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Numerical modeling of deposition-release mechanisms in long-term filtration: validation from experimental data

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ABSTRACT

A numerical phenomenological filtration model based on the combination of existing modeling approaches for simulating the transport of suspended particles in saturated porous medium is presented. The model accounts for the decreased physical straining with the distance from the inlet and the amount of deposited particles in the deposition kinetics. The particle release flux is a function of the local shear stress exerted by the flow on the pore surfaces. The proposed model is validated by interpreting a series of experimental data, realized in a laboratory sand column. The results show that the present model allows simulating the presence of a plateau in the breakthrough curves in the light of the shear stress conditions, and the spatial profile of deposited particles in the porous medium in the light of the straining profile.

1. Introduction

Filtration is a term used to describe the deposition and capture of solid particles from the transport of a fluid suspension through a porous medium. Filtration processes are encountered widely in the natural and industrial systems. Granular filtration is one of the widely implemented treatment methods for dilute aqueous suspensions. In this method, grains of the porous medium adsorb a substantial fraction of the suspended particles transported by water inside the filter bed. It is necessary to understand filtration kinetics and to predict filter performance for ensuring a high quality of the tap water. For a long time, the retention of particles by passage through a filter bed was determined using the classical colloid filtration theory (CFT) [1,2]. This theory is based on the assumption that particles are retained at a constant rate. Recent research shows that the CFT with a spatially constant kinetic approach was insufficient to predict the observed particle deposition profile. Li et al. [3] and Tufenkji and M. Elimelech [1,2] reported a reduction of the coefficient of deposition rate with transport distance. Lutterodt [4] found out that deposition rate coefficients decreasing with the distance were needed to predict accurately the shape of the profile of the observed retained particles in laboratory sand columns. In order to describe the shape of the profile of the retained particles in column tests, Bradford [5,6] incorporated two empirical kinetic terms for estimating two particle-retention mechanisms: (i) attachment–detachment to the grains surfaces of the filter and (ii) straining, which is the retention of particles in the smallest regions of the soil pore formed adjacent to points of grain–grain contact. Detachment and re-entrainment of previously filtered particles is handled by introducing a detachment term in the attachment–detachment kinetic term. The use of a depth-dependent function in the straining term enables accurate description of their observed retained particle profiles. Bai and Tien [7] introduced a dimensionless

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function in the deposition kinetic term in order to account for time-dependent retention. El Ganaoui et al. [8] showed that the release of deposited particles is induced by the hydrodynamic forces applied to the throat pore of porous media. A function of the pore shear stress was used for simulating the release process. Long-term effects in the filtration process are important in natural environments where backwashing of filters is not possible. A series of filtration experiments were conducted on laboratory columns in order to analyze long-term effects. Indeed, in these experimental conditions, deposition and mobilization mechanisms are complex and change greatly over time and space. In the present study, we present a mathematical model developed in order to characterize, through our experimental data, the main effects of long term in filtration process. Based on previous models of transport, deposition and mobilization phenomena, the present model incorporates several changes to take into account the non-linear deposition and mobilization mechanisms as well as their dependence on time and space. The model predictions are compared with experimental data from our laboratory filtration experiments.

2. Mathematical models

The filtration tests in laboratory columns can be described by the transport equation [9]:

$$\frac{\partial(\omega_c C)}{\partial t} = D\frac{\partial^2(\omega_c C)}{\partial x^2} - u\frac{\partial(\omega_c C)}{\partial x} - f \quad \text{with} \begin{cases} \omega_c = \omega_o - \omega_p \\ D = \alpha|u| \end{cases} \tag{1}$$

where ω_c is the kinetic porosity, ω_o the initial porosity of the porous medium, ω_p the specific deposit (volume of deposited particles per unit volume of the porous medium), C the concentration of suspended particles in the aqueous phase, D the dispersion coefficient, α the dispersivity, u the aqueous phase velocity, and f the source term. In the case of step-input experiments, the initial and boundary conditions are given by:

$$C(x \geq 0) = 0 \quad \text{and} \quad \omega_p(x \geq 0) = 0 \quad \text{for } t = 0 \tag{2}$$

$$C(x = 0) = C_o \quad \text{and} \quad \partial C(x = L)/\partial x = 0 \quad \text{for } t > 0 \tag{3}$$

with C_o the concentration of injected particles and L the length of the porous medium. The source term f, describing the deposition and the release of fine particles, is the sum of two kinetics:

$$f = q_{dep} + q_{rel} = \rho_p\frac{\partial \omega_p}{\partial t} \quad \text{with} \begin{cases} q_{dep} = K_{dep}\omega_c C\phi(\omega_p)\theta(x) \\ q_{rel} = -K_{rel}\omega_p\rho_p\zeta(\tau) \end{cases} \tag{4}$$

where K_{dep} and K_{rel} are respectively the deposition and release coefficients, ρ_p is the density of fine particles, and ϕ is a dimensionless function to account for time local dependent retention. It is given by [7]:

$$\phi(\omega_p) = 1 + a(\omega_p/\omega_{pmax}) + b(\omega_p/\omega_{pmax})^2 \tag{5}$$

where ω_{pmax} represents the maximum volume of deposited particles per the unit volume of the porous medium, a and b are dimensionless coefficients estimated by means of a matching of experimental data, and θ is a dimensionless function to account for the depth-dependent retention given by:

$$\theta(x) = \left((L_p + x)/L_p\right)^{-\beta} \tag{6}$$

This function is similar to that reported by Bradford et al. [5], where L_p is a parameter for the pore length set equal to d_{50}. β is a fitting parameter allowing one to control the shape of the curve. In our experiments, we observed deeper clogging. Using the Bradford function does not allow us to correctly predict the experimental results. A characteristic length that is better suited was then used. The parameter L_p used characterizes the penetration depth of the transported particle and it is evaluated using the equation $L_p = u/K_{dep}$. For the same reason, β is taken equal to unity. Based on the shear stress function proposed by [8], we incorporate in the release kinetic term the dimensionless shear stress function ζ:

$$\zeta(\tau) = \begin{cases} (1 - \tau_{cr}/\tau)^n & \text{if } \tau \geq \tau_{cr} \\ 0 & \text{if } \tau < \tau_{cr} \end{cases} \quad \text{with } \tau = \Delta P/\Delta L(2k/\omega_c)^{0.5} \tag{7}$$

τ is the local hydraulic shear stress [10], and τ_{cr} is the critical shear stress. n denotes an empirical parameter which is estimated by means of numerical tests. $\Delta P/\Delta L$ represents the local pressure gradient in the porous medium and k is the intrinsic permeability of the porous medium. The deposition and release of fine particles change the geometry of the porous medium. Thus the hydraulic characteristics of the porous medium are modified during the filtration of suspended particles. In order to take into account this modification, a flow equation is coupled with the filtration model. Under the assumption of a constant flow rate, the flow equation is given by:

$$u = \frac{Q}{\omega_c \pi R^2} \tag{8}$$

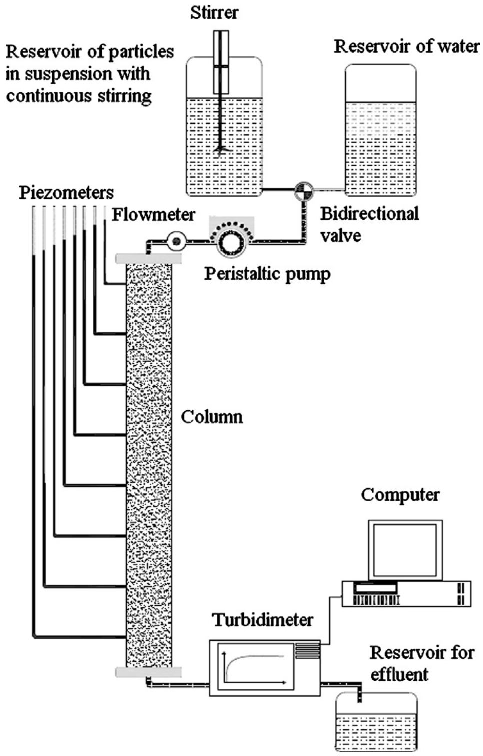

Fig. 1. Experimental setup for filtration tests.

where Q and R are the flow rate and the radius of the laboratory column, respectively. A Lagrangian approach, called vortex method, is used to solve the filtration model [11]. The vortex method allows checking easily the mass conservation and the boundary conditions. The coupling between the filtration model and the flow equation is performed by using a non-iterative sequential scheme. The filtration model and the flow equation are resolved successively.

3. Validation from experimental data

3.1. Experimental setup

The predictions of the present model are compared with experimental data obtained from laboratory long-term filtration tests [12]. The step-input injection technique is used in this experimental investigation for studying transport and filtration mechanisms of suspended particles (SP) in saturated porous medium (see Fig. 1). A Plexiglas column with an inner radius $R = 2.25$ cm and a length $L = 40$ cm was used. The column was vertically oriented and packed in 5-cm increments by slowly pouring sand into distilled water to avoid trapping air bubbles. The porous medium that filled the column consisted of quartz sand with a grain-size distribution ranging from 315 to 630 μm and a median diameter of 410 μm. The injected SP consisted of size-selected particles of kaolinite with a particle-size distribution ranging from 1.7 to 40 μm and a median diameter of 10.5 μm. Using the bulk-density method, the porosity of the sand was found to be $\omega_0 = 0.37$. The SP injection was done from a SP reservoir where a suspension with a desired particle concentration had been prepared previously. A motorized stirrer was used to prevent the deposition of particles on the interior surfaces of the reservoir and to keep the suspension stable and uniform during the injection experiment. A peristaltic pump was used to pump the influent suspension from the SP reservoir into the porous medium sample at a constant rate of 145 ml/min. The effluent coming out of the porous medium sample was passed through a continuous flow turbidimeter to record the turbidity values in term of nephelometric turbidity units (NTUs). The particle concentrations in the effluent were determined with the help of correlations made a priori between measured SP concentrations in the water and values in NTU given by the turbidimeter. The breakthrough curves are then obtained. Six SP concentrations were used: 0.25, 0.50, 1.00, 1.50, 2.00, and 3.00 g/l and a total volume of 83 pore volume of SP was injected in each experiment. Following each column experiment, the dirty sand filling the column was excavated and the mass of the deposited SP along the porous medium was determined. The profile of the retained particles was then determined.

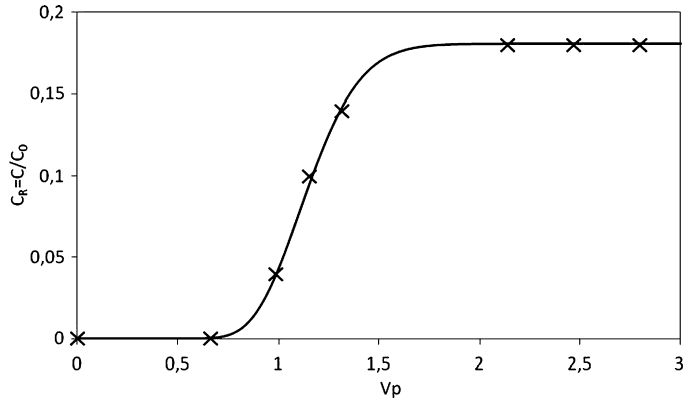

Fig. 2. Measured and predicted breakthrough curves C_R for $Q = 145$ ml/min and $C_o = 0.25$ g/l with $V_{inj} < 3V_p$ (crosses, experimental data; solid line, the present model).

Table 1
Fitting parameters for the present filtration model.

C_o (g/l)	α (cm)	K_{dep} (h^{-1})	K_{rel} (h^{-1})	τ_{cr} (Pa)	a	b
0.25	0.8	89.28	1.656	0.222	−0.1	30
0.5	0.8	86.4	1.476	0.158	−2.5	15
1	0.7	109.08	1.26	0.153	−2.5	6.5
1.5	0.4	91.8	1.62	0.1	−2.5	6.5
2	0.4	109.8	2.16	0.19	−2.5	7
3	0.4	144	2.88	0.176	−2.5	7

3.2. Fitting method

The large number of fitting parameters did not allow us to use effectively the optimization algorithms. In order to overcome this difficulty, a simple two-step procedure based on the analysis of experimental data has been used [13]. The analysis of breakthrough curves (BTC) from all experiments shows two distinct filtration stages. In the first times of the filtration process, the BTCs reached a plateau after a volume of about $2V_p$ has been injected and remained constant until a critical volume, which depends on the inlet concentration C_o, has been injected. In this stage of filtration, the particle deposit does not substantially modify the hydraulic properties of the porous medium and does not prevent the deposition of other particles in the suspension. The curve is typical of filtration in a clean bed medium. Beyond this critical injected volume, the accumulation of deposited particles becomes increasingly sufficient to modify the hydraulic characteristics of the medium. In addition, the amount of particles already deposited in the porous medium influences the filtration of other particles. As a consequence, SP removal decreases and SP concentration in the effluent increases with time. The experiment with $C_o = 0.25$ g/l is used to describe the fitting procedure. The first step consists in estimating the dispersivity α and the deposition coefficient K_{dep} from the adjustment of BTCs observed in the first times of the filtration process ($V_{inj} < V_p$) (see Fig. 2). In this stage of filtration, the deposited particle is not substantial and we can assume that the release phenomenon has not started yet and the deposition coefficient K_{dep} is constant. The value of K_{dep} impacts mainly the level of the concentration plateau and the value of α determines the spreading of BTCs around one injected pore volume. Fig. 2 presents the adjustment of the breakthrough curve with $\alpha = 0.8$ cm and $K_{dep} = 49.68$ h^{-1}. Table 1 gives the values of α and K_{dep} for all experiments. Note that these values are in agreement with the literature ones. In the second step of the fitting, the parameters of deposition and release functions (K_{rel}, τ_{cr}, a and b) are fitted to the results of BTCs' long-time filtration analysis and with the profile of the specific deposit ω_p obtained at the end of each experiment. From the experimental literature and a sensibility analysis, the parameters n and β were fixed to 0.3 and 1, respectively. The parameter L_p that characterizes the penetration depth of the transported particle is evaluated from the equation $L_p = u/K_{dep}$. Fitting is performed manually by minimizing the difference between the experimental data and the numerical results. Fig. 3 presents the adjustment of the experimental breakthrough curve and profile of the specific deposit ω_p with $a = -0.1$, $b = 30$, $K_{rel} = 1.656$ h^{-1} and $\tau_{cr} = 0.222$ Pa.

3.3. Results

Fig. 4 presents an example of comparison between experimental and predicted breakthrough curves. The predicted curves are obtained by the present model and the classical model of first-order kinetics, respectively. We can observe that the experimental data present a concentration plateau for $0 < V_p < 15$ and then an increase that is slowed down for $V_p > 60$.

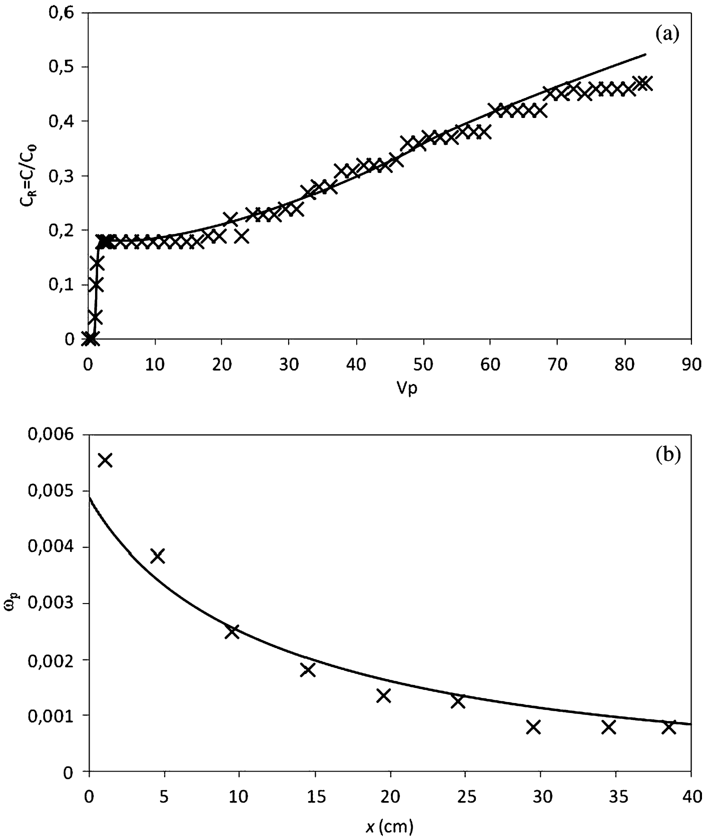

Fig. 3. Matching of the breakthrough curve C_R (a) and of the profile of specific deposit ω_p (b) for $Q = 145$ ml/min and $C_o = 0.25$ g/l (crosses, experimental data; solid line, the present model).

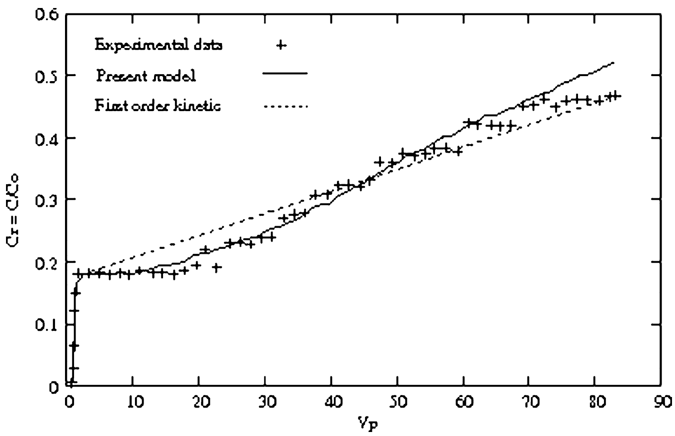

Fig. 4. Comparison between predicted breakthrough curves C_R obtained from various filtration models for $Q = 145$ ml/min and $C_o = 0.25$ g/l (squares, experimental data; solid line, the present model; dashed line, first-order kinetic model).

It is well shown that the first-order kinetic model is not able to accurately fit a non-monotonic breakthrough curve. The model does not allow one to simulate the presence of a concentration plateau at the start of the experiment, and a great discrepancy between predicted and measured curves is observed. On the other hand, the present model is able to predict accurately the whole curve and the presence of the concentration plateau is well simulated. The model is used to predict the results from all experiments performed. The fitting parameters used in the present model are given in Table 1. In Fig. 5a, the breakthrough curve for $C_o = 0.25$ g/l presents in the first 15 pore volumes a plateau close to 0.2 g/l. At the beginning of the filtration process, the intensity of the local shear stress τ is not sufficiently strong to detach the fine particles deposited in the porous medium. The rate of particles release q_{rel} is then zero, while the rate of particles deposition q_{dep} is non-zero. The progressive deposition of fine particles induces progressively an increase of τ. When the shear stress τ becomes larger

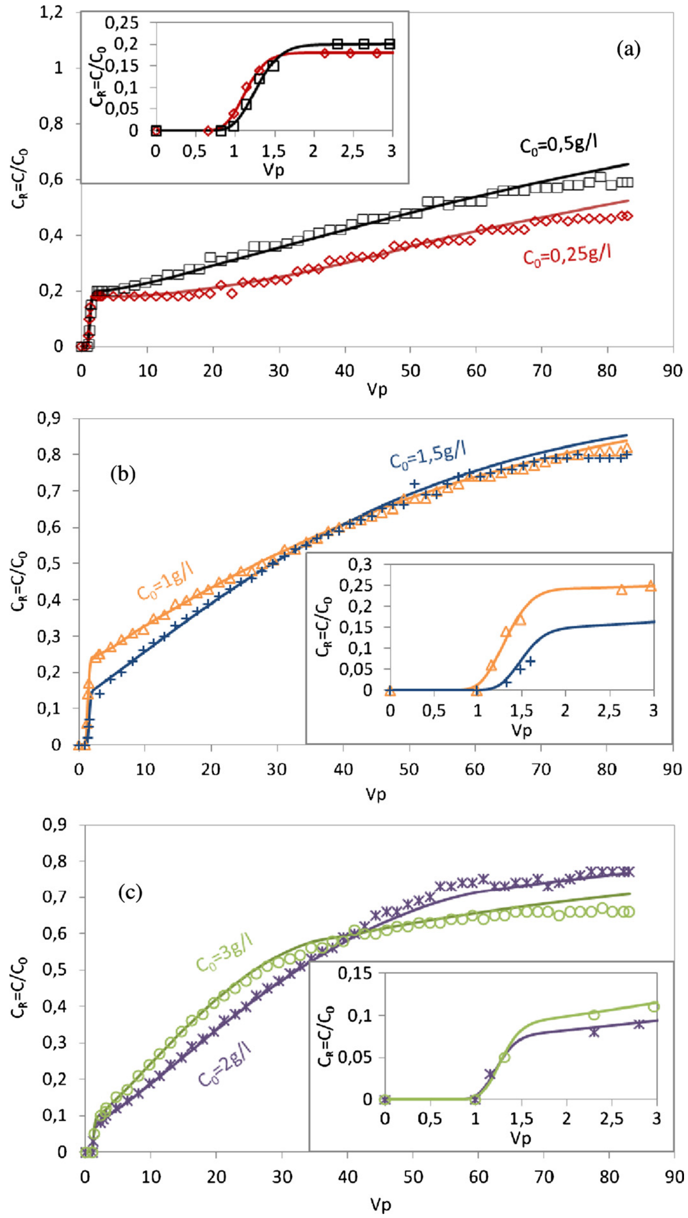

Fig. 5. (Color online.) Breakthrough curve (or relative concentration C_R as a function of the pore volume V_p) for a constant flow rate $Q = 145$ ml/min with various concentrations of injected particles ($C_o = 0.25$ and 0.5 g/l (a), 1 and 1.5 g/l (b), 2 and 3 g/l (c)).

than the critical shear stress τ_{cr}, the detachment of particles starts. The release rate increases progressively as τ increases. Thus the concentration measured at the outlet increases. The presence of a concentration plateau is also observed in all other tests. However, the time duration of the plateau is very short for tests with great inlet concentrations ($C_o = 2$ g/l and 3 g/l). For the above concentrations, the deposition rate is high and allows reaching τ_{cr} very quickly. We can conclude that the incorporation in the kinetic term of the release of the shear stress function $\zeta(\tau)$ (Eq. (7)) allows simulating correctly the breakthrough curve in the short time for all tests realized. Fig. 5a shows a non-monotonic increase of C_R with the injected volume beyond the critical volume ($15NV_p$) limiting the concentration plateau. This confirms the change in time of the kinetic of accumulation of the particles deposited in the porous medium. The change of q_{dep} is induced by the capacity of the grains of the porous medium for the capture of the suspended particles. When the particles deposit in the medium, the collector surface (surface of grain) is reduced. Thus q_{dep} decreases. When the deposited particles are released in the aqueous phase, the collector surface increases. Thus q_{dep} increases. This evolution is observed for all other tests. The measured deposition of suspended particles is not homogeneous in the porous medium. It is more important at the column inlet and decreases strongly with the distance from the inlet of the column. The incorporation of the shear stress function $\zeta(\tau)$ in the kinetic term of release and the functions of variation of the kinetic term of deposition in time and

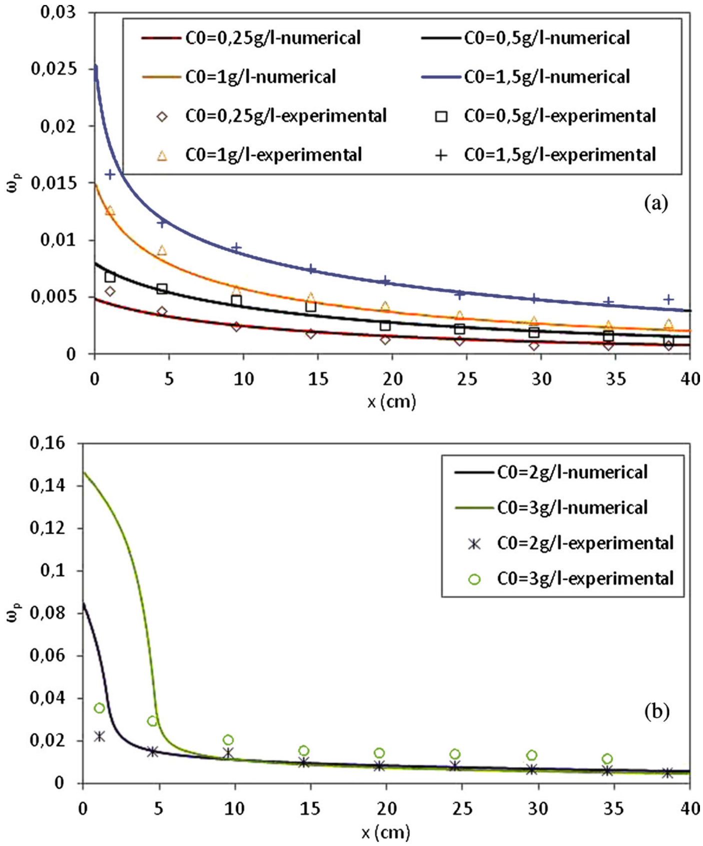

Fig. 6. (Color online.) Spatial distribution of ω_p in the laboratory column at the end of filtration tests for a constant flow rate $Q = 145$ ml/min with various concentrations of injected particles ($C_o = 0.25, 0.5, 1$ and 1.5 g/l (a), 2 and 3 g/l (b)).

depth allows simulating correctly both the whole breakthrough curve and the spatial distribution of the specific deposit ω_p obtained at the end of the experiment. The comparison between measured and predicted results is presented in Figs. 5 and 6 for all experiments realized. It is well shown that the novel formulations of the kinetic terms of deposition and release allows predicting accurately the breakthrough curves and spatial distributions of particle deposit through the porous medium. These results suggest that the present model simulates correctly the different mechanisms occurring in long-term filtration process.

4. Conclusions

In the present study, a phenomenological model of deep bed filtration is presented. The model combines an advection–dispersion equation with a non-linear equation of accumulation kinetic. The accumulation kinetic incorporates a kinetic term of deposition and a kinetic term of release. The deposition rate is time and depth dependent. The deposit is reversible and the mobilization and the re-entrainment of previous deposits can occur when the shear stress exerted by the flow on the pore surface exceeds the critical shear stress, which depends on the characteristics of the porous medium. The equations have been solved numerically using a Lagrangian approach. The values of the fitting parameters were set in the ranges reported in the literature. Predictions of the model are compared with experimental data taken from long-term filtration tests. The good agreement of the predictions with the experimental data suggests that the present model simulates correctly the different mechanisms occurring in long-term filtration processes.

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