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

I. Borsi
(joint work with A. Fasano)

Dipartimento di Matematica *U. Dini*, Università di Firenze (Italy)
borsi@math.unifi.it – http://web.math.unifi.it/users/borsi

IV UCM Modelling Week
Madrid – June 14-22, 2010

Outline

Introduction

Project **PURIFAST**
Advanced **PUR**ification Of **I**ndustrial And Mixed Wastewater By Combined Membrane **F**iltration **A**nd **S**onochemical **T**echnologies

LIFE +
Environmental Policy and Governance
Grant agreement n. LIFE07 ENV/IT/000439
Duration: January 2009 – December 2011

Partnership:

- *Coordinator*: Next Technology Tecnotessile (Italy)
- *Research and Technical activities*:
  University of Florence - Dep. of Civil Engineering (Italy)
  University of Florence - Dep. of Mathematics (Italy)
  IWW GmbH (Germany)
- *Manufactures industries*:
  Lavo (Italy) – Polymem SA (France) – **Inge AG** (Germany)
- *End-users industries*:
  Gestione Impianti Depurazione Acque S.p.A. (Italy)
  King Colour S.p.A. (Italy)

Introduction

Main tasks of our activity in the project

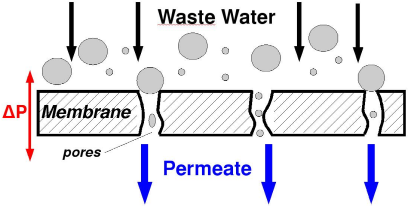
1. Modelling and simulation of filtration process at the meso-scale (i.e. single filter module)
2. Optimization of the parameters at the macro-scale (i.e. filtering plant)

Two filtering devices (based on polymeric membranes)

- Hollow fibre
- Multi-bore

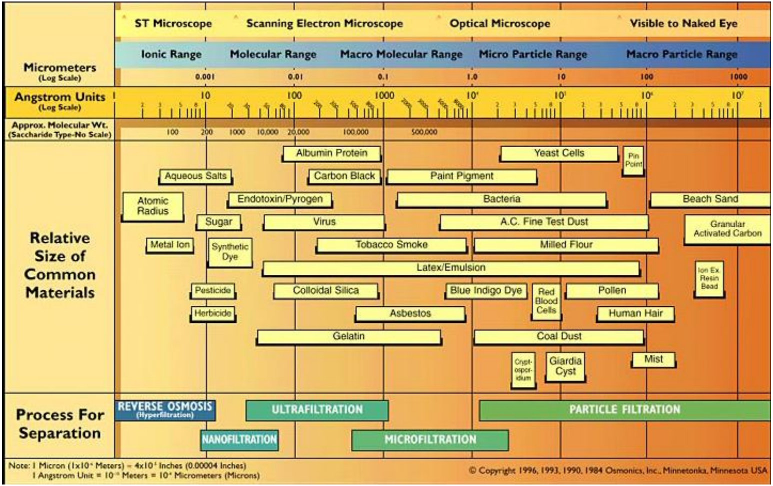
How the membrane works

- We deal with an **ultrafiltration** process:
  pores diameter 0.01 – 0.1 μm
- A pressure gradient ΔP is applied.
- All the particles larger than the pore diameter are cut off.



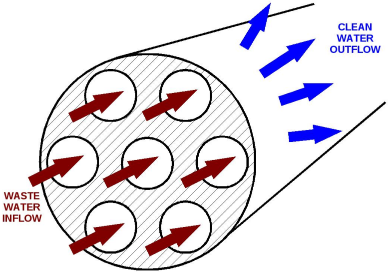
How the membrane works (ctd.)

Which materials can be removed:



How the membrane works (ctd.)

Different membrane's arrangements (some example):
plane, hollow fibre, spiral wound.
We are dealing with a particular hollow fibre: **multi-bore fibre**



How the membrane works (ctd.)

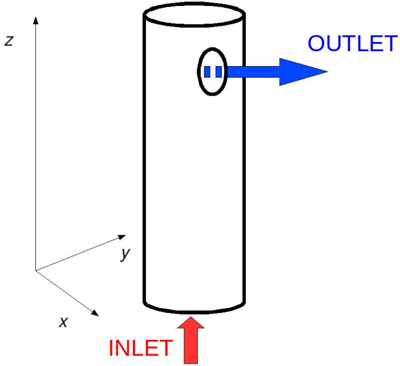
The main problem in these filtering systems is the membrane **fouling**: some of the particles attach on the membrane surface, soiling it and eventually reducing the filtration efficiency.

An example of **extreme** fouling, typical for filters immersed in bio-reactor...not our case!

To clean the membrane surface, a periodic back wash is imposed: the water flux is inverted and the clean water (partially) removes the fouling.

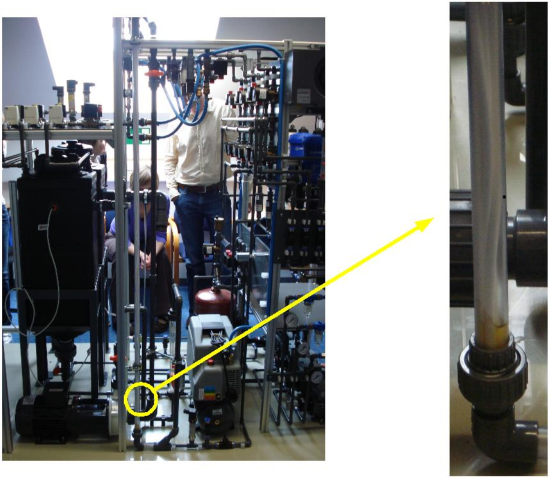
The Inge's module used for the project PURIFAST

Each module houses 7 multi-bore fibres. Length $\approx 1.5\ m$



The Inge's pilot plant within the project PURIFAST

The pilot consists of 3 modules:



Modelling the multi-bore module (macroscopic scale)

The approach of "coupled porous regions" (three-porosity, three-permeability medium)

We identify three regions:

- The capillary region: the total space occupied by the lumina of the capillaries within each fibre.
- The membrane region: the total space occupied by the membrane of each fibre.
- The shell region: the external space between the fibres.

These media are coupled each other by means of a spatially dependent source/sink term in the mass balance equation.

(Ref: Labecki et al., *Chem. Eng. Sci.*, 1995).

Modelling the hydrodynamics

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.

Steady-state mass conservation (with constant fluid density, ρ):

$$\nabla \cdot \mathbf{q}_c = -\Gamma_c, \tag{1}$$
$$\nabla \cdot \mathbf{q}_m = \Gamma_c - \Gamma, \tag{2}$$
$$\nabla \cdot \mathbf{q} = \Gamma \tag{3}$$

where: $\mathbf{q}$ is the Darcy's velocity and Γ_c, Γ are the source/sink terms.
Rate of mass loss per unit volume: $\rho\Gamma = \rho\dfrac{Q_{filt}}{V_{filt}} = \rho\dfrac{q_{filt}A_{filt}}{V_{filt}}$, where Q_{filt} and q_{filt} are the volume rate loss and the filtration specific discharge, respectively. V_{filt} is the filtering volume. A_{filt} the filtering area.

Modelling the hydrodynamics (ctd.)

The porous regions are characterized as follows:

1. **Membrane porosity and permeability**: they are given as datum (ε_m and k_m)
2. **Porosity and permeability in capillary and shell region**: they are calculated as a function of the structural parameters (inner and outer radius of the fibre, module radius, etc.). Such functions are assumed as constitutive law (Poiseuille, Happel, etc.)
3. Focus on **permeability**:
   - Capillary region: only longitudinal permeability, say k_c. Indeed, the capillaries are not connected with one another.
   - Membrane region: isotropic permeability tensor, say $k_m\mathbb{I}$.
   - Shell region: (symmetric) permeability tensor,

$$\mathbb{K} = \begin{pmatrix} k_x & 0 & 0 \\ 0 & k_y & 0 \\ 0 & 0 & k_z \end{pmatrix}.$$

Modelling the hydrodynamics (ctd.)

Darcy' law to express the velocity field:

$$\mathbf{q}_c = -\frac{k_c}{\mu}\left(\frac{\partial P_c}{\partial z} - \rho g \mathbf{e}_z\right),$$
$$\mathbf{q}_m = -\frac{k_m}{\mu}\left(\nabla P_m - \rho g \mathbf{e}_z\right),$$
$$\mathbf{q} = -\frac{\mathbb{K}}{\mu}\left(\nabla P - \rho g \mathbf{e}_z\right),$$

where P are the pressures.

Modelling the mass exchange and the effect of the fouling

The sink/source terms are defined as follows:

$$\Gamma_c = \alpha_c \frac{k_m}{\mu l} \left(P_c - P_m \right), \tag{4}$$

$$\Gamma = \alpha \frac{k_m}{\mu l} \left(P_m - P \right), \tag{5}$$

α_c and α are filtering efficiency coefficients ($[\alpha_c] = [\alpha] = L^{-1}$):

$$\alpha = \frac{\text{External surface of the membrane}}{\text{Volume of the shell}}. \tag{6}$$

The efficiency of the inner part decreases due to the pollutant soiling the membrane:

$$\alpha_c = \alpha_c(c_m) = A_v \frac{1}{1 + c_m/c_{ref}}, \tag{7}$$

where c_m is the concentration of the attached particles.
c_{ref} is a reference concentration. A_v is the specific filtering area.

Modelling the pollutant transport and attachment

Definitions:

1. c is the pollutant concentration in the volume of water flowing through the capillary region.
2. c_m is the concentration of matter attached on the inner part of the membrane's capillaries.

The pollutant transport takes place in the capillaries: therefore, the eq.s are coupled with the hydrodynamics of the capillaries region.

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

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

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

where γ is the attachment coefficient.

The complete system

$$-k_c \frac{\partial^2 P_c}{\partial z^2} = -\alpha_c(c_m)\frac{k_m}{l}\left(P_c - P_m\right)$$

$$-k_m \Delta P_m = \alpha_c(c_m)\frac{k_m}{l}\left(P_c - P_m\right) - \alpha\frac{k_m}{l}\left(P_m - P\right)$$

$$-\left(k_x \frac{\partial^2 P}{\partial x^2} + k_y \frac{\partial^2 P}{\partial y^2} + k_z \frac{\partial^2 P}{\partial z^2}\right) = \alpha\frac{k_m}{l}\left(P_m - P\right)$$

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

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

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

$+$ B.C. and I.C.

Boundary conditions (sketch)

We assume a **no flux condition** with the following exceptions:

1. **On the inlet**, in the capillary region: inward flux for the flow and assigned concentration (Dirichelet) for the pollutant.
2. **On the outlet**, in the shell region equation: outward flux for the flow.

The problem for the modelling week

Remarks & Critical points

1. A similar problem is defined for the **back wash** stage
2. For a realistic simulation we have to run **a long series of filtration/backwash cycles**.
   For instance: 5 days $\sim$ 450 cycles.
3. A 3D simulation of such process is time consuming. For instance: using *COMSOL Multiphysics*® in a 2D simulation of *just*, 1 cycle takes $\sim$ 5 *min*.
4. Actually, the dependence of the solution upon the horizontal (or radial) coordinates is significant **only very close to the outlet**.

The problem for the modelling week (ctd.)

Objectives (O) and actions (A)

(O.1) To reduce the simulation time.

(A.1) Averaging the model w.r.t. the horizontal coordinates $\Rightarrow$ **reducing the problem to a 1-D setting**.

(O.2) To find useful relationships for optimizing the module performance.

(A.2) Scaling analysis for the 1D problem.

(O.3) Calibration of the unknown model parameters

(A.3) To run a simulation of a single filtration/backwash cycle (by COMSOL or MATLAB) and compare it with experimental data.

The problem for the modelling week (ctd.)

Missing information...

All the data and further specifications needed to solve the problem will be supplied to the Working Group participants.

Thank you for your attention

Good work !