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DYNAMIC MODELLING OF A BIOFILTER USED FOR NITRIFICATION OF DRINKING WATER AT LOW INFLUENT AMMONIA CONCENTRATIONS

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Abstract: This paper reports on the development of a mathematical model of a packed bed biofilter operating at low influent ammonia concentrations. It is initially filled with biomass-free media, the adhesion by filtration of the bacteria present in the groundwater allowing colonization of the filter. The mathematical model is intended for simulation/optimization purposes, and should describe sufficiently well the start-up phase, as well as nominal operation. Unknown model parameters are estimated using experimental data collected on pilot plants. Validation and cross-validation results are discussed.

Keywords: Mathematical modelling; Distributed parameter systems; Parameter estimation; Biotechnology

1. INTRODUCTION

Generally, groundwater contains ammonia and is thus unsuitable for direct use as drinking water. Packed-bed biofilters enable a combination of biodegradation and physical retention, which ensures the capture of nitrifying bacteria carried by groundwater. Cell attachment and growth at the carrier surface create the biofilm. However, biofilters used for drinking water nitrification operate at lower ammonia concentrations than those usually observed in industrial wastewater treatment plants, and in most cases, the ammonia concentration is so low that it becomes the rate-limiting factor of biological nitrification. Moreover, a one- or two- month period is usually necessary to capture a sufficient amount of nitrifying bacteria, so as to reach the expected removal efficiency. For safe process operation, biofilter disinfection is also regularly performed, involving long stand-by phases where it is again necessary to wait for the biofilter colonization. Therefore, improving start-up of biofilters operating at low substrate concentrations is a major challenge related to the drinking water industry. Nitrites in the outflow of the biofilter must be avoided in all operating conditions.

In order to design a biofilter and optimize its operation, appropriate mathematical models would undoubtedly be very useful. The model should be complex enough to give a reliable representation of the physical and biological processes but simple enough to allow parameter identification from experimental data (practical parameter identifiability problem). A review of the published literature shows that only limited information is available on modelling of drinking water biofilters. A few papers report works on ammonia removal through biological filtration in aqua-

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culture industry (Grommen *et al.*, 2002), (Zhu and Chen, 1999). Numerical models were also developed to simulate the transient behaviour of biofilters used for biodegradable organic matter removal (Hozalski and Bouwer, 2001).

In the present work, experiments have been carried out under different conditions to explore the behavior of a packed-bed biofilter in the start-up and steady-state (nominal operation) phases. Taking into account the main biological processes, filtration and adsorption, a dynamic model based on a set of mass-balance partial differential equations (PDEs) is derived. Unknown model parameters are inferred from experimental data by minimizing an output-error criterion. Validation and cross-validation results are discussed.

2. MATERIALS AND METHODS

Two different filters were used in order to cover a larger range of operating conditions. The first filter structure, related in the following to experiments C1, is 21.5 *cm* in diameter and 180 *cm* in length, with a bed depth of 140 *cm*. The second filter (experiments C2) is 15 *cm* in diameter and 180 *cm* in length with a bed depth of 140 *cm*. Both beds are composed of (1.0-2.0 *mm*) manganese dioxide (ρ , 1.75-1.85 $g.cm^{-3}$; diameter, 0.36-1 *mm*). The filters are provided in different sites for water sampling (distributed vertically).

Groundwater is used in all experiments, whose average composition is ammonium: $0.2 \pm 0.02 mgN - NH_4^+ .l^{-1}$; nitrite: $0.01 \pm 0.005 mgN - NO_2^- .l^{-1}$; nitrate $0.01 \pm 0.005 mgN - NO_3^- .l^{-1}$. In experiments C2, additional ammonium was added to increase the influent water composition to 1.1 or 5 $mgN - NH_4^+ .l^{-1}$. Flow rates were set to 254 $l.h^{-1}$ and 140 $l.h^{-1}$ for filters 1 and 2, respectively, so as to impose the same liquid superficial velocity of about 8-10 $m.h^{-1}$. The water temperature inside the biofilter was 16^oC and 24^oC for experiments C1 and C2, respectively. The monitored variables were the dissolved oxygen concentration, conductivity and pH. In all cases, the biofilter was initially filled with biomass-free media, before eventually being uniformly inoculated with nitrifying bacteria previously grown in an aerated batch reactor.

Ammonia, nitrite and nitrate concentrations in the bulk phase were measured according to French standards (Afnor, 1994).

3. MODELLING

3.1 Bacterial growth and inactivation

Nitrification is a reaction chain oxidizing ammonia into nitrate, which consists of two main biological reactions (Henze *et al.*, 2002) associated to bacterial growth. It is commonly assumed that the production of nitrite and nitrate is associated to the growth of *Nitrosomonas* and *Nitrobacter*, respectively, which are formed with yields Y_{NS} and Y_{NB}.

The reaction rates are known to be limited by their nitrogeneous substrates at low concentrations as well as by oxygen. The temperature is also known to have a strong influence on these rates. The specific growth rates are then formulated according to classical Monod laws, where the dependency on the temperature is given by:

$$\mu_{\mathrm{i,max}}(T) = \mu_{\mathrm{i,max}}(20\,^{\circ}\mathrm{C}) 1.103^{T-20} \ , \ \mathrm{i} = \mathrm{NS \ or \ NB}$$

The biomass forms a biofilm around the particles. The growth of bacteria is counterbalanced by an inactivation process, i.e., part of the biomass can be considered as inactive despite its presence in the biofilm. This leads to a maximum active biomass concentration $X^{\mathrm{F}}_{\mathrm{max}}$ of both bacteria types, which compete for a place at the interface of the biofilm (Haag *et al.*, 2004). In agreement with the growth and inactivation kinetics introduced by Jacob (Jacob, 1994), the balance of growth/inactivation for each type of bacteria present in the biofilm is expressed as follows:

$$\dot{X}^{\mathrm{F}}_{\mathrm{NS}} = \mu_{\mathrm{NS}} X^{\mathrm{F}}_{\mathrm{NS}} - \frac{X^{\mathrm{F}}_{\mathrm{NS}}}{X^{\mathrm{F}}_{\mathrm{max}}} \left(\mu_{\mathrm{NS}} X^{\mathrm{F}}_{\mathrm{NS}} + \mu_{\mathrm{NB}} X^{\mathrm{F}}_{\mathrm{NB}} \right) \quad (1)$$

$$\dot{X}^{\mathrm{F}}_{\mathrm{NB}} = \mu_{\mathrm{NB}} X^{\mathrm{F}}_{\mathrm{NB}} - \frac{X^{\mathrm{F}}_{\mathrm{NB}}}{X^{\mathrm{F}}_{\mathrm{max}}} \left(\mu_{\mathrm{NS}} X^{\mathrm{F}}_{\mathrm{NS}} + \mu_{\mathrm{NB}} X^{\mathrm{F}}_{\mathrm{NB}} \right) \quad (2)$$

3.2 Filtration

The adhesion of the bacteria present in the groundwater to the solid bed is mainly due to filtration. The basic equation used in filtration theory to represent the removal of particles (suspended particle concentration $X^{\mathrm{B}}_{\mathrm{tot}}$) with distance z in a packed filter was first empirically derived by (Iwasaki, 1937). Various attempts were made to find a simple correlation between the filter coefficient k_f and key variables such as particle size, filtration velocity, porous media. In the simplest case, the filter coefficient is assumed to be constant. Assuming that transport by dispersion and detachment process can be neglected, the filtration process is described by two equations:

$$\frac{\partial X^{\mathrm{F}}_{\mathrm{tot}}}{\partial t} = k_{\mathrm{f}} \frac{Q}{A} X^{\mathrm{B}}_{\mathrm{tot}} \quad (3)$$

$$\frac{\partial (\varepsilon X^{\mathrm{B}}_{\mathrm{tot}})}{\partial t} = -\frac{Q}{A} \frac{\partial X^{\mathrm{B}}_{\mathrm{tot}}}{\partial z} - k_{\mathrm{f}} \frac{Q}{A} X^{\mathrm{B}}_{\mathrm{tot}} \quad (4)$$

where superscript B and F refer to the bulk and solid phases, respectively, and k_f is the filtration constant.

3.3 Decay

The decay cycle involves a loss of bacteria, part of which is transformed into ammonia by hydrolysis. The whole cycle of decay is fully described in (Henze *et al.*, 2002). It involves the decay with specific rate *b*,

to produce particulate biodegradable organic nitrogen X_{ND}, with yield $\nu = i_{XB} - f_p i_{XP}$, then its transformation into soluble biodegradable organic nitrogen and finally into ammonia nitrogen. The less favorable case where the hydrolysis and ammonification are assumed to be instantaneous is considered here:

$$X_{NS} + X_{NB} \xrightarrow{b} \nu X_{ND} \xrightarrow{\infty} \nu NH_4^+ \qquad (5)$$

Of course, this assumption does not reflect the reality, but allows the number of equations to be to reduced, while considering an approximate decay cycle.

3.4 Adsorption

A common way to describe sorption processes is based on the boundary layer theory which assumes an adsorption equilibrium at the interface between the mobile and stationary phases. A widely used isotherm for the sorption equilibrium was proposed in (Freundlich, 1906), involving the Freundlich constant K_{Fr}, the exponent $0 < n_{Fr} \leq 1$ and adsorption specific rate k_{ads}, which all depend on the media used.

3.5 The PDE model

The biological and physical transformations described in the previous subsections are schematically represented in Figure 1.

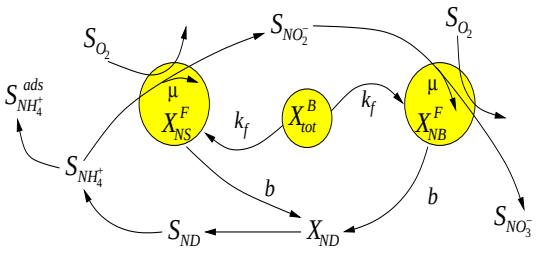

Fig. 1. Scheme of biological and physical phenomena involved in the biofilter nitrification process

The dynamic model equations are derived from mass balances. Since the biofilter is a spatially distributed system, these balances have to consider the state variables as functions of time and space. Height different states are considered in the proposed modeling approach leading to the state vector:

$$x^T = [S_{NH_4^+} \;\; S_{NO_2^-} \;\; S_{NO_3^-} \;\; S_{O_2} \;\; X_{tot}^B \;\; S_{NH_4^+}^{ads} \;\; X_{NS}^F \;\; X_{NB}^F \;]$$

The model PDEs are derived by expressing the dynamic mass balances around a infinitesimal slice along the column axis (Haag *et al.*, 2004). Under the assumption that the biofilm density is large enough so that the variation of porosity ε related to biomass growth can be neglected, i.e. ε is constant, the system of partial differential equations describing the biofilter is given by:

$$\dot{S}_{NH_4^+} = -\frac{Q}{\varepsilon A}\frac{\partial S_{NH_4^+}}{\partial z} + \nu b \frac{(X_{NS}^F + X_{NB}^F)}{\varepsilon} - \frac{\mu_{NS}}{Y_{NS}}\frac{X_{NS}^F}{\varepsilon} - \frac{k_{ads}}{\varepsilon}\left(S_{NH_4^+} - \left(\frac{S_{NH_4^+}^{ads}}{K_{Fr}}\right)^{1/n_{Fr}}\right) \qquad (6)$$

$$\dot{S}_{NO_2^-} = -\frac{Q}{\varepsilon A}\frac{\partial S_{NO_2^-}}{\partial z} + \frac{Y_{NO_2^-}}{Y_{NS}}\mu_{NS}\frac{X_{NS}^F}{\varepsilon} - \frac{1}{Y_{NB}}\mu_{NB}\frac{X_{NB}^F}{\varepsilon} \qquad (7)$$

$$\dot{S}_{NO_3^-} = -\frac{Q}{\varepsilon A}\frac{\partial S_{NO_3^-}}{\partial z} + \frac{Y_{NO_3^-}}{Y_{NB}}\mu_{NB}\frac{X_{NB}^F}{\varepsilon} \qquad (8)$$

$$\dot{S}_{O_2} = -\frac{Q}{\varepsilon A}\frac{\partial S_{O_2}}{\partial z} - \left(\frac{Y_{O_2,NS}}{Y_{NS}}\mu_{NS}\frac{X_{NS}^F}{\varepsilon} + \frac{Y_{O_2,NB}}{Y_{NB}}\mu_{NB}\frac{X_{NB}^F}{\varepsilon}\right) \qquad (9)$$

$$\dot{X}_{tot}^B = -\frac{Q}{\varepsilon A}\frac{\partial X_{tot}^B}{\partial z} - k_f\frac{Q}{\varepsilon A}X_{tot}^B \qquad (10)$$

$$\dot{S}_{NH_4^+}^{ads} = \frac{\varepsilon}{1-\varepsilon}k_{ads}\left(S_{NH_4^+} - \left(\frac{S_{NH_4^+}^{ads}}{K_{Fr}}\right)^{1/n_{Fr}}\right) \qquad (11)$$

$$\dot{X}_{NS}^F = \mu_{NS}X_{NS}^F + f_{NS,in}k_f\frac{Q}{A}X_{tot}^B - bX_{NS}^F - \frac{X_{NS}^F}{X_{max}^F}\left(\mu_{NS}X_{NS}^F + \mu_{NB}X_{NB}^F - b(X_{NS}^F + X_{NB}^F) + k_f\frac{Q}{A}X_{tot}^B\right) \qquad (12)$$

$$\dot{X}_{NB}^F = \mu_{NB}X_{NB}^F + (1 - f_{NS,in})k_f\frac{Q}{A}X_{tot}^B - bX_{NB}^F - \frac{X_{NB}^F}{X_{max}^F}\left(\mu_{NS}X_{NS}^F + \mu_{NB}X_{NB}^F - b(X_{NS}^F + X_{NB}^F) + k_f\frac{Q}{A}X_{tot}^B\right) \qquad (13)$$

The derived PDE system has to be supplemented with appropriate initial and boundary conditions:

- initial spatial profile: $x(t_0, z) = x_0(z)$,
- inflow ($z = z_0$) boundary conditions: $x(t, z_0) = x_{in}(t)$, which have to be consistent at $(t_0, z = 0)$.

3.6 Model simulation

The non-linear PDE system described above is solved numerically using a *Method of Lines* strategy, which proceeds in two steps: (a) the spatial domain is discretized and the spatial derivatives are approximated by finite differences, (b) the resulting system of semi-discrete ODEs is integrated in time.

4. MODEL IDENTIFICATION

Several model parameters are involved in the PDE model, whose values have been published in the literature. The parameters relative to nitrification are generally considered as well known in the case of fully stirred bioreactors (Henze *et al.*, 2002). However, it is considered in the present study that the affinity of the micro-organisms for their substrates is influenced by the porous support.

Another key parameter of the model is the maximum active biomass concentration X_{max}^F, the value of which is unknown and has to be identified.

The parameters relative to adsorption can be either identified, or evaluated through specific experiments. The second way has been used in this study. The set of model parameters is summarized in Table 1.

Table 1. Model parameters

symbol (unit)	value
Y_{NS} ($^{\mathrm{gDCO}}/_{\mathrm{gN-NH_4^+}}$)	0.142
Y_{NB} ($^{\mathrm{gDCO}}/_{\mathrm{gN-NO_2^-}}$)	0.084
$Y_{\mathrm{NO_2^-}}$ ($^{\mathrm{gN-NO_2^-}}/_{\mathrm{gN-NH_4^+}}$)	0.988
$Y_{\mathrm{NO_3^-}}$ ($^{\mathrm{gN-NO_3^-}}/_{\mathrm{gN-NO_2^-}}$)	0.993
$Y_{\mathrm{O_2,NS}}$ ($^{\mathrm{gDCO}}/_{\mathrm{gN-NH_4^+}}$)	$3.42 - Y_{\mathrm{NS}}$
$Y_{\mathrm{O_2,NB}}$ ($^{\mathrm{gDCO}}/_{\mathrm{gN-NO_2^-}}$)	$1.14 - Y_{\mathrm{NB}}$
$\mu_{\mathrm{NS,max}}$ (d^{-1})	0.7
$\mu_{\mathrm{NB,max}}$ (d^{-1})	0.8
K_{NS} ($mg\mathrm{N-NH_4^+}.\mathrm{l}^{-1}$)	to be estimated
K_{NB} ($mg\mathrm{N-NO_2^-}.\mathrm{l}^{-1}$)	to be estimated
$K_{\mathrm{O_2}}$ ($mg\mathrm{O_2}.\mathrm{l}^{-1}$)	0.8
b (d^{-1})	0.05
$\nu = i_{\mathrm{XB}} - f_{\mathrm{p}} i_{\mathrm{XP}}$ ($^{\mathrm{gN}}/_{\mathrm{gDCO}}$)	0.0812
X_{max} ($g\mathrm{DCO}.\mathrm{m}^{-3}$)	to be estimated
k_{f} (m^{-1})	0.2
ε (-)	0.12
dp (dm)	0.0094
K_{Fr} (-)	0.26
k_{ads} (d^{-1})	162
n_{Fr} (-)	1

Besides the model parameters, the initial and input conditions have to be specified for each experiment. At the initial time, the concentration of bacteria in the bulk phase, the free and adsorbed ammonia, nitrite and nitrate concentrations are set equal to 0. The oxygen is saturated (10 $mg.l^{-1}$). In the cases where additional nitrifying bacteria are inoculated, the initial concentration of *Nitrosomonas* and *Nitrobacter* have to be estimated. The initial conditions are summarized in Table 2.

Table 2. Initial concentrations

Initial concentration	value
$S_{NH_4^+}(t=0,z)$	0 or known
$S_{NO_2^-}(t=0,z)$	0 or known
$S_{NO_3^-}(t=0,z)$	0 or known
$S_{0_2}(t=0,z)$	9
$X^{\mathrm{B}}_{\mathrm{tot}}(t=0,z)$	0
$S^{ads}_{NH_4^+}(t=0,z)$	0 or known
$X^{\mathrm{F}}_{\mathrm{NS}}(t=0,z)$	to be estimated
$X^{\mathrm{F}}_{\mathrm{NB}}(t=0,z)$	to be estimated

The boundary conditions for the state variables in the bulk phase are fixed by the column inflow. Influent concentrations of ammonia, nitrite, nitrate and oxygen are potentially time-varying, but measured. The influent concentration of bacteria in the bulk phase $X^{\mathrm{B}}_{\mathrm{tot,in}}$ is unknown, but constant. The influent concentrations are summarized in Table 3.

For parameter estimation, a classical least-squares criterion is used, which is minimized using the Nelder-Mead simplex method, implemented in MATLAB routines.

Table 3. Influent concentrations

Initial concentration	value
$S_{NH_4^+}(t,z=0)$	measured - time-varying
$S_{NO_2^-}(t,z=0)$	measured - time-varying
$S_{NO_3^-}(t,z=0)$	measured - time-varying
$S_{0_2}(t,z=0)$	10
$X^{\mathrm{B}}_{\mathrm{tot,in}} = X^{\mathrm{B}}_{\mathrm{tot}}(t,z=0)$	to be estimated
$f_{NS,in}$	to be estimated

5. RESULTS AND DISCUSSION

5.1 Few considerations about the estimation procedure

Parameter estimation problem is particularly delicate in biological water treatment processes, due to the complexity of the models (and associated number of parameters) and the difficulty of collecting experimental data in well-defined and reproducible conditions. Particularly, real-life experiments involve unmodeled phenomena, random perturbations, sampling errors, and limited accuracy of the analysis procedures. For all these reasons, it is illusory to estimate accurate parameter values, and in the present study, our objective is mostly to validate the proposed model structure and to determine representative parameter estimates. Of course, in order to alleviate the above mentioned difficulties, independent experiments corresponding to various operating conditions have been carefully conducted. More precisely, two different datasets, corresponding to two different packed bed biofilters, are available. The first dataset involves two experiments:

- C1Exp1: $X^{\mathrm{F}}_{\mathrm{NS}}(t=0,z)=0$, $X^{\mathrm{F}}_{\mathrm{NB}}(t=0,z)=0$, $X^{\mathrm{B}}_{\mathrm{tot,in}} \neq 0$ unknown, known low level of ammonia concentration at input (around 0.2 $mg\mathrm{N-NH_4^+}.\mathrm{l}^{-1}$);
- C1Exp2: $X^{\mathrm{F}}_{\mathrm{NS}}(t=0,z) \neq 0$ unknown, $X^{\mathrm{F}}_{\mathrm{NB}}(t=0,z) \neq 0$ unknown, $X^{\mathrm{B}}_{\mathrm{tot,in}} \neq 0$ unknown but the same as in the previous experiment, known low level of ammonia concentration at input (around 0.2 $mg\mathrm{N-NH_4^+}.\mathrm{l}^{-1}$).

For such experiments of about one month, initiated with very low concentrations of bacteria and rather slow growth rates, the maximum active biomass concentration has a minor effect on the model transients, i.e., sensitivity with respect to X_{max} is very low in a wide range of values above 100 $mg\mathrm{DCO}.\mathrm{l}^{-1}$. On the other hand, the limiting conditions of these experiments allow the half-saturation constants to be estimated. This can be seen on Figure 2 where the cost function measuring the deviation between simulated and measured outputs is plotted for different values of the half-saturation constants. The minimum of the function is achieved for $K_{\mathrm{NS}} = 0.4 mg\mathrm{N-NH_4^+}.\mathrm{l}^{-1}$ and $K_{\mathrm{NB}} = 0.175 mg\mathrm{N-NO_3^-}.\mathrm{l}^{-1}$. These values are not affected for any X_{max} belonging to the interval $[100...500]$.

Moreover, experiment C1Exp1 can be used to estimate the concentration of particles in the influent water, and the fraction $f_{\mathrm{NS,in}}$ of *Nitromosonas*. Ac-

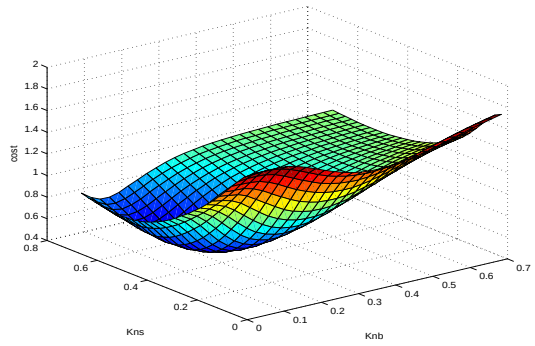

Fig. 2. C1Exp1 - Cost function evolution with the half-saturation constants K_{NS} and K_{NB} for given values $X_{\max} = 200 mg\mathrm{DCO}.\mathrm{l}^{-1}$, $X^{\mathrm{B}}_{\mathrm{tot,in}} = 0.0001 mg\mathrm{DCO}.\mathrm{l}^{-1}$ and $f_{\mathrm{NS,in}} = 0.9$

cording to the growth yields Y_{NS} and Y_{NB}, an initial guess would be $f_{\mathrm{NS,in}} = 0.63$. However, this fraction is strongly influenced by the conditions of conservation of the groundwater. Figure 3 illustrates this fact, i.e. the output least-square cost function is plotted for different values of the influent particle concentration and repartition between *Nitrosomonas* and *Nitrobacter*. The minimum of the cost function corresponds to $X^{\mathrm{B}}_{\mathrm{tot,in}} = 0.0012 mg\mathrm{DCO}.\mathrm{l}^{-1}$ and $f_{\mathrm{NS,in}} = 0.9$.

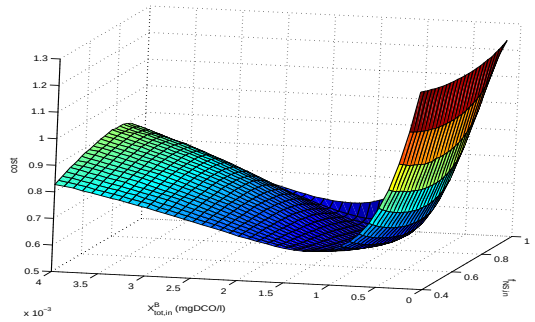

Fig. 3. C1Exp1 - Cost function evolution with the influent concentration of bacteria $X^{\mathrm{B}}_{\mathrm{tot,in}}$ and fraction of *Nitrosomonas* $f_{\mathrm{NS,in}}$ for given $X_{\max} = 200 mg\mathrm{DCO}.\mathrm{l}^{-1}$, $K_{\mathrm{NS}} = 0.4 mg\mathrm{N} - \mathrm{NH}^{+}_{4}.\mathrm{l}^{-1}$ and $K_{\mathrm{NB}} = 0.2 mg\mathrm{N} - \mathrm{NO}^{-}_{3}.\mathrm{l}^{-1}$

The second dataset contains one experiment:

- C2Exp1: High but unknown initial concentration $X^{\mathrm{F}}_{\mathrm{NS}}(t=0,z)$ and $X^{\mathrm{F}}_{\mathrm{NB}}(t=0,z)$, $X^{\mathrm{B}}_{\mathrm{tot,in}} = 0$, known high level of ammonia concentration at input (over 1 $mg\mathrm{N} - \mathrm{NH}^{+}_{4}.\mathrm{l}^{-1}$).

When studying this second dataset, the half-saturation constants K_{NS} and K_{NB} are assumed to be known (values determined from the first series of experiments at low influent ammonia concentration) and attention is focused on the estimation of $X_{\max}$, $X^{\mathrm{F}}_{\mathrm{NS}}(t=0,z)$ and $X^{\mathrm{F}}_{\mathrm{NB}}(t=0,z)$. Moreover, since the initial concentration of bacteria is provided by a nitrifying sludge previously acclimated from an activated sludge reactor for 40 days, the fraction of *Nitrosomonas* is set to its standard value $f_{\mathrm{NS}} = 0.63$. The biofilter is in fact inoculated with a so high concentration of *Nitrosomonas* and *Nitrobacter* that it can be verified in Figure 4 that this initial concentration corresponds more or less to the maximum active biomass concentration, i.e. the optimal cost function is given for $X^{\mathrm{F}}_{\mathrm{tot}}(t=0,z) = X_{\max} = 200 mg\mathrm{DCO}.\mathrm{l}^{-1}$.

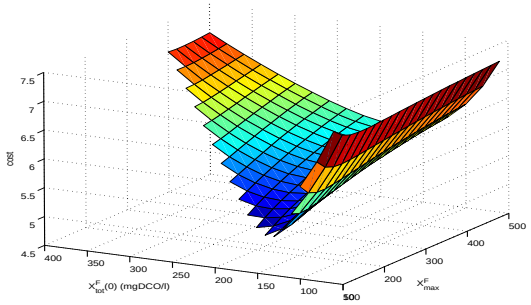

Fig. 4. C2Exp1 - Cost function evolution with the initial concentration of bacteria $X^{\mathrm{F}}_{\mathrm{tot}}(t=0,z)$ and maximum active biomass concentration $X_{\max}$ (only cases where $X^{\mathrm{F}}_{\mathrm{tot}}(t=0,z) \leq X_{\max}$ are considered), for given $f_{\mathrm{NS}} = 0.63$, $K_{\mathrm{NS}} = 0.4 mg\mathrm{N} - \mathrm{NH}^{+}_{4}.\mathrm{l}^{-1}$ and $K_{\mathrm{NB}} = 0.2 mg\mathrm{N} - \mathrm{NO}^{-}_{3}.\mathrm{l}^{-1}$

5.2 *Model fitting*

The numerical values of the estimated model parameters and particle concentrations are given in Table 4 and 5, respectively. Bounds on the standard deviations and correlations between parameters can be computed using the inverse of the Fisher information matrix. The main correlations are between $X^{\mathrm{F}}_{\mathrm{NS}}(t=0,z)$ and K_{NS} on the one hand, and between $X^{\mathrm{F}}_{\mathrm{NB}}(t=0,z)$, K_{NB}, $X^{\mathrm{B}}_{\mathrm{tot,in}}$ and $f_{NS,in}$ on the other hand. $X^{\mathrm{F}}_{\max}$ is also partly correlated with K_{NS} and K_{NB}. This shows that it is more suitable to estimate the half-saturation constants based on experiments without inoculation of biomass if the inoculum concentrations are not precisely known.

Table 4. Estimated model parameters

Model parameter	value
K_{NS} ($mg\mathrm{N} - \mathrm{NH}^{+}_{4}.\mathrm{l}^{-1}$)	0.4
K_{NB} ($mg\mathrm{N} - \mathrm{NO}^{-}_{3}.\mathrm{l}^{-1}$)	0.2
$X^{\mathrm{F}}_{\max}$ ($mg\mathrm{DCO}.\mathrm{l}^{-1}$)	200

Table 5. Estimated influent and initial particles concentrations

Particle ($mg\mathrm{DCO}.\mathrm{l}^{-1}$)	C1Exp1	C1Exp2	C2Exp1
$X^{\mathrm{F}}_{\mathrm{NS}}(0,z)$	0	0.25	126
$X^{\mathrm{F}}_{\mathrm{NB}}(0,z)$	0	0.25	74
$X^{\mathrm{B}}_{\mathrm{tot,in}}$		0.001	0
$f_{NS,in}$		0.9	0

Figures 5 to 7 show the spatial profiles of the nitrogenous components in the liquid phase and biomass fixed on the porous bed as snapshots of Experiment C1Exp1, at time t = 6 days, 9 days and 22 days, respectively. Figure 8 and 9 show the spatial profiles at time t = 3 days and 18 days relative to Experiment C2Exp1. The graphical results confirm the good agreement between the model and the experimental data.

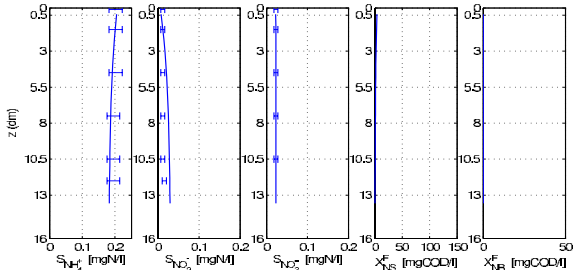

Fig. 5. C1Exp1 - Spatial profiles at t = 6 days. model prediction (solid line) and measurements (dash symbol)

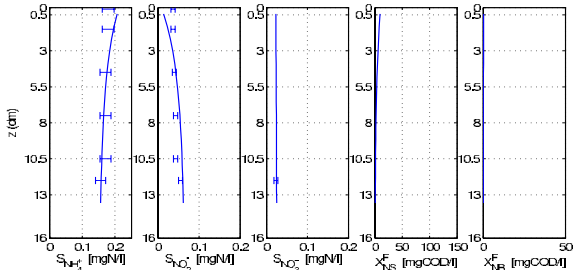

Fig. 6. C1Exp1 - Spatial profiles at t = 9 days. model prediction (solid line) and measurements (dash symbol)

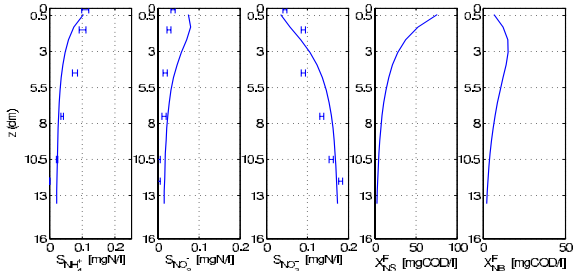

Fig. 7. C1Exp1 - Spatial profiles at t = 22 days. model prediction (solid line) and measurements (dash symbol)

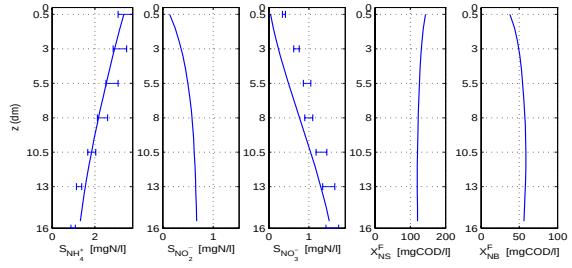

Fig. 8. C2Exp1 - Spatial profiles at t = 3 days. model prediction (solid line) and measurements (dash symbol)

6. CONCLUSION

A mass-balance PDE model has been set up, based on main biological reactions, filtration and adsorption phenomena, and calibrated with experiments carried out with two packed bed biofilters operating under different conditions (e.g., influent water composition, temperature, inoculum, operational events). Parameter estimation was discussed, taking into account the

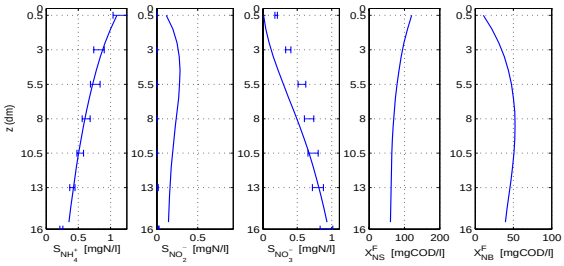

Fig. 9. C2Exp1 - Spatial profiles at t = 18 days. model prediction (solid line) and measurements (dash symbol)

published results, parameter sensitivity analysis, and identification of selected parameters. Validation results show that the model is in good agreement with experimental data (accepting the idea that experiments with biological water treatment systems are delicate to achieve, and are unavoidably corrupted by random perturbations and measurement errors).

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