Modelling Waste Water Flow in Hollow Fibre Filters

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Abstract: In this paper we present a model to describe the process of waste water filtration based on hollow-fibre membrane filters. In particular, we deal with membranes whose pores diameter is in the range $0.01 - 0.1\ \mu m$, i.e. we consider the so-called *ultrafiltration* process. The main problem in these filtering systems is the membrane *fouling*: some of the particles to be filtered attaches on the membrane outer surface, soiling the medium and reducing the filtration efficiency.
The mathematical model consists in two equations for the Darcy's flow through the filter, coupled with an advection-diffusion-reaction equation and an evolution equation.
We solved the model by COMSOL, exploiting the Earth Science module and the Diffusion mode. The preliminary result of simulations shows that the qualitative behaviour of the solution is coherent with the experimental evidence.

Keywords: Flow in porous media, waste water filtration, membrane fouling

1 Introduction

The application of polymeric membranes to filter waste waters is a technique widely used by industry and municipal companies devoted to the control of the water quality. In particular, the filtration based on membranes is competitive due to the low cost of the materials and the management of the plants, compared to other filtration methods.
In our context, we deal with a filtration module consisting in a pressure vessel housing a number of bundles *U-shaped*; in turn, each bundle consists of a series of hollow fibre membranes, whose pores diameter is in the range $0.01 - 0.1\ \mu m$, which means that we are considering the so-called *ultrafiltration* process. The water to be filtered occupies the void space outside the fibres. A pressure gradient is applied between the interior part of the fibre and the outer one, so that the water flows through the membrane and the pollutant particles larger than the pore diameter are cut off outside the membrane. The clean water (the so–called *permeate*) is then collected and it flows away by the outlet.
The main problem in these filtering systems is the membrane *fouling*. As a the matter of fact, a part of the filtered particles can attach on the outer surface of the membrane, forming a thin layer (the so–called *cake*) which eventually soils the medium and reduces the filtration efficiency. To remove such a material, periodically a back wash process is imposed to the system, inverting the flux and let the clean water flow through the membrane.
In Fig.1 we show a picture of the filtering module we are considering, while in Fig 2 a magnified picture of a single fibre is reported. The filtration takes place in a *dead-end* configuration, i.e. the polluted water (*feed*) entering the module can flow away just going through the membranes. The feed goes into the module from an edge and flows in the space outside the fibres: in other words we are dealing with the so–called *outside/in* filtration. The permeate flows away by the outlet placed at the opposite edge of the inlet.
A single cycle of production takes almost one hour; afterwards a backwash cycle (almost 60 *sec.*) is imposed, along with an air scouring in order to make easier the removal of the cake from the membrane.

Figure 1: An example of hollow-fibre module (Courtesy of *Polymem* - Toulouse, France)

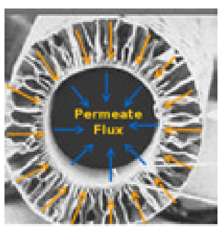

Figure 2: A magnified picture of a single hollow-fibre.

2 Model definition

In order to describe the process, we consider the module as a double porosity and double permeability porous medium. We define two regions:
(A) the *lumina region*, consisting in the volume occupied by the inner part of the fibres.
(B) the *shell region*, consisting in the space outside the fibres.
Therefore, the total membrane area is the interface between these regions, which are linked each other by a source/sink term representing the water flux through the membrane. A similar approach can be found in [1].
In the sequel we will use the following notation: subscript $(\cdot)_s$ is referred to the shell region, while $(\cdot)_l$ is referred to the lumina region.
Exploiting the axial symmetry of the module, we study the problem in a 2D domain using cylindrical coordinates. In particular, referring to Fig. 3 we denote by x the longitudinal coordinate pointing upward and by r the radial coordinate. Moreover, L is the length of the module and R its radius. In our model we neglect the effect of gravity, therefore the choice of the orientation of the coordinate x does not affect the model solution.

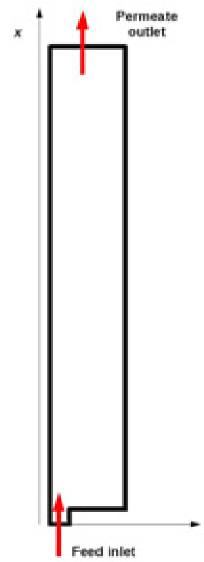

Figure 3: Domain of the problem for the hollow-fiber module

In such a domain, we write the mass conservation equation in each medium, i.e.

$$\nabla \cdot \mathbf{q}_s = -\Gamma, \qquad (1)$$

$$\nabla \cdot \mathbf{q}_l = \Gamma, \qquad (2)$$

where we have assumed a constant fluid density, ρ, and $\mathbf{q}$ is the specific discharge (or superficial velocity). Moreover Γ is the source/sink term, which will be defined later.

Concerning the characterization of the porous media, we assume the following:

- Since we are dealing with a tertiary water treatment, we stipulate that the fouling affects the filtration efficiency but it does not change the porosity and the permeability of the shell region. Therefore, in each medium we consider a constant porosity and permeability.

- In the lumina region, we have only the longitudinal permeability. Indeed, the inner parts of the fibres are not connected with one another. Therefore, we define k_l as the permeability of the lumina region (along the x coordinate).

- Conversely, in the shell region we introduce a permeability tensor

$$\mathbb{K} = \begin{pmatrix} k_{s,r} & 0 \\ 0 & k_{s,x} \end{pmatrix}.$$

  with $k_{s,x}$ and $k_{s,r}$ permeability along longitudinal and radial coordinate, respectively.

Shell and lumina porosity are defined in the usual way, i.e.

$$\varepsilon_s = 1 - N\left(\frac{r_o}{R}\right)^2, \tag{3}$$

$$\varepsilon_l = N\left(\frac{r_i}{R}\right)^2, \tag{4}$$

where N is the number of fibres and r_i, r_o are the inner and outer fibre radius, respectively.
Concerning k_l we use the well-known formula derived for media of capillary tubes and based on Hagen-Poiseuille flows (see [2], for instance),

$$k_l = \frac{N r_i^4}{8R^2} \tag{5}$$

For what concerns the shell, we use the formulas defined by Happel (see [3]), i.e.

$$k_{s,x} = \frac{r_o^2}{4\varphi}\left(-\log\varphi - \frac{3}{2} + 2\varphi - \frac{1}{2}\varphi^2\right) \tag{6}$$

$$k_{s,r} = \frac{r_o^2}{4\varphi}\left(-\log\varphi + \frac{\varphi^2-1}{\varphi^2+1}\right), \tag{7}$$

where $\varphi = 1 - \varepsilon_s$.

2.0.1 Darcy's flow

Using the parameters selected for the problem solution, we evaluate the Reynolds number of filtration and backwash process. During filtration the leading flow is the one in the shell, while the main flow during backwashing takes place in the lumina. Moreover, as usual in dealing with porous media, as characteristic length we consider the square root of the permeability. According to this argument, we get,

$$Re_{filtration} \approx 1.53$$

and

$$Re_{backwash} \approx 0.16$$

Therefore, in both cycles we are allowed to consider a Darcy's flow and thus we define

$$\mathbf{q}_s = -\left(\frac{k_{s,x}}{\mu}\frac{\partial P_s}{\partial x}\mathbf{e}_x + \frac{k_{s,r}}{\mu}\frac{\partial P_s}{\partial r}\mathbf{e}_r\right) \tag{8}$$

$$q_l = -\frac{k_l}{\mu}\frac{\partial P_l}{\partial x}. \tag{9}$$

where P_s and P_l are the pressure in the shell and in the lumina region, respectively.

As we said, the term Γ represents the rate of water loss per unit volume. Therefore it is linked to the averaged Darcy's velocity within the membrane, so that it is proportional to the pressure difference $(P_s - P_l)$.
We define,

$$\Gamma = \frac{A_v}{\mu\,(R_m + R_c)}(P_s - P_l) \tag{10}$$

where:

- A_v is the ratio between filtering area and filtering volume (specific filtering area), $[A_v] = L^{-1}$,

$$A_v = \frac{2 r_o N}{R^2 - N r_o^2}.$$

- R_m is the membrane resistance, $[R_m] = L^{-1}$, which is linked to the membrane permeability.

- R_c is the cake resistance, $[R_c] = L^{-1}$, namely the additional resistance due to the presence of the cake onto the membrane surface. The definition of R_c will be specified later on.

Exploiting (8), (9) and (10), the mass balance (1)-(2) rewrites as

$$\frac{k_{s,x}}{\mu}\frac{\partial^2 P_s}{\partial x^2} + \frac{k_{s,r}}{\mu}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial P_s}{\partial r}\right) = = \frac{A_v(P_s - P_l)}{\mu\,(R_m + R_c)} \tag{11}$$

$$\frac{k_l}{\mu}\frac{\partial^2 P_l}{\partial x^2} = -\frac{A_v(P_s - P_l)}{\mu\,(R_m + R_c)} \tag{12}$$

In next section we define the equations for the pollutant concentration which will be coupled with the previous system.

2.0.2 Modelling the fouling process

We denote by c the pollutant concentration in the volume of water, $[c] = ML^{-3}$, assuming the presence of only one species. Since the pollutant is completely cut off by the membranes, it is transported only by the water in the shell region.
Then we denote by c_m the concentration of

the cake, namely the mass of the cake per unit volume of the shell region, $[c_m] = ML^{-3}$. The growth rate of c_m is proportional to Γ, since the attachment process is driven by the filtration flux. Accordingly, it represents a sink term for the transport equation of c. Finally, we define the following system

$$\begin{aligned} \frac{\partial}{\partial t}(\varepsilon_s c) + \nabla \cdot (c\mathbf{q}_s) &= \nabla \cdot (\varepsilon_s D \nabla c) \\ &\quad -\alpha\Gamma\,(\varepsilon_s c)\,, \quad (13) \\ \frac{\partial c_m}{\partial t} &= \alpha\,\Gamma\,\,(\varepsilon_s c)\,, \quad (14) \end{aligned}$$

where D is the hydrodynamic dispersion coefficient and α is the attachment coefficient.
The resistance due to the cake is function of c_m. We model such a dependence by the following relationship

$$R_c(x, r, t) = \gamma_c r_0 c_m(x, r, t) \qquad (15)$$

where γ_c is a constant parameter.

2.0.3 The complete system

Summarizing, the process is described by the following system

$$k_{s,x}\frac{\partial^2 P_s}{\partial x^2} + k_{s,r}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial P_s}{\partial r}\right) = \frac{A_v(P_s - P_l)}{(R_m + R_c)}, \qquad (16)$$

$$k_l\frac{\partial^2 P_l}{\partial^2 x} = -\frac{A_v(P_s - P_l)}{(R_m + R_c)}, \qquad (17)$$

$$\frac{\partial}{\partial t}(\varepsilon_s c) + \nabla \cdot (c\mathbf{q}_s) = \nabla \cdot (\varepsilon_s D \nabla c) -\alpha\left[\frac{A_v}{\mu}\frac{(P_s - P_l)}{R_m + R_c}\right]\,(\varepsilon_s c), \qquad (18)$$

$$\frac{\partial c_m}{\partial t} = \alpha\left[\frac{A_v}{\mu}\frac{(P_s - P_l)}{R_m + R_c}\right]\,(\varepsilon_s c), \qquad (19)$$

$$R_c(x, r, t) = \gamma_c r_0 c_m(x, r, t). \qquad (20)$$

2.0.4 Boundary conditions

The module houses completely the bundle, so that there is no flux into or from the module unless at inlet and outlet: thus the inlet flux (feed) equals the outlet flux (permeate). Moreover, we assume a constant value for the concentration of pollutant entering the module, say c_{in}. Therefore, denoting the feed flux by J_f, $[J_f] = LT^{-1}$, we set the boundary conditions as follows:

- On the inlet boundary:

  $\mathbf{q}_s \cdot \mathbf{n} = J_f.$
  $\mathbf{q}_l \cdot \mathbf{n} = 0.$
  $c = c_{in}.$

- On the outlet boundary:

  $\mathbf{q}_s \cdot \mathbf{n} = 0.$
  $\mathbf{q}_l \cdot \mathbf{n} = -J_f.$
  No flux condition for c.

- Elsewhere: *no flux condition* for both the hydrodynamic and the transport–reaction problem.

2.1 Back wash

During the back wash step, we have a counterflux, say J_{back}, entering the lumen region at the outlet. Moreover, an air flux is added in the shell to aid the cake removal. Therefore, the model is similar to the previous step with the exception of the evolution equation for c_m, which acquires the following form:

$$\begin{aligned} \frac{\partial c_{m,back}}{\partial t} &= -\alpha\left[\frac{A_v}{\mu}\frac{(P_s - P_l)}{R_m + R_c}\right]\,c_{m,back} \\ &- \beta J_{back} c_{m,back}. \qquad (21) \end{aligned}$$

where $\beta J_{back} c_{m,back}$ is the term accounting for the air scouring, with β parameter to be calibrated via experiments, $[\beta] = L^{-1}$, and

$$R_c = R_c\,(c_{m,back})\,.$$

The initial condition for equation (21) is the value of c_m at the end of the previous step.
The boundary conditions for the PDEs are:

- On the outlet boundary:

  $\mathbf{q}_s \cdot \mathbf{n} = 0.$
  $\mathbf{q}_l \cdot \mathbf{n} = J_{back}.$
  No flux condition for c.

- On the inlet boundary:

  $\mathbf{q}_s \cdot \mathbf{n} = -J_{back}.$
  $\mathbf{q}_l \cdot \mathbf{n} = 0.$
  Vanishing dispersive flux for c (i.e. only advective flux).

- Elsewhere: *no flux condition* for both the hydrodynamic and the transport problem.

2.2 Characteristic time scales

Since in this problem several phenomena take place, it is useful to consider the different time scales involved and evaluate them using the selected parameters, namely

- Time of advection along the radial coordinate r,

$$t_{adv,r} = \left(\frac{\varepsilon_s \mu R^2}{P^* k_{s,r}} \right) \sim O(10^{-4}) sec.$$

- Time of advection along the longitudinal coordinate x,

$$t_{adv,x} = \left(\frac{\varepsilon_s \mu L^2}{P^* k_{s,x}} \right) \sim O(10^{-1}) sec.$$

- Time of diffusion along the radial coordinate r,

$$t_{diff,r} = \left(\frac{R^2}{D} \right) \sim O(10^{2}) sec.$$

- Time of diffusion along the longitudinal coordinate x,

$$t_{diff,x} = \left(\frac{L^2}{D} \right) \sim O(10^{5}) sec.$$

- Characteristic time for the filtration process (without cake influence),

$$t_{filt} = \left(\frac{\mu R_m}{A_v P^*} \right) \sim O(1) sec.$$

- Characteristic time of the attachment,

$$t_{attach} = \frac{1}{\alpha} t_{filt} \sim \frac{1}{\alpha} O(1) sec.$$

where P^* is a characteristic pressure (e.g. we set $P^* = 1\ bar$). Therefore, setting as characteristic time of the problem the duration of filtration,

$$T_{filt} \sim O(10^3),$$

we note that

(A) $T_{filt} \ll t_{diff,x}$, so that diffusion along x is negligible.

(B) Conversely, the advection is the leading phenomenon.

The order of magnitude of the attachment coefficient α has to be set according to the experimental evidence, by evaluating the ratio between attachment process and advection. For instance, if during the experiments a variable thickness of the cake is noticed along the module, then it means that attachment is comparable with advection and for sure we have to set $\alpha \leq 1$.

3 Use of COMSOL Multiphysics

To approach the problem with COMSOL, we solved separately the two stages of the process (i.e the filtration and the back wash step, respectively). Exploiting the axial symmetry, we define a 2D geometry and for each stage we applied the following modes:

- The *Darcy's law - Pressure* for a saturated medium (*Earth Science Module*), to solve equations (16)-(17).

- The *Solute Transport* mode (*Earth Science Module*) for equation (18).

- The *Diffusion* mode for equation (19).

In particular, we notice that the *Diffusion* mode was applied with a vanishing diffusion coefficient: even if this approach seems far to the mathematical character of equation (19) — in fact the unknown c_m does not depend directly on the spatial coordinates (r, x) – it allows to couple this equation with the system of PDEs (16)-(18) better than considering it properly as an evolution equation.
The term Γ is the one coupling each equation with another in a nonlinear way, accordingly to definitions (10) and (15). Therefore, this term was defined as *Global Expression*.
Finally, we remark that (16)-(17) are stationary equations. Nevertheless, after preliminary tests we decided to analyze them in a *transient* mode with a zero storage term (see [4] for more details): this factitious numerical approach ensures a better coupling between the hydrodynamic problem and the transport–reaction one, which were solved all together using the *time dependent segregated* solver.
After the filtration stage, the solution was stored and used as initial condition for the backwas step, which was solved in a similar way.

4 Results of preliminary simulations

In this section we report the results obtained for a simulation considering only a cycle of filtration and back wash step. In particular, we note that as TMP (transmembrane pressure) we report the difference between the pressure at inlet and outlet; such an approach follows the specifications given by the companies producing filters.
Moreover, in the simulation we selected $\alpha = 1$, recalling that this choice has to be carefully taken after an experimental validation of the model. The same argument applies to the air scouring process, for which we have selected $\beta = 1$.
Hereafter we report the simulation time (in *sec.*) for each cycle:

Filtration	Back wash
147.112 *sec.*	175.258 *sec.*

In Fig. 4-9 we report the surface plot of the cake resistance R_c during the two stages: accordingly to what defined in the model, the resistance increases during filtration and decreases due to the back wash, even if the initial state is never reached. In Fig. 10-11 we report the TMP according to the definition given above. In all figures the time is scaled to $T_{filt} = 1$ *h.* for filtration and $T_{back} = 30$ *sec.* for backwash
These results show that the model definition is in accordance with the experimental evidence. As future work we envisage an iterative application of filtration/backwashing cycles, in order to simulate the process taking place in real industrial plants.

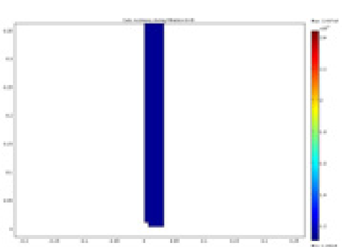

Figure 4: Cake resistance during production at the initial time (zoom close to the inlet).

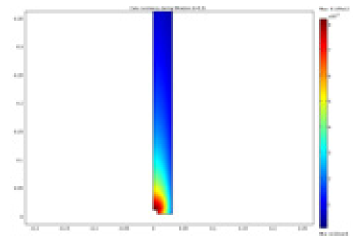

Figure 5: Cake resistance during production at times $t = 0.3$. (The time is dimensionless).

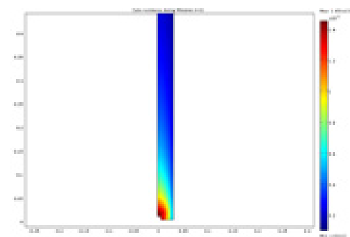

Figure 6: Cake resistance during production at times $t = 1$. (The time is dimensionless).

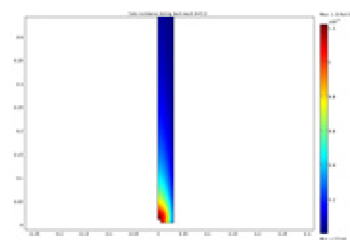

Figure 7: Cake resistance during back wash at times $t = 0.1$. (The time is dimensionless).

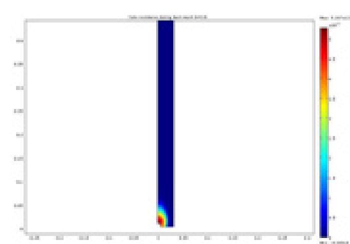

Figure 8: Cake resistance during back wash at times $t = 0.4$. (The time is dimensionless).

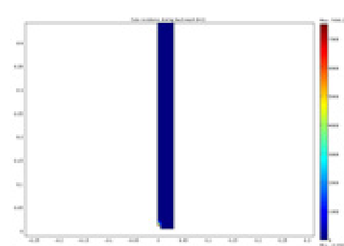

Figure 9: Cake resistance during back wash at final time $t = 1$. (The time is dimensionless).

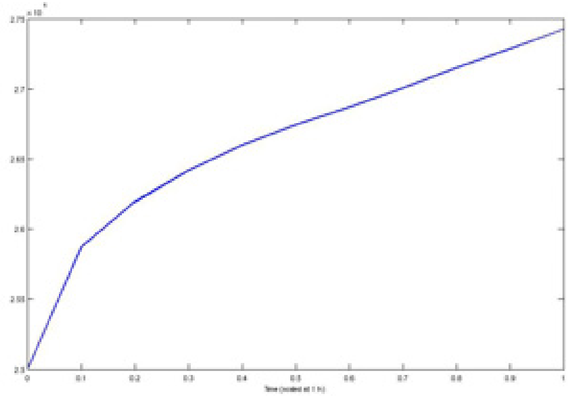

Figure 10: TMP during filtration.

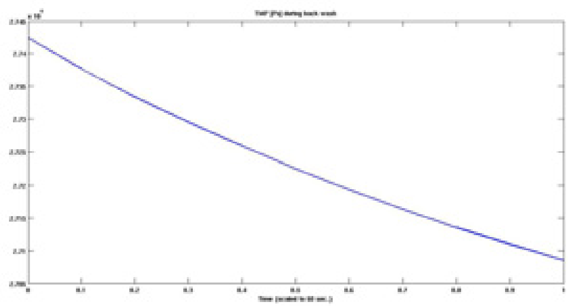

Figure 11: TMP during back wash.

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Acknowledgements

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