

## Modeling and simulation of iron/sand filters Modélisation et simulation des filtres à eau faits de particules de fer et de sable

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[See table of contents](#)

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Article abstract

Water pollution is increasingly becoming an issue of global concern, especially in developing countries. Therefore, the development of affordable, reliable, low-maintenance, electricity-free technologies for reducing biological and chemical pollutants in drinking water to an acceptable level for human consumption is an interesting topic of research. The suitability of metallic iron ( $\text{Fe}^0$ ) as a universal filter material has been recently discussed. Iron/sand filters have a great potential for rural regions where source water may be subjected to various microbial and chemical contaminations. This is based on the fact that corroding iron has the ability to remove all soluble species by an unspecific mechanism. This article develops a mathematical model of iron( $\text{Fe}^0$ )/sand filter taking into account the loss of porosity during the filtration process. The porosity loss with time is calculated using the rate of formation of corrosion products. The time after which the porosity is reduced to zero indicating a zero flow rate is estimated. 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. The control parameters are the iron proportion, the volume of sand particles, the height of the filter and the sorption coefficient. 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.

For instance, taking the guideline equal to be 25% of the influent concentration, simulation results demonstrated that by mixing sand and iron particles in proportion of 40 vol%  $\text{Fe}^0$ , the filter can be used continuously for 83 months.

# MODELLING AND SIMULATION OF IRON/SAND FILTERS

*Modélisation et simulation des filtres à eau faits de particules de fer et de sable*

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## ABSTRACT

Water pollution is increasingly becoming an issue of global concern, especially in developing countries. Therefore, the development of affordable, reliable, low-maintenance, electricity-free technologies for reducing biological and chemical pollutants in drinking water to an acceptable level for human consumption is an interesting topic of research. The suitability of metallic iron ( $\text{Fe}^0$ ) as a universal filter material has been recently discussed. Iron/sand filters have a great potential for rural regions where source water may be subjected to various microbial and chemical contaminations. This is based on the fact that corroding iron has the ability to remove all soluble species by an unspecific mechanism. This article develops a mathematical model of iron( $\text{Fe}^0$ )/sand filter taking into account the loss of porosity during the filtration process. The porosity loss with time is calculated using the rate of formation of corrosion products. The time after which the porosity is reduced to zero indicating a zero flow rate is estimated. 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. The control parameters are the iron proportion, the volume of sand particles, the height of the filter and the sorption coefficient. 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.

For instance, taking the guideline equal to be 25% of the influent concentration, simulation results demonstrated that by mixing sand and iron particles in proportion of 40 vol%  $\text{Fe}^0$ , the filter can be used continuously for 83 months.

**Keywords:** *iron/sand filters; loss of filter porosity; advection-diffusion equation; numerical simulation; distribution of pollutants; filter service life.*

## RÉSUMÉ

La pollution des eaux devient de plus en plus un problème d'intérêt mondial, particulièrement dans les pays en voie de développement. Par conséquent, le développement de technologies à faible coût et faciles à maintenir, pour réduire les polluants dans les sources d'eau à boire à un niveau acceptable pour la consommation, est un sujet de recherche intéressant. Cet article développe un modèle mathématique de filtre à base de particules de fer ( $\text{Fe}^0$ ) et de sable en tenant compte de la perte de porosité au cours du processus de traitement de l'eau. La réduction de la porosité au cours du temps est calculée

en tenant compte de la vitesse de formation des produits de corrosion. Le temps après lequel la porosité est réduite à zéro, impliquant un débit d'eau nul à travers le filtre, est calculé. 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 paramètres de contrôle sont la proportion de fer, la taille des particules de fer, la hauteur de la colonne et le coefficient de sorption. Il est trouvé que le pourcentage de dépollution et la durée de vie du filtre dépendent des proportions relatives des particules de sable et du fer. Par exemple, prenant un seuil tolérable de 25 % de la concentration des polluants à l'entrée 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.

**Mots clés :** *filtres fer/sable; modèle mathématique; perte de porosité du filtre; équation 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 extend the filter service life.

In this paper, an approximate and feasible mathematical model that allows for the prediction of concentration profiles of aqueous pollutants 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 than the maximum contaminant levels (KÜMMERER, 2011). 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 Figure 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 where 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:

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

with  $\varphi(t) = \varphi_0 (1 - n_{Fe} \cdot \alpha_p \cdot t)$ ,  $\alpha_p = \frac{\delta d_0^3}{\epsilon D^2 H}$ ,  $\delta = 3.8 \times 10^{-5}$   $\rho$  is the density of water,  $d_0$  is the diameter of iron and sand particles,  $H$  is the height of the cylinder,  $\varphi$  is the porosity based on porosity loss kinetics (MACKENZIE *et al.*, 1999),  $h_{\text{water}}$  the height of water,  $\mu$  the dynamic viscosity.  $n_{Fe}$  is the number of iron particles,  $\alpha_p$  is the porosity losses rate and  $t$

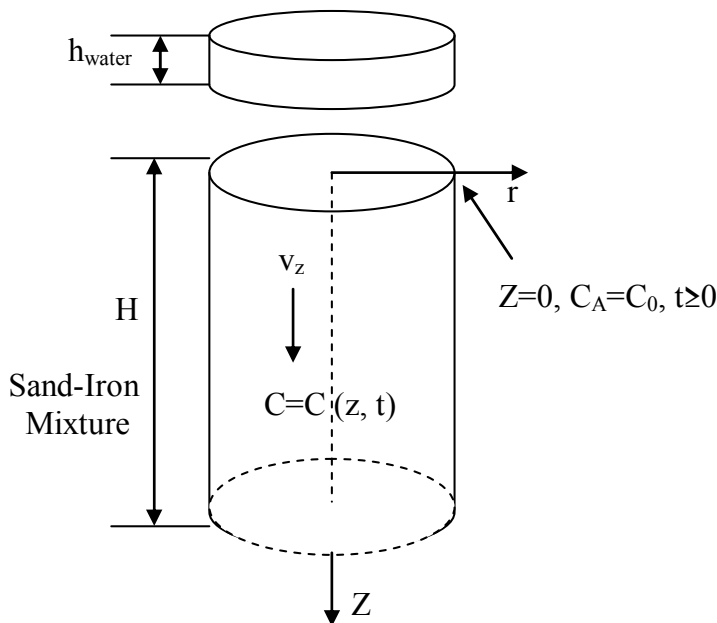


Figure 1. Schematic of analyzed system, including initial condition in the column.  
 Schéma du système analysé, y compris la condition initiale dans la colonne.

the operation time.  $\delta$  is the fraction volume of particles. This expression of the porosity has been derived recently by the authors (NOUBACTEP *et al.*, 2010).

### 2.2 Mass transport equation for pollutants in the filter

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

$$\frac{\partial C}{\partial t} = \frac{1}{R_0} \left( D_z \frac{\partial^2 C}{\partial z^2} - \frac{q}{\phi} \frac{\partial C}{\partial z} \right) \quad (2)$$

with,  $R_0 = 1 + \frac{\rho_b \cdot n \cdot K_f \cdot C^{n-1}}{\phi}$

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.  $\rho_b$  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  $\phi$ . 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 a 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.  $\rho = 1000 \text{ kg}\cdot\text{m}^{-3}$ ,  $g = 9.81 \text{ m}\cdot\text{s}^{-2}$ ,  $d_0 = 1.2 \text{ mm}$ ,  $\mu = 0.01 \text{ g}\cdot\text{s}^{-1}\cdot\text{cm}^{-1}$ ,  $h_{\text{water}} = 20 \text{ cm}$ ,  $H = 50 \text{ cm}$ ,  $\delta = 0.64$ ,  $D = 50 \text{ cm}$  (this gives a cylindrical bed volume equal to 98 L),  $D_z = 0.14 \text{ cm}^2\cdot\text{min}^{-1}$  (WILLIAMS *et al.*, 2003),  $\rho_b = 7800 \text{ kg}\cdot\text{m}^{-3}$ ,  $n = 0.32$ ,  $K_f = 278 \text{ L}\cdot\text{kg}^{-1}$ . We remind the reader that the sand density is equal to  $2650 \text{ kg}\cdot\text{m}^{-3}$ . 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 it is found that  $n_c \approx 20 \times 10^6$  (which corresponds to about 141 kg of iron).

### 3. RESULTS AND DISCUSSION

#### 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  $C_0 = 0.35 \text{ mg}\cdot\text{L}^{-1}$ . 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  $20 \times 10^6$  iron particles. In contrast, Figure 2b shows that for  $20 \times 10^6$  iron particles and assuming that the porosity is constant (as 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 (YOU *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 (2005) is used (see Figure 2 of this reference). The transport Equation 2 is then solved numerically with input parameters provided by the same authors ( $C_0 = 2 \text{ mg}\cdot\text{L}^{-1}$ ,  $n = 0.53$ ,  $K_f = 2.67 \text{ L}\cdot\text{g}^{-1}$ ,  $V = 0.41 \text{ m}\cdot\text{min}^{-1}$ ). For three different bed depths, Figure 3 shows the results obtained from our simulation for a 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 the long-term performance of filters.

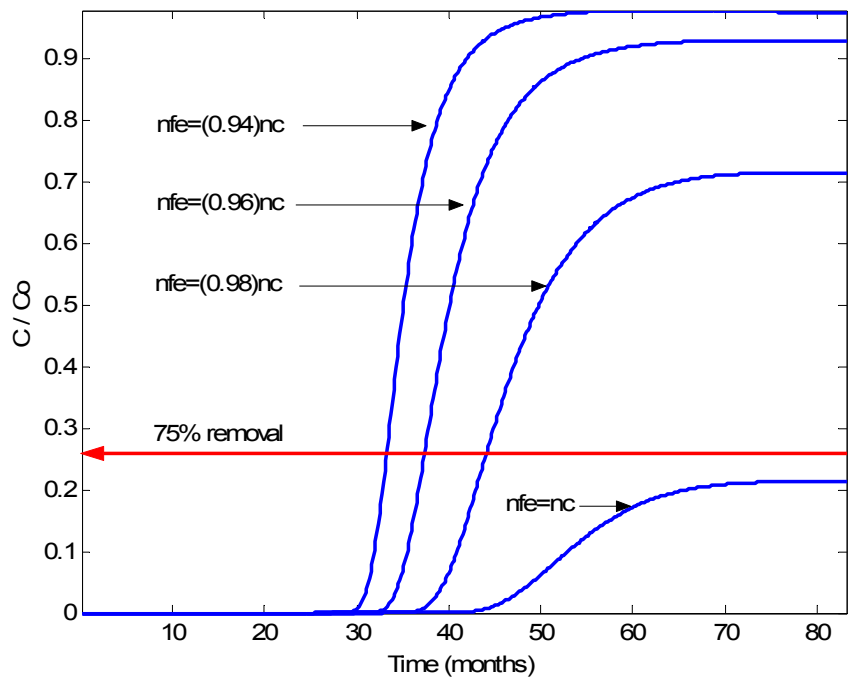
### 4. CONCLUSION

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 pollutant concentration in the filter has been developed. The numerical simulation has been used to monitor the spatial and temporal variation of the pollutant 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.

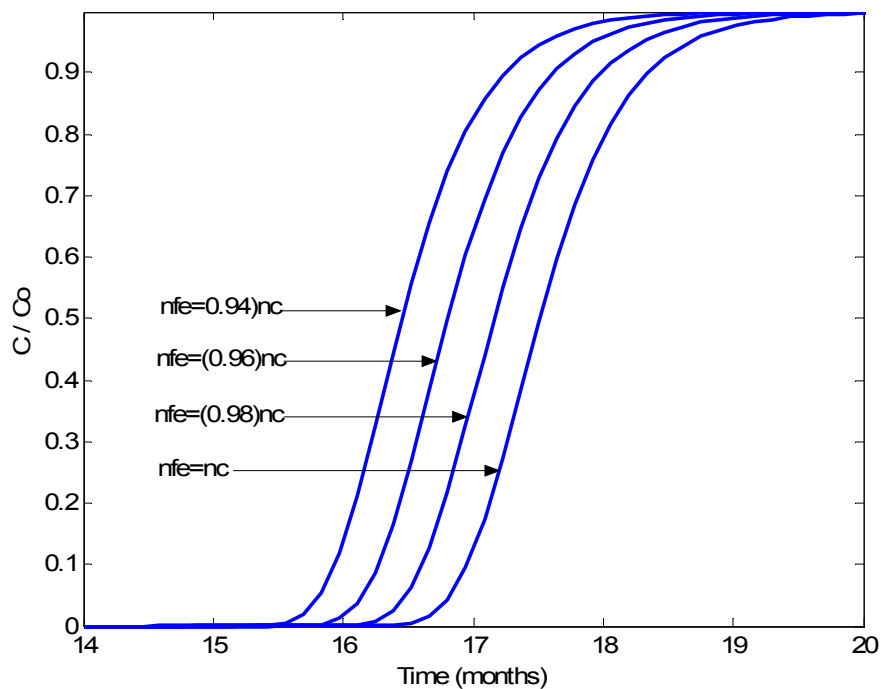
This study constitutes a step towards a more complete design of an affordable filter that can be for community access to safe drinking water. But this requires further studies such as, for instance, long-term experimental data for fixed bed column operations on pollutant removal by sorption onto iron/sand filters, 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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(a)



(b)

Figure 2. Temporal distribution of the pollutant concentration at the filter exit ( $z = H$ ) for different values of the number of iron particles, (a) for time-dependent porosity, and (b) for a constant porosity.  $n_c$  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, (a) pour une porosité dépendante du temps, et (b) pour une porosité constante.  $n_c$  est le nombre de particules de fer nécessaire pour remplir le volume initial des pores.*



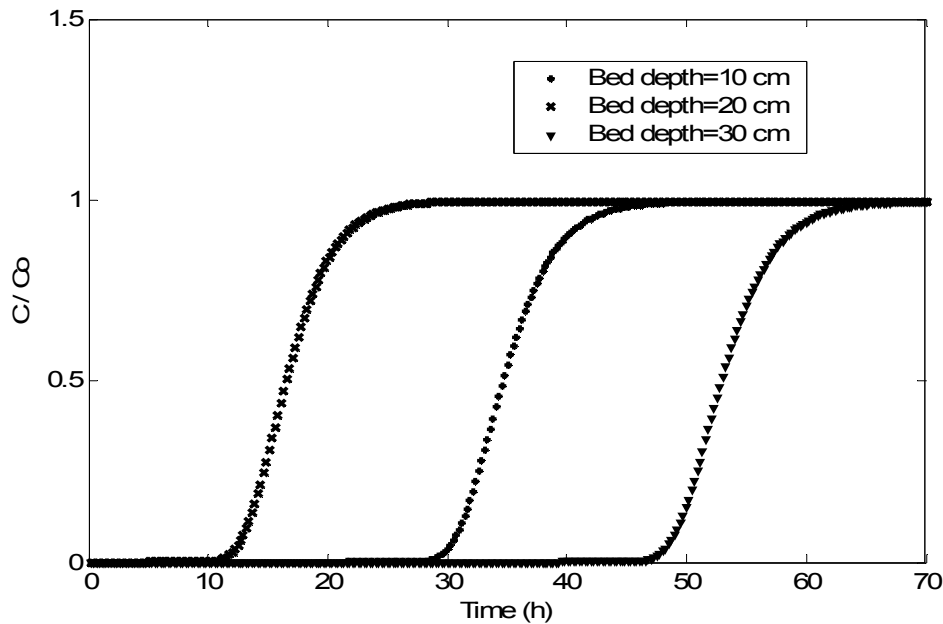


Figure 3. Breakthrough profiles for As- (V) adsorption on iron oxide-coated cement (IOCC) at three different bed heights (for the validation of our model).  
*Profil de l'adsorption de As- (V) sur du ciment enduit d'oxyde de fer à trois hauteurs différentes du lit (pour la validation de notre modèle).*

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