

On The Purification Of Waste Waters Using Multi-Bore Filters: Simulation of a Long-Term Filtration Stage

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COMSOL Conference 2010
Paris, November 17 – 19, 2010

Introduction

Project **PURIFAST**

Advanced **PUR**ification Of **I**ndustrial And Mixed Wastewater By
Combined Membrane **F**iltration And **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

Final goal of the project:

Demonstration of a tertiary treatment system based on ultrafiltration and sonochemical technologies for purification and reuse of textile and mixed effluents.

Main tasks of our activity in the project

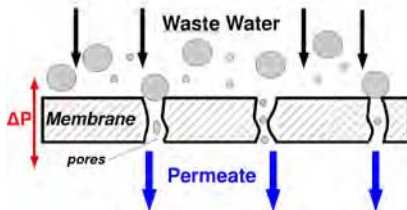
1. Modelling and simulation of filtration process at the meso-scale (i.e. single filter module)
2. Optimization of the parameters at the macro-scale (i.e. filtering plant)

Two filtering devices (based on polymeric membranes)

- ▶ Hollow fibre
- ▶ **Multi-bore**

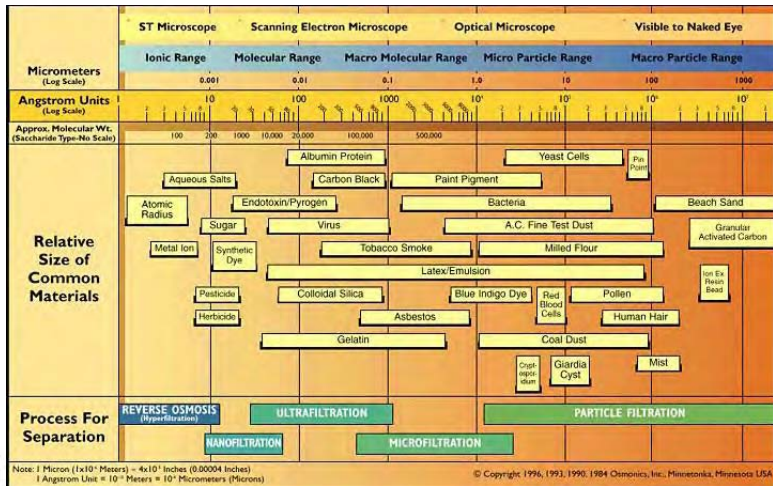
How the membrane works

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



How the membrane works (ctd.)

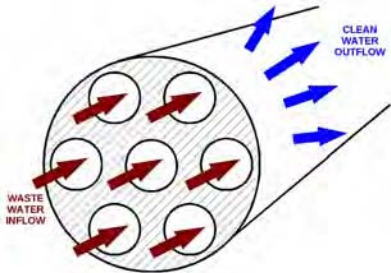
Which materials can be removed:



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.)

Fouling

The main problem in these filtering systems is the membrane **fouling**. Actually, we have two different fouling processes:

1. **Reversible fouling**: some of the particles attach on the membrane outer surface, soiling it and eventually reducing the filtration efficiency. To clean the membrane surface, a periodic **back wash** is imposed: the water flux is inverted and the clean water (partially) removes the fouling.
2. **Irreversible fouling**: the one due to the *adsorption* of matter within the membrane pores. It cannot be removed at all!

The pilot plant within the project PURIFAST

The pilot consists of 3 **modules**:
everyone houses **7 multi-bore fibres**.



Modelling a 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).

Model definition: general considerations

Physical assumptions:

- ▶ Saturated porous media.
- ▶ Typical Reynolds number: $Re < 5 \implies$ Darcy's law applies.
- ▶ Only one chemical species (for the sake of simplicity).
- ▶ In shell and capillary region permeability and porosity are constant. Conversely, porosity and permeability of the membrane depend on pollutant concentration.

Model definition: general considerations (ctd.)

Remarks

1. We first considered the full 3D model, and we solved it with *COMSOL Multiphysics*
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 very time consuming. For instance: using also a simplified 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**.

Therefore:

To reduce the simulation time, we average the model w.r.t. the horizontal coordinates \Rightarrow **1-D setting of the problem**.

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):

$$\frac{\partial}{\partial z} q_c = -\Gamma_c, \quad (1)$$

$$\frac{\partial}{\partial z} q_m = \Gamma_c - \Gamma, \quad (2)$$

$$\frac{\partial}{\partial z} q = \Gamma - \frac{1}{\pi R^2} \frac{Q}{A_{out}} \chi(z) (2\pi R_{out}) \quad (3)$$

where: q is the superficial velocity (specific discharge) and Γ_c , Γ are the **source/sink terms** (= mass exchange between regions).

The second term in the r.h.s. of (3) accounts for the water flowing out from the outlet: A_{out} , R_{out} are the area and radius of the outlet. Q is the volumetric flux. $\chi(z)$ is the characteristic function of the outlet position.

Modelling the hydrodynamics (ctd.)

The porous regions are characterized as follows:

1. **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 laws (*Poiseuille*, *Happel*, etc.)
2. **Membrane porosity and permeability** (ε_m and k_m): they are function of the pollutant concentration (see later on).

Modelling the hydrodynamics (ctd.)

Darcy' law to express the velocity field:

$$q_c = -\frac{k_c}{\mu} \left(\frac{\partial P_c}{\partial z} - \rho g \right),$$

$$q_m = -\frac{k_m}{\mu} \left(\frac{\partial P_m}{\partial z} - \rho g \right),$$

$$q = -\frac{k}{\mu} \left(\frac{\partial P}{\partial z} - \rho g \right),$$

where P are the pressures, ρ, μ are the water density and viscosity (assumed constant), g is the gravity acceleration.

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_p is the mass fraction of **adsorbed** pollutant (on the membrane)
3. 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.

$$[\text{TRANSPORT}] \quad \varepsilon_c \frac{\partial c}{\partial t} + \frac{\partial}{\partial z}(cq_c) = \varepsilon_c D \frac{\partial^2 c}{\partial z^2} - \gamma \Gamma_c(\varepsilon_c c) - \rho_b \frac{\partial c_p}{\partial t}$$

$$[\text{ADSORPTION}] \quad c_p = \frac{\bar{s}K_L c}{1 + K_L c},$$

$$[\text{ATTACHMENT}] \quad \frac{\partial c_m}{\partial t} = \gamma \Gamma_c(\varepsilon_c c)$$

Modelling the mass exchange: the attachment effect

The sink/source terms are defined as follows:

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

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

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

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

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

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

where c_m is the concentration of the attached particles.

c_{ref} is a reference concentration. A_v is the specific filtering area.

Adsorption and its effect on pores diameter

We assume there is an equilibrium relationship between c and the mass fraction of adsorbed pollutant (p.u. mass of the membrane), c_m :

$$c_p = \frac{\bar{s}K_L c}{1 + K_L c}$$

which is the well-known *Langmuir* adsorption isotherm (K_L and \bar{s} are constant).

The mass fraction c_p is proportional to the volume occupied into the pores. Assuming a capillary tubes structure:

$$c_p(x, t) = \eta (d_0^2 - d(x, t))$$

with η constant.

The effects on porosity and permeability

We assume a **Poiseuille-type** law:

$$\varepsilon_m(x, t) = \frac{N_p \pi}{4A_{filt}} d^2(x, t) \quad (8)$$

$$k_m = \varepsilon_m(x, t) d^2(x, t) \quad (9)$$

where $N_p = \#$ pores and A_{filt} is the filtering area.

If in (8) and (9) we use the dependence of d upon the adsorbed pollutant, we get the variation of porosity and permeability due to the adsorption.

The back wash has no effect on this process: the value of ε_m and k_m before and after backwashing are the same (\Rightarrow **irreversible fouling !**)

Boundary and initial conditions

B.C.

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

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

$$q_c = Q/A, \quad c = c_{in}$$

I.C.

The apparatus measures the pressure at inlet and outlet. Therefore:

1. **In the capillary region**: pressure in the hydrostatic equilibrium with the inlet.
 2. **In the shell region**: pressure in the hydrostatic equilibrium with the outlet.
 3. **In the membrane**: an average of the two.
- ▶ The initial concentrations are set to zero.

The complete system

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

$$-k_m(c_p) \frac{\partial^2 P_m}{\partial z^2} = \alpha_c(c_m) \frac{k_m(c_p)}{l} (P_c - P_m) - \alpha \frac{k_m(c_p)}{l} (P_m - P)$$

$$-k_z \frac{\partial^2 P}{\partial z^2} = \alpha \frac{k_m(c_p)}{l} (P_m - P) - \frac{\mu}{\pi R^2} \frac{Q}{A_{out}} \chi(z) (2R_{out})$$

$$\left(\varepsilon_c + \rho_b \frac{\partial c_p}{\partial c} \frac{\partial c}{\partial t} \right) + \frac{\partial(cq_c)}{\partial z} = \varepsilon_c D \frac{\partial^2 c}{\partial z^2} - \gamma \left[\alpha_c(c_m) \frac{k_m(c_p)}{\mu l} (P_c - P_m) \right] (\varepsilon_c c)$$

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

$$c_p = \frac{\bar{s} K_L c}{1 + K_L c}; \quad \alpha_c(c_m) = A_v \frac{1}{1 + c_m/c_0}.$$

REMARK: A similar system has been defined for the **back wash stage**.

Use of COMSOL Multiphysics

The system was solved separating the two stages of the process (i.e the filtration and the back wash step, respectively).

For each stage we applied the following:

1. The *Darcy's law - Pressure (Earth Science Module)*, to solve the pressure eq.s
2. The *Solute Transport mode (Earth Science Module)* to solve the eq. for c , selecting the *Langmuir adsorption* model. The attachment term is included in the source option.
3. The *Diffusion mode* to solve eq. for c_m [with a vanishing diffusion coefficient, since actually is a ODE !!]
4. In the *Global Expressions* we included the expression for Γ , Γ_c , α_c , ε_m and k_m .

Simulations

Actually, the filtration module has 2 inlet options: bottom and top.
Therefore, we have **four steps**:

- (A) Filtration 1: the waste water enters from the **bottom**.
- (B) Back wash 1: the clean water enters from the outlet and exits from the **bottom** .
- (C) Filtration 2: the waste water enters from the inlet at the **top**.
- (D) Back wash 2: the clean water enters from the outlet and exits from the inlet at the **top**.

MATLAB[®] + COMSOL[®] simulation

We provided a MATLAB simulation code.

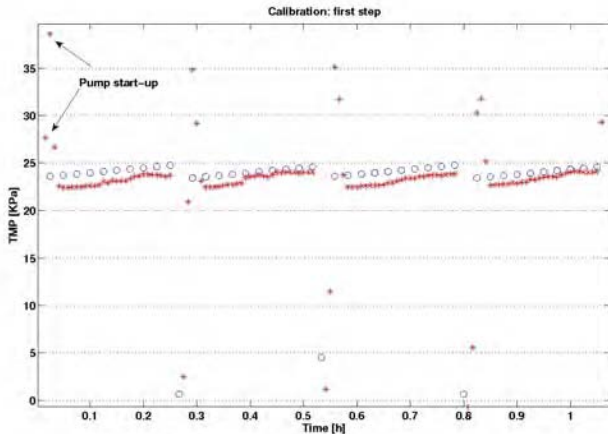
The main steps of our work:

- ▶ Once a single-cycle simulation has been performed using the COMSOL User Interface, we derived from it the four specialized MATLAB-functions (one for each step of the process).
- ▶ In a *main file* we give all the needed input data.
- ▶ From the main file, the 4 functions (in the right order) are called iteratively, launching at each time the COMSOL solver algorithm.
- ▶ The final value of the concentrations are the initial values for next step.

Example 1: calibration on a short period

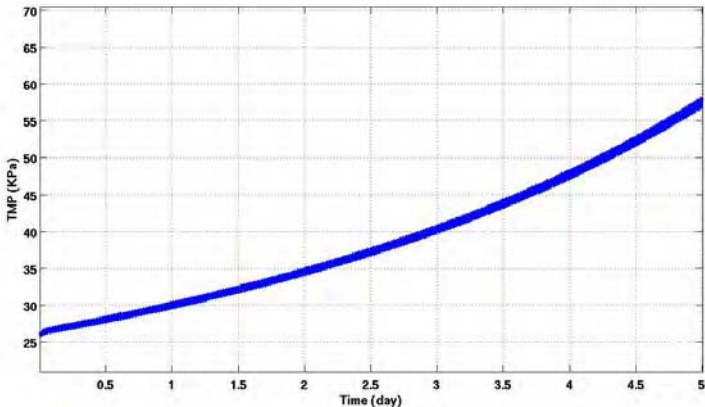
An example of 1 hour process (= 4 cycles).

Red: data; Blue: simulation.



Example 2: a long term simulation

After the calibration we run a 5-day simulation (225 *cycles*).
We obtain a good qualitative behaviour.



Conclusions

Remarks

- ▶ The 1D problem allows to easily simulate a process of several days. due to the faster procedure: e.g. a 5–day simulation (=225 cycles) ~ 2.05 hours
- ▶ The introduction of the porosity and permeability variation allows to recover the behaviour of the experimental curves