Mathematical modelling of a waste water filtration process based on membrane filters

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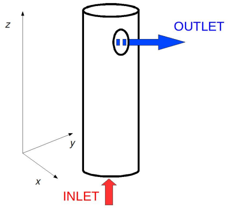
Outline

As a reminder, three porosity approach



Subscripts notation:
$(\,\cdot\,)_c$ is referred to the capillary region.
$(\,\cdot\,)_m$ is referred to the membrane region.
$(\,\cdot\,)$ is referred to the shell region.

Main tasks of our project:

- Modelling and simulation of filtration process
- Optimization of the parameters of the filters

The complete system

$$\nabla \cdot \mathbf{q_c} = -\alpha_c(c_m)\frac{k_m}{\mu l}(P_c - P_m)$$

$$\nabla \cdot \mathbf{q_m} = \alpha_c(c_m)\frac{k_m}{\mu l}(P_c - P_m) - \alpha\frac{k_m}{l}(P_m - P)$$

$$\nabla \cdot \mathbf{q} = \alpha\frac{k_m}{\mu l}(P_m - P)$$

$$\varepsilon_c\frac{\partial c}{\partial t} + \nabla \cdot (c\,\mathbf{q}_c) = \varepsilon_c\nabla \cdot (D\nabla c) - \gamma\left[\alpha_c(c_m)\frac{k_m}{\mu l}(P_c - P_m)\right](\varepsilon_c c)$$

$$\frac{\partial c_m}{\partial t} = \gamma\left[\alpha_c(c_m)\frac{k_m}{\mu l}(P_c - P_m)\right](\varepsilon_c c)$$

$$\alpha_c(c_m) = A_v\frac{1}{1 + c_m/c_{ref}}.$$

Boundary conditions

- On the inlet boundary:

  $$\mathbf{q}_c \cdot \mathbf{n} = -J_{in}.$$
  $$\mathbf{q}_m \cdot \mathbf{n} = 0.$$
  $$\mathbf{q} \cdot \mathbf{n} = 0.$$
  $$c = c_{in}.$$

- On the outlet boundary:

  $$\mathbf{q}_c \cdot \mathbf{n} = 0.$$
  $$\mathbf{q}_m \cdot \mathbf{n} = 0.$$
  $$\mathbf{q} \cdot \mathbf{n} = J_{out}.$$

  No flux condition for c.

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

Averaging

How could we reduce our 3D problem?

- We define the mean value:

$$\langle F \rangle (z,t) \equiv \frac{1}{\pi R^2} \int_0^R \int_0^{2\pi} F(x,y,z,t) r \, \mathrm{d}r \mathrm{d}\theta$$

- We use,

$$\int_V \nabla \cdot \mathbf{F} \, \mathrm{d}V = \oint_s \mathbf{F} \cdot \mathbf{n} \, \mathrm{d}S$$

- We suppose,

$$\langle \alpha_c(c_m) \cdot (P_c - P_m) \rangle \approx \langle \alpha_c(c_m) \rangle \cdot \langle (P_c - P_m) \rangle$$

Getting the 1D problem

$$
\begin{aligned}
-k_c \frac{\partial^2 P_c}{\partial z^2} &= -\alpha_c(c_m) \frac{k_m}{l} (P_c - P_m) \\
-k_m \frac{\partial^2 P_m}{\partial z^2} &= \alpha_c(c_m) \frac{k_m}{l} (P_c - P_m) - \alpha \frac{k_m}{l} (P_m - P) \\
-k_z \frac{\partial^2 P}{\partial z^2} &= \alpha \frac{k_m}{l} (P_m - P) - \frac{\mu}{\pi R^2} \frac{Q_{in}}{A_{out}} \chi(z)(2R_{out}) \\
\varepsilon_c \frac{\partial c}{\partial t} + \frac{\partial}{\partial z} (c\, \mathbf{q}_c) &= \varepsilon_c D \frac{\partial c^2}{\partial z^2} - \gamma \left[\alpha_c(c_m) \frac{k_m}{\mu l} (P_c - P_m) \right] (\varepsilon_c c) \\
\frac{\partial c_m}{\partial t} &= \gamma \left[\alpha_c(c_m) \frac{k_m}{\mu l} (P_c - P_m) \right] (\varepsilon_s c) \\
\alpha_c(c_m) &= A_v \frac{1}{1 + c_m / c_{ref}},
\end{aligned}
$$

Getting the 1D problem (cont.)

+ B.C. and I.C.

On the inlet boundary $(z = 0)$:

$$q_c = -J_{in}$$

$$q_m = 0 = q$$

$$c = c_{in}.$$

On the outlet boundary $(z = L)$:

No flux condition for all the eq.s

The dimensionless form:

$$\frac{1}{T_c}\frac{\partial c}{\partial t} + \left(\frac{k_c P^*}{\varepsilon_c \mu L^2}\right)\frac{\partial (c q_c)}{\partial z} =$$

$$= \left(\frac{D}{L^2}\right)\frac{\partial^2 c}{\partial z^2} - \left(\gamma A_v \frac{k_m P^*}{\mu l}\right)(P_c - P_m)\left[\frac{1}{1 + c_m/c_{ref}}\right] c$$

Define:

$$t_{adv} = \frac{\varepsilon_c \mu L^2}{k_c P^*}, \quad t_{diff} = \frac{L^2}{D}, \quad t_{filt} = \frac{\mu l}{A_v k_m P^*}, \quad t_{attach} = \frac{1}{\gamma} t_{filt}.$$

Remark:

$$T_c = T_{filt} \sim O(10^3)\, s; \quad t_{diff} \sim O(10^5)\, s \Longrightarrow \frac{T_c}{t_{diff}} \ll 1$$

Therefore, **the diffusion is negligible**.

Our request:

$$t_{adv} \ll t_{filt} \Longrightarrow \frac{\varepsilon_c \mu L^2}{k_c P^*} \ll \frac{\mu l}{A_v k_m P^*},$$

$$\Phi := \varepsilon_c L^2 \frac{k_m}{k_c} \frac{A_v}{l} \ll 1.$$

Substituting the definition of k_c, A_v and ε_c, we have the following condition:

$$\Phi = \frac{16 k_m L^2}{l r_i^3} \ll 1.$$

Notice that:

- Φ depends only on the filter and the membrane parameters (no dependence upon the process).
- Φ depends on r_i but not on r_o; that's a good point, since the pollutant flows only through the capillary region.

Different Approaches:

1. Simplified model using **Matlab**
2. **Comsol Multiphysics** software built-in models

A simplified approach

Additional scaling leads to the following non-dimensional equations for the pressures

$$\frac{\partial^2 p_c}{\partial z^2} = \theta_c \alpha_c(c_m)(p_c - p_m),$$
$$\frac{\partial^2 p_m}{\partial z^2} = \theta_m \left[\beta(p_m - p_s) - \alpha_c(c_m)(p_c - p_m)\right],$$
$$\frac{\partial^2 p_s}{\partial z^2} = \theta_s (p_s - p_m) + \zeta \chi(z),$$

and for the concentrations

$$\frac{\partial c}{\partial t} + \frac{\tau_{\text{filt}}}{\tau_{\text{adv}}} \frac{\partial}{\partial z}(c q_c) = \frac{\tau_{\text{filt}}}{\tau_{\text{diff}}} \frac{\partial^2 c}{\partial z^2} - \gamma \alpha_c(c_m)(p_c - p_m) c,$$
$$\frac{\partial c_m}{\partial t} = \gamma \alpha_c(c_m)(p_c - p_m) c.$$

Leading order equations

Pressure equations become much simpler

$$\frac{\partial^2 p_c}{\partial z^2} = \theta_c \alpha_c(c_m)(p_c - p_m),$$
$$0 = \beta(p_m - p_s) - \alpha_c(c_m)(p_c - p_m),$$
$$\frac{\mathrm{d}^2 p_s}{\mathrm{d}z^2} = 0.$$

Concentration equation now hyperbolic

$$\frac{\partial c}{\partial t} + \frac{\tau_{\mathsf{filt}}}{\tau_{\mathsf{adv}}} \frac{\partial}{\partial z}(c q_c) = -\gamma \alpha_c(c_m)(p_c - p_m)c,$$
$$\frac{\partial c_m}{\partial t} = \gamma \alpha_c(c_m)(p_c - p_m)c,$$

where the capillary flux is given by

$$q_c = -\frac{\partial p_c}{\partial z} - p_h$$

First implementation

Even the simplified system cannot be solved completely by hand

- Implement a simple numerical scheme in MATLAB
- Idea is to decompose the problem into two smaller problems; one for the pressure and one for the concentration

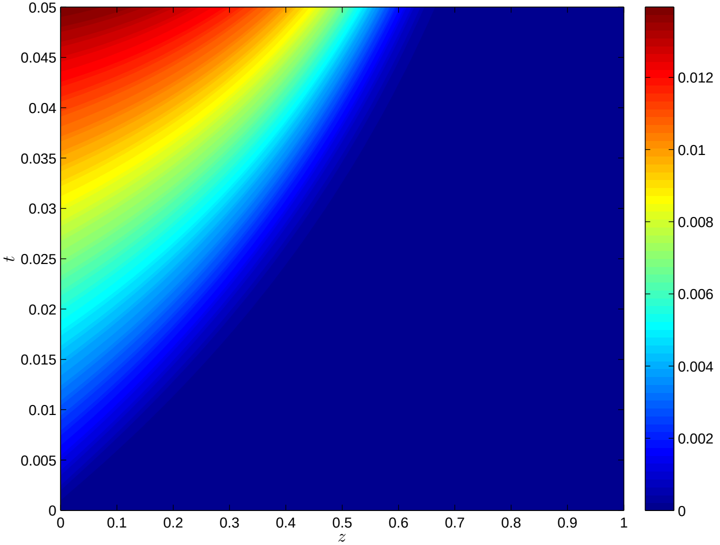
Outline of algorithm:

1. Assume concentration at time-step i is known (initial condition, for example)
2. Solve an elliptic equation for the capillary pressure at time-step i
3. Use new pressures to advance concentrations in time
4. Repeat

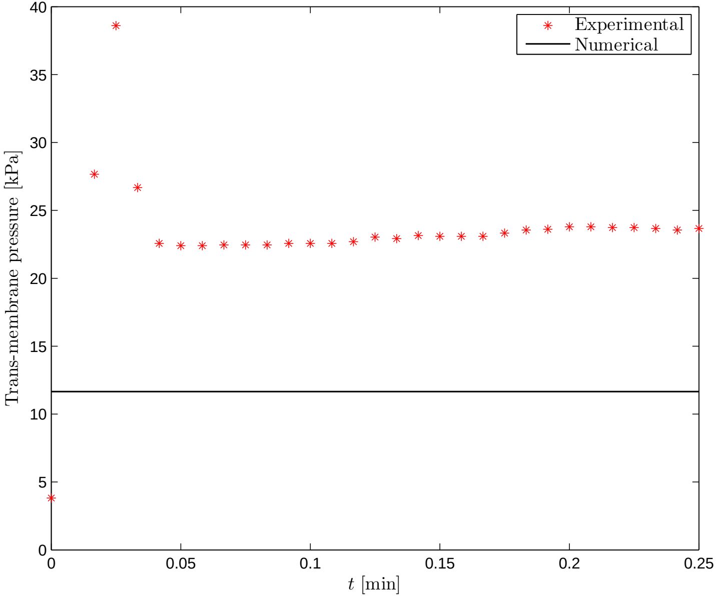
Further numerical details

- Spatial discretizations using finite differencing
- First order upwinding used for concentration equation
- Elliptic equation for capillary pressure linear, solved using \
- Time-stepping handled using `ode15s`

Results: attached matter



Results: trans-membrane pressure



Comsol Approach (I)

- **Earth Science Module** was used
- Application Modes:
  - **Darcy's law** for pressures (3 pde's)
  - **Solute Transport** for transport of pollutant (2 pde's)
- Transient analysis for the whole system ($t \in [0, 1]$)
- Process made of several cycles
- Each cycle has two stages, *filtration* (F) and *backwash* (BW)
- Matlab scripting to reproduce filtration-backwash cycles
- Physical parameters calibrated for one F-BW cycle

Comsol Approach (II)

Darcy's law application mode for p_c, p_m and p:

$$\delta_S S \frac{\partial p}{\partial t} + \nabla \cdot \left[-\delta_\kappa \frac{\kappa}{\eta} \nabla \left(p + \rho_f \mathbf{g} D \right) \right] = \delta_Q Q_S$$

S : Storage coefficient ($S = 10^{-4} \Rightarrow$ pseudo-stationary problem)

p : Pressure in the porous media

κ : Permeability

η : Dynamic viscosity

ρ_f : Fluid density

D : Vertical elevation

Q_S : Flow source/sink

$\delta_{S,\kappa,Q}$: Scaling coefficients ($\delta_S = 1/\tau_{\text{filt}}$ or $1/\tau_{\text{back}}$ for filtration/backwash)

Comsol Approach (III)

Solute Transport application mode for c and c_m:

$$\delta_{ts1}\theta_s \frac{\partial c}{\partial t} + \nabla \cdot (-\theta_s D_L \nabla c) = -\mathbf{u} \cdot \nabla c + S_c$$

- δ_{ts1} : Time scaling coefficient ($= 1/\tau_{\text{filt}}$ or $1/\tau_{\text{back}}$ for filtration/backwash)
- θ_s : Porosity
- c : Solute concentration
- D_L : Diffusion coefficient (10^{-5} for numerical stability)
- $\mathbf{u}$: Darcy's velocity ($\mathbf{u} = 0$ for c_m)
- S_c : Solute source/sink

o.d.e. for c_m is solved as a diffusion equation with very low diffusivity

Comsol Approach (IV)

Matlab scripting for process simulation:

- One main file defines all parameters, cycles and function calling
- Two functions are called to solve F and BW stages
- Each function solves the 5 pde's according to I.C. and B.C. of each stage of the cycles
- $c^{f=i}_{(x,t=Tf)} = c^{bw=i}_{(x,t=0)}$, $c^{bw=i}_{(x,t=Tbw)} = c^{f=i+1}_{(x,t=0)}$, ...
- Concentrations are averaged along the filter after each stage (assumed constant, see Φ parameter)

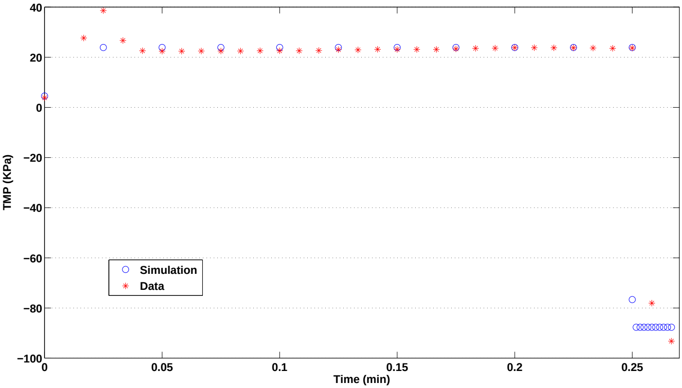
Comsol Approach (V)

Matlab scripting for process simulation (cont.):

- Filter parameters (κ_m, γ) calibrated to fit experimental data ($TMP \simeq (P_{in} + P_{out})/2$)
- Once parameters are calibrated, the process is optimized depending on τ_{filt}, τ_{back} and number of cycles
- Goal: maximize the ratio purified/used water of the process for given operation conditions

Comsol Approach (VI)

Parameter fitting depending on κ_m, γ and operation condition:



Final Remarks

- Averaging leads to a set of simplified equations
- Not simple enough to solve by hand
- Two different numerical approaches were implemented
  1. Using MATLAB: Simplest case, but unable to match experimental data
  2. Using COMSOL: Filtration data could be reproduced. Not enough data to compare backwash stage

Future work:

- Explore higher order behaviour in the simple model
- Model pore adsorption in the membrane, reduction in permeability
- Spatially dependent filter properties (permeability, etc.)
- Simulate filtration/backwash process over several cycles

Thank you for your attention