MODELING AND SIMULATION OF IRON/SAND FILTERS

Titre en français : Modélisation et simulation des filtres à eau faits de particules de fer et de sable

Short title: Modeling and simulation of Iron/sand filters

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Abstract:

This article develops a mathematical model of Iron (Fe^0) /sand filter taking into account the loss of porosity during the filtration process. The mass transport advection-dispersion equation is derived to predict, through numerical simulation, the spatiotemporal distribution of pollutants and the flow rate in the filter as well as the water quality at the exit of the filter. Simulation results demonstrated that by mixing sand and iron particles in proportion of 40 vol% Fe^0, the filter can be used continuously for 83 months.

Author keywords: Iron/sand filters; Mathematical model; Loss of Filter porosity; Advection-diffusion equation; Numerical Simulation; Distribution of pollutants; Filter service life.

RESUME :

Cet article développe un modèle mathématique de filtre à base de particules de fer (Fe^0) et de sable en tenant compte de la perte de porosité au cours du processus de traitement de l'eau. L'équation d'advection-dispersion est établie pour prédire, par simulation numérique, la répartition spatiotemporelle des polluants et le débit d'eau à travers le filtre ainsi que la qualité de l'eau à la sortie du filtre. Les résultats des simulations montrent qu'en mélangeant le fer et le sable dans une proportion de 40% en volume de fer, le filtre peut être utilisé en continu pendant une période de 83 mois.

Mot clés : Filtres fer/sable ; Modèle mathématique ; Perte de porosité du filtre ; Equation d'advection-dispersion ; Simulation numérique ; Répartition des polluants ; Durée de vie du filtre.

1.INTRODUCTION

Water pollution mostly results from (i) natural mobilization/leaching, (ii) mining activities, (iii) industrial discharge, (iv) agricultural discharge (e.g. fertilizers, herbicides, pesticides), (v) solid waste disposal, and (vi) unplanned urban and rural development. Poor water quality has damaging impacts on human health, aquaculture and ecology. In general, water quality problems for human health fall into two major categories: (i) microbiological contamination responsible for immediate acute diseases and (ii) chemical contamination, which poses cumulative and chronic health risks to human beings and aquatic life (Ahamed et al., 2009**)**.

The scientific community is on schedule to develop universal water treatment units for domestic use (Clasen et al., 2009). The suitability of metallic iron (Fe^0) as universal filter material has been recently discussed (Noubactep et al., 2010). It is based on the fact that corroding iron has the ability to remove all soluble species by an unspecific mechanism. There are however two main modifications in the design of Fe^0/sand filter in comparison to the Kanchan Arsenic Filter (KAF) developed and distributed in Nepal by Ngai et al. (2007): (i) the Fe-oxide-producing unit (Fe^0/sand bed) is placed after the conventional Biosand filter (BSF) and (ii) the Fe^0/sand bed contains an optimal proportion of Fe^0 mixed to sand to extent the filter service life.

In this paper, an approximate and feasible mathematical model that allows for the prediction of concentration profiles of aqueous pollutant is developed. The prediction is based on time and height measurements in a Fe^0/sand bed according to the variation of the pore space within the filter as expansive corrosion proceeds. The service life of the filter is operationally defined as the time to reach (i) 75 % porosity loss and (ii) more than 75% removal from a 100% influent contaminant concentration. This assumption is justified by the fact that chemical pollutants typically occur in trace amounts, rarely considerably larger that the maximum contaminant levels (Schwarzenbach et al., 2010). It is found that the pollutant removal percentage and the service life of the filter depend on the relative proportions of sand and iron in the filter.

2 PHYSICAL MODEL DESCRIPTION

Let us consider a layer of water containing contaminants as shown in Fig.1. *H* is the height and *D* the diameter of the bed. Water which is considered as an incompressible and Newtonian fluid flows toward the bottom of the column (porous medium) by gravity. The column which contains a mixture of spherical particles (sand + metallic iron) of equal size constitutes the filter.

2.1 Filtration velocity and Variation of porosity of the filter

In the case the water flows towards the column by gravity, the filtration velocity, follows the Darcy law (Marle, 2006). Therefore the flow velocity modulus in the filter is a temporal function given as

$$q(t)=\frac{\rho g d_0^2\varphi^3}{180\mu(1-\varphi)^2}\left(\frac{h_{water}}{H}+1\right) \tag{1}$$

with $\varphi(t)=\varphi_0\left(1-n_{Fe}.a_p.t\right)$, $a_p=\frac{\delta \mathrm{d}_0^3}{\varepsilon D^2 H}$, $\delta=3.8\mathrm{x}10^{-5}$. ρ is the density of water, d_0 is the diameter of iron and sand particles, *H* is the height of the cylinder, φ is the porosity based on porosity losses kinetics (Mackenzie et al., 1999), h_{water} the height of water, μ the dynamic viscosity. n_{Fe} is the number of iron particle, a_p is the porosity losses rate and *t* the operation time. □ is the fraction volume of particles. This expression of the porosity has been derived recently by the authors (Noubactep *et al.,* 2010).

2.4.2 Mass transport equation for pollutants in the filter

The spatiotemporal variation of pollutants in the filter obeys the following equation

$$\frac{\partial C}{\partial t}=\frac{1}{R_0}\left(D_z\frac{\partial^2 C}{\partial z^2}-\frac{q}{\varphi}\frac{\partial C}{\partial z}\right)$$
$$with,\ R_0=1+\frac{\rho_b.n.K_f C^{n-1}}{\varphi} \tag{2}$$

This equation describes a microscopic mass balance using Fick's law adapted to macrodispersion (Rooklidge et al., 2005). The hydrodynamic dispersion coefficient, D_z, includes turbulence effects caused by species and gravity. ρ_b is the iron bulk density of the porous media, n the sorption intensity parameter and K_f the sorption capacity parameter (Williams et al., 2003). The main feature of this equation (2) is the time dependence of the flow velocity q and the porosity φ. This time dependence is seen hereafter to be an important factor that makes the theoretical prediction similar to what is found from the experimental investigation. This equation (2) can be coupled to transfer equation that describes the transfer of water and its pollutants to the filter (Peel et al., 1980; 1981). However, this equation is not necessary here since it is assumed that the pollutant concentration at the entrance of the filter is assumed known and constant. The main concern is to find out how the effects of time dependence of the porosity affects the concentration of pollutants at the exit or at any point of the filter.

The initial and boundary conditions related to the transport equation are C (z, 0) = C_0 if z=0, if not C (z, 0) = 0, i.e. initially uncontaminated column; **C** (0, t) = C_0, where C_0 is the concentration of pollutants at the entrance of the filter and H the depth of the filter. The following values of the parameters are used. ρ= 1000 kg/m^3, g= 9.81 m.s^{-2}, d_0=1.2 mm, μ = 0.01 g/s.cm, h_{water}=20 cm, H=50 cm, □ =0.64, D=50 cm (this gives a cylindrical bed volume equal to 98 L), Dz=0.14 cm^2/min (Williams et al. 2003), ρ_b=7800 kg/m^3, n=0.32, K_f=278 L/kg. We remind the reader that the sand density is equal to 2650 kg/m^3. The determination of n_c, which is the threshold number of iron particles necessary to fill completely the initial volume of pores, is obtained as the ratio between total volume of pores in the filter and the volume of expansive corrosion product minus the mean value of the iron particle (Caré et al., 2008, Noubactep et al., 2010). With the above values of it is found that nc≈20 millions (which corresponds to about 141 kg of iron).

3 RESULTS AND DISCUSSIONS

3.1 Temporal distribution of solutes

Equation (2) is solved numerically. The spatial derivative is discretized using the backward finite difference scheme while the time derivative is handled using the fourth order Runge-Kutta computer routine written in FORTRAN**.** The value of concentration of the pollutant at the entrance of the filter is C0= 0.35 mg/L. Figure 2a presents the time variation of the pollutant concentration at the filter exit for different values of the number of iron particles. It is found that the pollutant concentration at the exit increases with time and decreases when the number of iron particles increases. If one assumes that 25% of the pollutant concentration is tolerable, then the service time of the filter is found to be more than 83 months for 20 millions of iron particles. In contrast, Figure 2b shows that for 20 millions of iron particles and assuming that the porosity is constant (as it considered in most of the scientific papers), the service time of the filter is approximately 17.2 months. This demonstrates that the long-term performance of the filter is assured by the iron corrosion product formed continuously over the iron surface. To end this section, we note that the numerical simulation can help to find out how the pollutant concentration evolves over the filter length showing the action of the zero valent iron in the removal process of pollutants (Youwen et al., 2005).

3.2 Validation of the model implementation

To validate the correct implementation of the model, the experimental breakthrough curve obtained by Sanghamitra and Gupta in 2005 is used (see Fig. 2 of this reference). The transport Eq. (2) is then solved numerically with input parameters provided by the same authors (C_0=2 mg/L, n=0.53, K_f=2.67L/g, V=0.41 m/min) For three different bed depths, Figure 3 shows the results obtained from our simulation for pollutant in the influent against time (in hours, h). Our Figure and that of Sanghamitra and Gupta (2005) reveal agreement for the treated pollutant system. Therefore, our model can be used to predict the breakthrough curves. By taking into account the porosity loss which is one factor that affects the performance and lifetime of the granular iron media, the new model developed in this work can therefore be used to predict long-term performance of filters.

4 CONCLUSION

From an analysis on a typical cylindrical sand/iron filter and the kinetics of iron corrosion in water, an equation describing the spatiotemporal variation of pollutants concentration in the filter has been developed. The numerical simulation has been used to monitor the spatial and temporal variation of the pollutants concentration. It has been found that by taking into account the time variation of the porosity due to the reduction of porosity by the corrosion products, the mathematical model gives results similar to what is obtained from experimental investigations.

This study constitutes a step for a more complete design of an affordable filter that can be for community access to safe drinking water. But, this requires further studies, as for instance, long term experimental data of fixed bed column operations on pollutants removal by sorption onto iron/sand filter, after the model has taken into account the transfer processes between the liquid phase (water) and the surface of the filter (entrance side).

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Figure Caption

Figure 1. Schematic of analyzed system, including initial condition in the column.

Schéma du système analysé, y compris la condition initiale dans la colonne

Figure 2. Temporal distribution of the pollutants concentration at the filter exit (z=H) for different values of the number of iron particles, for time dependent porosity (Figure 2a), and for a constant porosity (Figure 2b). n_c is the threshold number of iron particles necessary to fill completely the initial volume of pores.

Distribution Temporelle de la concentration du polluant à la sortie du filtre (z=H) pour différentes valeurs du nombre de particules du fer, pour une porosité dépendante du temps (Figure 2a), et pour une porosité constante (Figure 2b). n_c *est le nombre de particules de fer nécessaire pour remplir le volume initial des pores.*

Figure 3. Breakthrough profiles for As (V) adsorption on iron oxide-coated cement (IOCC) at three different bed heights (for the validation of our model).

Profil de l'adsorption de As (V) sur du ciment enduit d'oxyde de Fer à trois hauteurs différentes du lit (pour la validation de notre modèle).

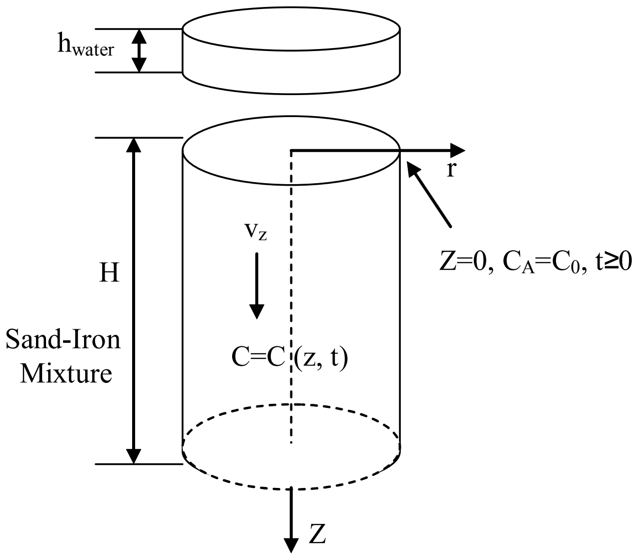
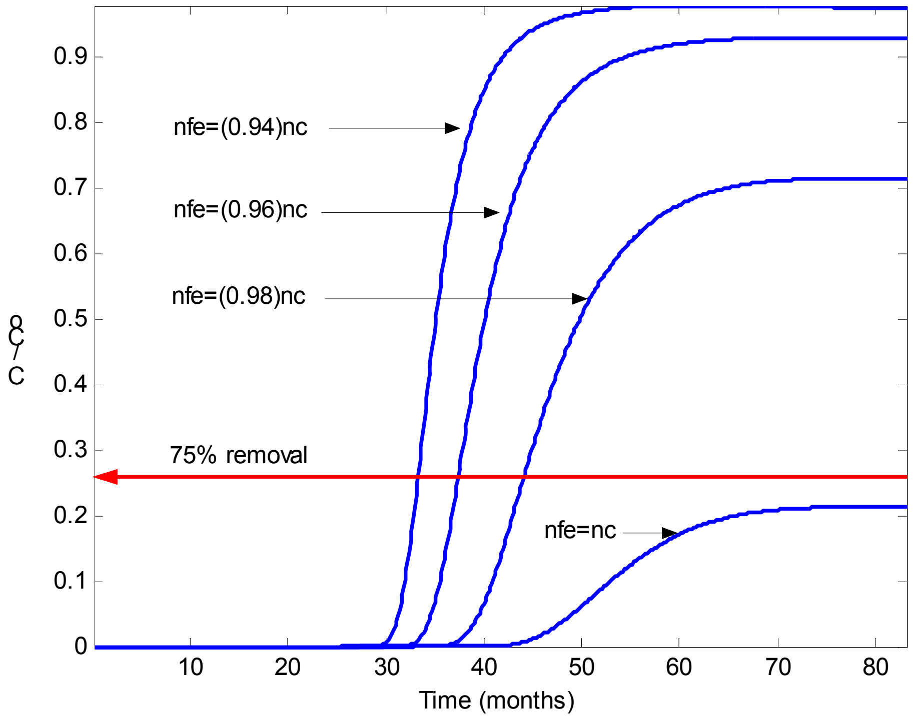
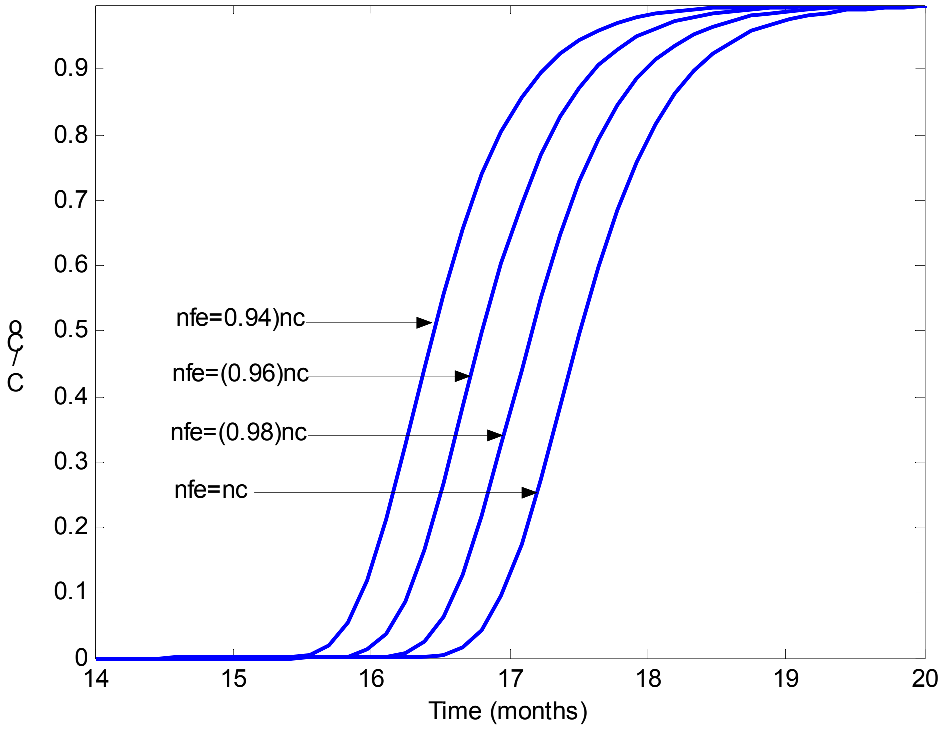


Figure 1.



(a)

Figure 2 a.



(b)

Fig. 2 b

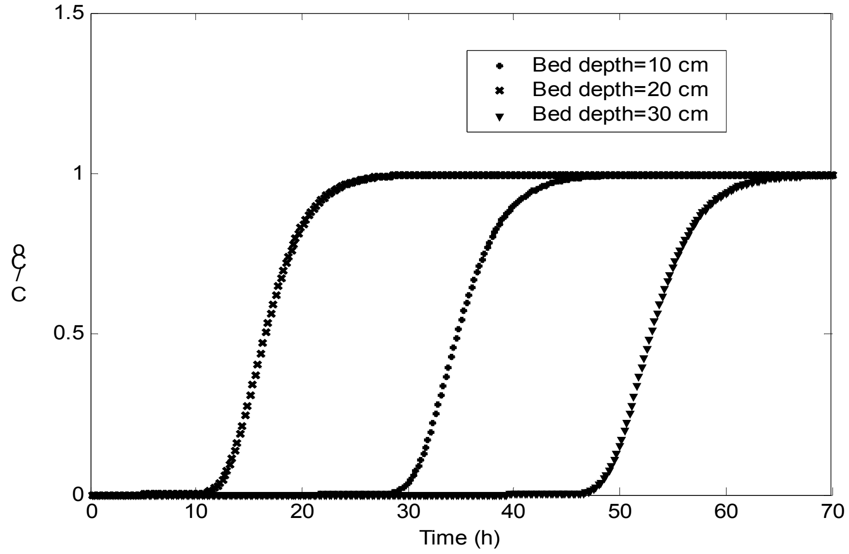

1.5
1
0.5
0
C/Co
0
10
20
30
40
50
60
70
Time (h)
Bed depth=10 cm
Bed depth=20 cm
Bed depth=30 cm

Figure 3.