A comparative study of three membrane fouling models

Towards a generic model for optimization purposes

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ABSTRACT. Most of the published models of membrane fouling are too complex and contain too many parameters to be estimated from experimental data. This works aims to justify the choice from the literature of a simple model of membrane fouling for control and optimization design purposes. To do so, we identify a simple and generic model from the literature and we show, using preliminary results, that this model can reproduce the same results than those much more complicated and specific published models with less parameters to estimate.

RÉSUMÉ. La plupart des modèles de colmatage de la membrane sont compliqués avec beaucoup de paramètres à estimer à partir des données expérimentales. L'objectif de ce travail est de justifier le choix, à partir de la littérature, d'un model simple de colmatage de la membrane pour des fins de contrôle et d'optimisation. Pour ce faire, on identifie un modèle simple et générique et on montre que ce modèle peut reproduire les mêmes résultats que d'autres modèles publiés plus compliqués et spécifiques, avec moins de paramètres à estimer.

KEYWORDS: membrane bioreactor(MBR), fouling, modeling, mathematical models, optimization.

MOTS-CLÉS : bioréacteur à membrane (BRM), colmatage, modélisation, modèles mathématiques, optimisation.

1. Introduction

The membrane bioreactors (MBR) are an increasingly used technology in wastewater treatment. Such a process combines a biological reactor with a filtration membrane that separates microorganisms and suspended matters from the purified water. The advantages are: a high quality effluent, a high solid retention time (SRT), a high possible biomass concentration and a small footprint. Despite its benefits and its widespread use, the MBR technology is constrained by membrane fouling. Fouling is due to the attachment of particles on membrane surface which leads to sever flux decline and an increase of the operating costs. Therefore, several authors have proposed different mathematical models to simulate the MBR process in order to be used in the prediction and control of membrane fouling. However, those models either include a lot of parameters to be estimated from experimental data and they are thus too complex to be really operational, or they make too many assumptions that limit their interest. In this paper, we propose to evaluate a simple generic mathematical model proposed by Benyahia et al. [1] by comparing this model to two other models published in the literature: the model of Pimentel et al. [2] and the model of Di Bella et al. [3]. In particular, we are interested in investigating the generic character of the model proposed by Benyahia et al. [1] for two purposes. The first is to illustrate its usefulness for control and optimization design purposes by justifying the high prediction capabilities of this model despite its simplicity. The second is to prove that if MBRs are very complex systems, yet they can be modeled by simple and generic mathematical models.

To do so, the models [2] and [3] are used as virtual processes to generate data that are then utilized to identify the model parameters of Benyahia et al. model [1] by using an optimization strategy. Model simulations and parameter estimation were conducted using Matlab.

2. The model proposed by Pimentel et al.

Pimentel et al. [2] have proposed an integrated model coupling a biological model and a filtration model. The coupled model is formed of eight ordinary differential equations (ODEs) with six parameters to be estimated from experimental data. The biological model is designed using a simple chemostat reactor, involving one substrate and one biomass. The short-term evolution of the cake deposit on the membrane surface was modeled by equation (1) and the long-term evolution due to irreversible clogging was described by equation (2). In this model, the total resistance is calculated as the cake resistance while the intrinsic resistance of the membrane was neglected (equations (3) and (4)). The trans-membrane pressure can be determined according to equation (5).

For the relaxation phase, the model is represented by equations (6) to (7). The nomenclature used in the model is presented in Appendix 1.

- Coupled model for the filtration phase:

$$\dot{m} = Q_{perm}\,X - J_{air}\,\mu_{air}\,m \tag{1}$$

$$\dot{\beta} = -\gamma\,\beta \tag{2}$$

$$R_{tot} = R_{cake} \tag{3}$$

$$R_{cake} = \rho\,\frac{m + m_0}{A} \tag{4}$$

$$TMP = \frac{Q_{perm}}{A}\,\eta\,R_{tot} \tag{5}$$

- Coupled model for the relaxation phase :

$$\dot{m} = -J_{air}\,\mu_{air}\,m \tag{6}$$

$$\dot{\beta} = -\gamma\,\beta \tag{7}$$

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3. The model proposed by Di Bella et al.

The membrane bioreactor mathematical model of Di Bella et al. [3] consists of two sub-models. The biological activity is described in the first sub-model through twenty-six ODEs. This sub-model is a modified version of the well-know ASM1 [4] to consider the influence of the Soluble Microbial Products (SMPs), known as playing a key role in membrane fouling [5]. The cake layer formation was modeled by equation (10). The latter is regulated by two opposite phenomena: the suction which leads to attachment and the friction drag caused by the turbulent air flow. The attachment is proportional to the total suspended concentration as expressed by equation (8) while the friction drag is proportional to the local shear intensity as in equation (9). During backwashing phase, the detachment action of the cake layer is evaluated by equation (11) where η_c is a calibrated parameter. The nomenclature used in Di Bella et al.'s model is given in Appendix 2.

- The model for the filtration phase:

$$MLSS = i_{SS,X_I}\,X_I + i_{SS,X_S}\,X_S + i_{SS,BH}\,X_{BH} + i_{SS,BA}\,X_{BA} \tag{8}$$

$$G = \sqrt{\frac{\rho_S\,g\,Q_a}{\mu_S}} \tag{9}$$

$$\dot{M}_{sf} = \frac{24\,MLSS\,Q_{perm}^2}{24\,Q_{perm} + C_d\,d_p\,G} - \frac{\beta\,(1-\alpha)G\,M_{sf}^2}{\gamma\,V_f\,t_f + M_{sf}} \tag{10}$$

- The model for the backwashing phase:

$$\dot{M_{sf}} = -\eta_c \, M_{sf} \tag{11}$$

Di Bella et al. model includes forty-four parameters to be estimated from experimental data and it does not give equations to calculate the resistance of membrane fouling and thus the transmembrane pressure (*TMP*).

4. The model proposed by Benyahia et al.

Benyahia et al. [1] have proposed a simple model of membrane fouling and have connected it to a biological process to demonstrate its utility in a large number of situations. In this model, two main fouling phenomena were considered: the attachment of solids onto the membrane surface (cake formation) and the retention of compounds inside the pores (pores clogging), in particular the SMP.

The coupled model of Benyahia et al. is formed of fourteen ODEs: ten ODEs to describe the biological activity and four ODEs to represent the filtration process, with twenty-six parameters. In their work, the authors [1] assume that total filtering membrane surface is not constant, contrary to many models of the literature. Instead, it is modeled by a decreasing function of both the mass of matter attached on the surface of the membrane *m(t)* and the mass of deposited matter into pores *Sp(t)* (notably *SMP*). The dynamic of *m(t)* is proportional to the particulate matter (X_T) and the total soluble (S_T and *SMP*), as in equation (12). The evolution of *Sp(t)* is proportional to *SMP* (cf equation 13). The filtration model of Benyahia et al. [1] is represented by the following dynamical equations and the nomenclature used in this model is given in Appendix 3:

- The model for the filtration phase:

$$\dot{m} = \delta \, Q_{out} \, (C_S \, S_T + C_x \, X_T + C_{SMP} \, SMP) - f_m \, m \tag{12}$$

$$\dot{S_p} = \delta' \, Q_{out} \, (\beta \, SMP + \frac{\beta}{15} \, (S_1 + S_2)) \tag{13}$$

$$R_{tot} = R_0 + \alpha \, \frac{m}{A} + \alpha' \, \frac{V_p \, S_p}{\epsilon \, A} \tag{14}$$

$$TMP = \frac{Q_{perm}}{A} \, \eta \, R_{tot} \tag{15}$$

- The model for the relaxation/backwashing phase:

$$\dot{m} = -\omega \, m \tag{16}$$

$$\dot{S_p} = -\omega' \, S_p \tag{17}$$

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5. Identification of Benyahia et al. 's model parameters using Pimentel data

At this stage, Pimentel et al. model [2] is considered as a virtual process to generate data in order to identify the parameter of the model [1]. All the hypothesis considered in Pimentel et al. model [2] were applied to Benyahia et al. model [1]. Therefore, the parameter to be optimized of the model [1] are: $\delta\ C_X$, f_m , α and ω.

The optimization of these parameters was done by the least squares method programmed with Matlab R2013a. The functional cost that was minimized is the sum of the error between the mass of attached matter calculated according to the model [1] and that determined according to the model [2] and the difference between the trans-membrane pressure calculated with the model [1] and that determined with the model [2]. It should be noticed here that in the model [1] the contribution of the SMP in the fouling was neglected in order to fit the hypothesis considered in [2].

The optimal values of the different parameters of the model [1] are presented in the table 1. The results of the simulation of the optimization problem are shown in the Figs.1 and 2. The comparison of the simulated data of the two models confirms the possibility of the model proposed by Benyahia et al. [1] to capture the mean value and the dynamics of the attached mass and the trans-membrane pressure.

Table 1 *Optimal results for parameter estimation of the model [1] from the data of the model [3]*

Parameters	Unit	Value	Lower bound	Upper bound
$\delta\ C_X$	dimensionless	1	0.9	1
f_m	day^{-1}	184.2	160	190
ω	day^{-1}	184.2	160	190
α	m.g^{-1}	2.371e+07	2.2e+07	2.4e+07

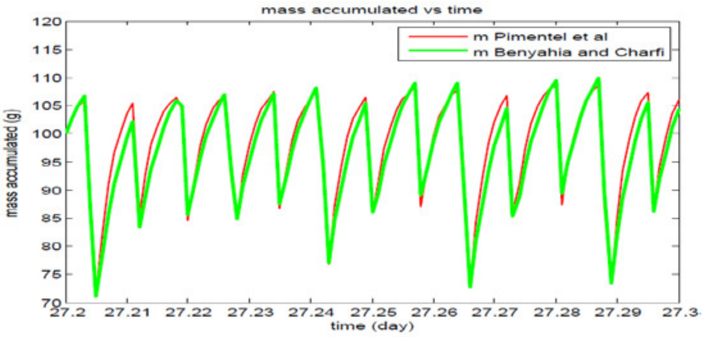

Figure 1. *the accumulated mass on the membrane surface versus time*

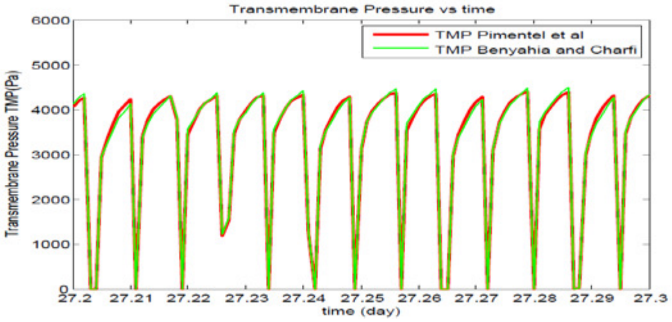

Figure 2. *the TMP trends versus time*

6. Identification of Benyahia et al. 's model parameters using Di Bella data

In this part, the model of Di Bella et al.[3] was considered to evaluate the genericity of Benyahia et al. model [1]. To do that, the same approach as before was considered. The objective function that was minimized by the optimization problem is the difference between the mass of attached matter calculated according to the model [1] and that determined according to the model [3]. The optimal solution and the search ranges of the unknown parameters of Benyahia et al. model are presented in the table 2.

Table 2. *Optimal results for parameter estimation of the model [1] from the data of the model [3]*

Parameters	Unit	Value	Lower bound	Upper bound
$\delta\ C_x$	dimensionless	0.3	0	1
f_m	day^{-1}	3.25e+3	1e+3	3.5e+3
ω	$m.kg^{-1}$	3300	3000	3500

Fig.3 shows the simulation results of the mass attached. These results demonstrate that the model proposed by Benyahia et al. [1] can reproduce well the dynamic of the mass attachment on the membrane. However, this model estimate a mean value of the attached mass slightly different from that evaluated with the model [3]. We explain this difference by the fact that DiBella et al. suppose in their model that the friction drag (the second term of the equation (10)) is a function of the square of the sludge cake which reduce the rate of the sludge deposition in the time. Contrary to DiBella et al., Benyahia et al. model consider that the friction drag is proportional only to the mass attached. For that, the attachment rate evaluated with the model [1] increase much more than that calculated with the model proposed by DiBella et al.

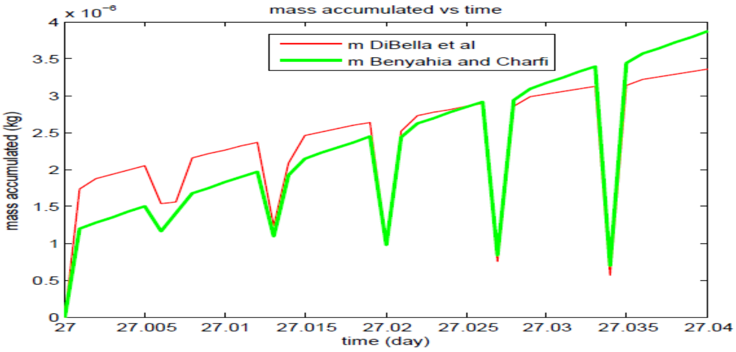

Figure 3. *the mass accumulated on the membrane surface versus time*

7. Conclusion

The aim of this paper is to investigate the capability of the model of Benyahia et al.[1] to capture the dynamics of more complex models. For this purpose, simulations of two models of the literature, the model of Pimentel el al.[2] and Di Bella et al.[3], were performed. The generated data are used to identify Benyahia et al. model [1] parameters by minimizing the difference between the models predictions. Simulations of the different models were performed by solving a set of differential equation by using the Matlab function ODE. The optimization problem was resolved with the fmincon function in MATLAB. Certainly the model of Pimentel et al. [2] is a simple model but with many assumptions which limit its application. Likewise, comparing to the model of Benyahia et al.[1], the model of DiBella et al. [3] is not taking into account all the fouling mechanisms and it is composed of large number of ODE with many parameters to estimate.

The optimization results show that Benyahia et al. model [1] can capture important properties of the model proposed by Pimentel et al. [2] as the mean value of the trans-membrane pressure and the attached mass on the membrane and their dynamics. The model of Benyahia et al. [1] was able to reproduce the evolution of the attached mass of the model proposed by DiBella et al. [3] but with a little deviation in the values. This deviation can be explained by the difference in the mathematical formulation of the two models [1] and [3]. So, we suggest to add to the drag force of the model of Benyahia et al. a squared term in order to increase the applicability of this model.

Finally, we conclude that the model of Benyahia et al. is generic enough to be used for optimization and control purposes.

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8. Bibliography

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Annexe 1: Pimentel et al. model nomenclature

Symbol	Meaning and Unit
A	The membrane area [m^2]
J_{air}	Air crossflow [$m^3/m^2.d$]
m	Mass cake state [g]
m_0	Initial value of solids m(t) attached onto the membrane area
Q_{in}	Inflow [m^3/d]
Q_w	Waste flux [m^3/d]
Q_{perm}	Permeate flux [m^3/d]
R_{tot}	The total fouling resistance [m^{-1}]
R_{cake}	The cake resistance [m^{-1}]
S	Substrate concentration [g/m^3]
S_{in}	Input substrate concentration [g/m^3]
TMP	The trans-membrane pressure [Pa]
V	Tank volume [m^3]
X	Solid matter concentration [g/m^3]
Y	Yield coefficient of the substrate consumption [-]
μ	Monod's law [1/d]
γ	Constant [day^{-1}]
β	Resistance of detachable cake by air crossflow [m^{-1}]
ρ	The specific cake resistance [m/g]
η	The apparent bulk viscosity [Pa.s]

Annexe 2: Di Bella et al. model nomenclature

Symbol	**Meaning and Unit**
C_d	Lifting force coefficient [dimensionless]
d_p	Particle size [m]
G	Local shear intensity [day^{-1}]
g	Gravity acceleration [$m\ s^2$]
i_{SS,X_I}	Mass particular inert/mass COD in biomass [$kg\ X_I\ kgcod^{-1}$]
i_{SS,X_S}	Mass biodegradable organic matter/mass COD in biomass [$kg\ X_S\ kgcod^{-1}$]
$i_{SS,BH}$	Mass active heterotrophic biomass/mass COD in biomass [$kg\ X_{BH}\ kgcod^{-1}$]
$i_{SS,BA}$	Mass active autotrophic biomass/mass COD in biomass [$kg\ X_{BA}\ kgcod^{-1}$]
MLSS	The mixed liquor suspended solids
M_{sf}	Dynamic sludge film cake on the membrane [$kg\ m^2$]
Q_a	Air flow [$m^3\ day^{-1}$]
Q_{perm}	Effluent flow rate [$m^3\ day^{-1}$]
V_f	Volume of permeate produced [m^3]
X_I	Particulate inert organic matter [$kg\ COD\ m^{-3}$]
X_S	Particulate biodegradable organic matter [$kg\ COD\ m^{-3}$]
X_{BH}	Active heterotrophic biomass [$kg\ COD\ m^{-3}$]
X_{BA}	Active autotrophic biomass [$kg\ COD\ m^{-3}$]
α	Stickiness of biomass [dimensionless]
β	Erosion rate coefficient of dynamic sludge film [dimensionless]
γ	Compression coefficient for dynamic sludge layer [$kg\ m^{-3}\ day^{-1}$]
ρ_S	Density of activated sludge [$kg\ m^{-3}$]
η_c	Efficiency of backwashing [dimensionless]
μ_S	Viscosity of activated sludge [Pa s]

Annexe 3: Benyahia et al. model nomenclature

Symbol	Meaning and Unit
A	Membrane surface [m^2]
C_S	Fraction of ST = S1 + S2 attached onto the membrane at a given time [day^{-1}]
C_x	Fraction of $X_T = X_1 + X_2$ attached onto the membrane at a given time [day^{-1}]
C_{SMP}	Fraction of SMP attached onto the membrane at a given time [day^{-1}]
f_m	Coefficient [day^{-1}]
Q_{out}	The output flow of the bioreactor [m^3. Day^{-1}]
R_{tot}	The total membrane resistance
R_0	Intrinsic membrane resistance
m	Value of solids attached onto the membrane area [kg]
SMP	Soluble microbial products [$kg.m^{-3}$]
S_T	Total substrate [$kg.m^{-3}$]
S_p	Value of the suspended solids blocked into the pores [$kg.m^{-3}$]
V_p	The total volume of the pores [m^3]
X_T	Total biomass [$kg.m^{-3}$]
α	Specific resistance of the sludge [$m.kg^{-1}$]
α'	Specific resistance of the sludge [$m.kg^{-1}$]
β	SMP fraction leaving the bioreactor [-]
δ	Parameter to normalize units [day]
δ'	Parameter to normalize units [-]
ω	Efficiency of backwashing/relaxation [dimensionless]
ω'	Efficiency of backwashing/relaxation [dimensionless]
η	The permeate viscosity [Pa.s]
$\in A$	The porous surface [m^2]