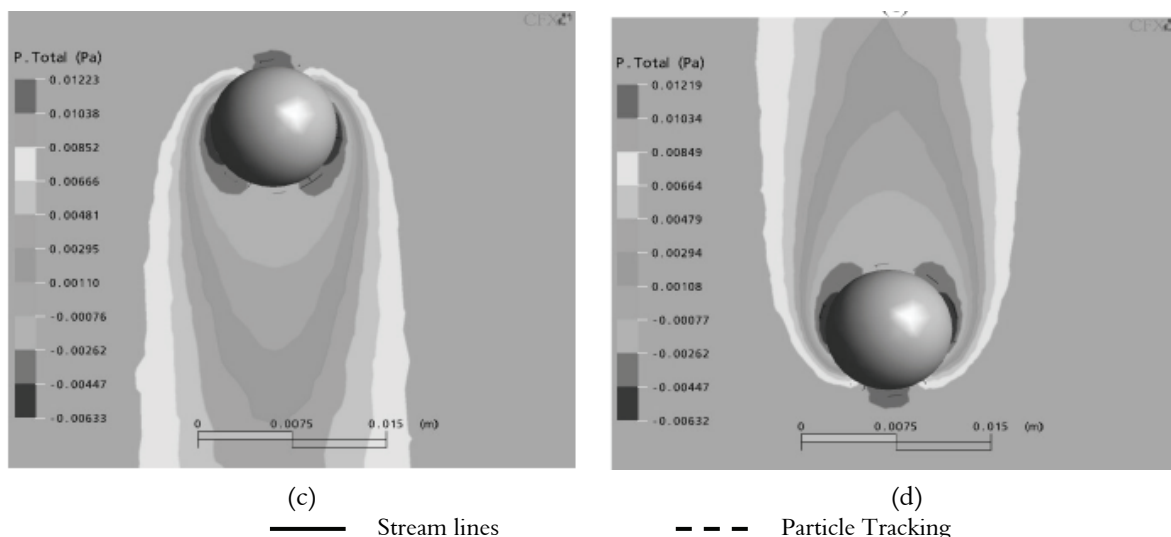


Figure 8 (continuation). CFD modeling results: Velocity vectors (m s^{-1}) for (a) Downflow and (b) Upflow; Total Pressure Field (Pa) for (c) Downflow and (d) Upflow.

Conclusion

In this work, a fundamental approach for incorporating the effect of flow direction in the clean-bed filtration model has been described. Specific conclusions are:

the gravity effect was demonstrated by the observation that effluent turbidity and total particle concentration depended on flow direction through the bed;

the initial efficiency collector values are lower for upflow than for downflow;

further work should be done in order to develop a filtration model incorporating the flow direction and the practical aspects regarding upflow direct filtration.

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References

- BERGENDAHL, J.; GRASSO, D. Prediction of colloid detachment in a model porous media: thermodynamics. *AIChE Journal*, v. 45, n. 3, p. 475-484, 1999.
- CFX. *Cfx 5 Solver Theory*. Waterloo: Ansys Canada Ltda., 2004.

GEBHART, J.; ROTH, C.; STAHLHOFEN, W. Filtration properties of glass bead media for aerosol particles in the $0,1 - 2 \mu\text{m}$ size range. *Aerosol Science*, v. 4, n. 5, p. 355-371, 1973.

PARETSKY, L.; THEODORE, L.; PFEIFFER, R.; SQUIRES, A. M. Panel bed for simultaneous removal of fly ash and sulfur dioxide: II. Filtration of dilute aerosols by sand beds. *Journal of the Air Pollution Control Association*, v. 21, n. 4, p. 204-209, 1971.

THOMAS, J. W.; RIMBERG, D.; MILLER, T. J. Gravity effect in air filtration. *Aerosol Science*, v. 2, n. 1, p. 31-38, 1971.

TIEN, C. A. *Granular filtration of aerosols and hydrosols*. London: Butterworth publishers, 1989. (Series in chemical engineering).

TUFENKJI, N.; ELIMELECH, M. Correlation equation for predicting single-collector efficiency in physicochemical filtration in saturated porous media. *Environmental Science and Technology*, v. 38, n. 2, p. 529-536, 2004.

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