BIOMASS RECONSTRUCTION IN A WASTEWATER TREATMENT BIOFILTER

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Abstract: this paper is concerned with a pilot-scale fixed-bed biofilter used for nitrogen removal from municipal wastewater. Process dynamics is described by a set of mass balance partial differential equations, which allow the evolution of the several component concentrations along the biofilter axis to be reproduced. Based on sets of experimental data collected over a several-month period, unknown model parameters are estimated by minimizing an output error criterion. The resulting distributed parameter model and a few pointwise measurements of nitrate, nitrite, and ethanol concentrations can be used to design observers, which allow the unmeasured biomass concentrations to be reconstructed on-line. First, it is demonstrated that asymptotic observers are unsuitable for the model structure. Then, a receding-horizon observer is designed and tested, which shows very satisfactory performance. *Copyright © 2002 IFAC*

Keywords – distributed parameter systems, state estimation, identification, biotechnology.

1. INTRODUCTION

Nitrogen removal is an important step in the treatment of municipal wastewater. Over the past several years, biofilter systems have received considerable attention; see for instance the conference proceedings and journals of the International Water Association (IWA) (e.g. Oh *et al.*, 2001). The main advantages of these wastewater treatment systems are their ease of use, compactness, efficiency, and low energy consumption.

In a previous study (Vande Wouwer et al., 2002), a dynamic model was developed based on experimental data collected from a pilot-scale plant. The resulting model can be used for simulation purposes (e.g. for system analysis and design) or as a basis for the development of a software sensor (which can be used to estimate unmeasured variables on-line). In contrast to a similar study by Bourrel et al. (1996; 2000), the proposed model does not assume that steady state biomass conditions are achieved, but on the opposite explains the very long transient phases observed experimentally by growth and inactivation processes associated to the biomass.

The biomass distribution inside the biofilter therefore appears as a primary determinant of the plant performance. Based on a few pointwise measurements of nitrate, nitrite and ethanol concentrations, and on the biofilter model, the objective of this paper is to design distributed parameter observers of the unmeasured biomass concentration profiles. Asymptotic observers (Bastin and Dochain, 1990), which do not rely on the knowledge of the kinetic model and which have good convergence properties in the case of continuous systems, would a priori be a very appealing solution. However, they appear unsuitable for the model structure, and attention is therefore focused on receding-horizon observers (Allgöwer et al., 1999; Bogaerts and Hanus, 2001), which allow the state estimation problem for nonlinear distributed parameter systems to be solved in a very elegant way.

This paper is organized as follows. In the next section, the experimental setup is described. Section 3 briefly discusses biofilter modeling, i.e. the derivation of a reaction scheme, reaction kinetics, and a system of mass balance PDEs. In Section 4, distributed parameter asymptotic observers and receding-horizon observers for the unmeasured biomass concentration profiles are examined. Finally, Section 5 is devoted to some conclusions.

2. PROCESS DESCRIPTION

The pilot plant under consideration (Fig. 1) is a submerged biofilter packed with lava rock (pouzzolane). The biofilter is fed with a synthesis water composed of raw municipal wastewater and additions of a concentrated nitrate solution. Several biological reactions take place inside the biofilter, e.g. removal of soluble COD and removal of nitrate and nitrite.

The denitrification process consists of several consecutive reactions of oxydo-reduction and implies a transient accumulation of nitrite in the biofilter

$$NO_3^- \xrightarrow{(1)} NO_2^- \xrightarrow{(2)} N_2$$

Oxydo-reduction is achieved thanks to an organic carbon source (as donor of electrons). In this case, ethanol is used.

Eight sampling points are evenly distributed along the reactor axis, which allow the several component concentration profiles (COD, nitrate and nitrite) to be measured. The manipulated variables are the feed flow rate F(t) to the biofilter and the inlet ethanol concentration $S_{C,in}(t)$.

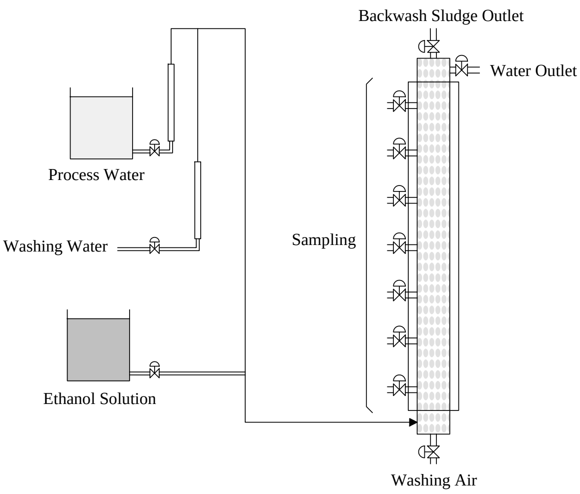

Fig. 1. Experimental setup

The experiments accomplished with the pilot plant aimed at sweeping the range of operating conditions (various C/N and feed-flow rates; on the other hand, the temperature was kept constant) observed in a full-scale wastewater treatment plant located in Montargis, France. The experiments were carried out at the Institut National des Sciences Appliquées de Toulouse (INSAT), France (Bascoul, 1995).

3. MODEL DEVELOPMENT

In this section, a system of mass-balance PDEs is derived, and the unknown model parameters are estimated from experimental data (for more details see (Vande Wouwer et al., 2002)).

3.1 Reaction scheme

A macroscopic biological reaction scheme based on the concept of "pseudo-stoichiometry" (Bastin and Dochain, 1990) is used

$$\nu_1 \text{carbon} + \frac{\nu_2}{\alpha_1}\text{nitrate} \rightarrow \text{biomass} + \frac{\nu_2}{\alpha_2}\text{nitrite} \quad (1)$$

$$\nu_3 \text{carbon} + \frac{\nu_4}{\alpha_2}\text{nitrite} \rightarrow \text{biomass} + \nu_5 \text{nitrogen} \quad (2)$$

$$\text{active biomass} \rightarrow \text{inactive biomass} \quad (3)$$

where ν_i , i = 1,…,5 are the pseudo-stoichiometric coefficients, and α_1 = 1.14, α_2 = 1.71 are Chemical Oxygen Demand (COD) conversion factors.

3.2. Reaction kinetics

The specific growth rates are taken in the form

$$\mu_1 = \mu_{1,max} \frac{S_{NO3}}{S_{NO3} + K_{NO3}} \frac{1}{1 + X_a / K_{Xa1}} \quad (4)$$

$$\mu_2 = \mu_{2,max} \frac{S_{NO2}}{S_{NO2} + K_{NO2}} \frac{1}{1 + X_a / K_{Xa2}} \quad (5)$$

$$\mu_3 = \mu_{3,max} \quad (6)$$

where the limiting substrates are nitrate (S_{NO3}) and nitrite (S_{NO2}). The active biomass X_a has an inhibition effect on the two growth-associated reactions (1-2). The inactivation process is assumed to have first-order kinetics (the simplest possible model in the absence of detailed knowledge about this process). In the experiments considered in this study, the carbon source is always in excess so that its limiting effect cannot be quantified.

3.3. Mass balances

Based on this reaction scheme and kinetics, it is straightforward to derive the following mass balance PDEs

$$\frac{\partial S_{NO3}}{\partial t} = -v\frac{\partial S_{NO3}}{\partial z} - \frac{\nu'_2}{\alpha_1}\mu_1 X_a \qquad (7)$$

$$\frac{\partial S_{NO2}}{\partial t} = -v\frac{\partial S_{NO2}}{\partial z} + \left(\frac{\nu'_2}{\alpha_2}\mu_1 - \frac{\nu'_4}{\alpha_2}\mu_2\right)X_a \qquad (8)$$

$$\frac{\partial S_C}{\partial t} = -v\frac{\partial S_C}{\partial z} - \left(\nu'_1\mu_1 - \nu'_3\mu_2\right)X_a \qquad (9)$$

$$\frac{\partial X_a}{\partial t} = \left(\mu_1 + \mu_2 - \mu_3\right)X_a \qquad (10)$$

where plug-flow conditions are assumed, $v = \frac{F}{\varepsilon A}$ is the fluid flow velocity (A: cross-section area of the biofilter, ε : bed porosity), and $\nu'_i = \frac{1-\varepsilon}{\varepsilon}\nu_i$.

These equations are supplemented by boundary conditions corresponding to the inlet concentrations.

PDEs (7-10) are solved numerically using a standard method of lines procedure (finite differences with about 30 nodes).

3.4. Parameter estimation

Pseudo-stoichiometry and kinetics involve 11 unknown model parameters (ν_i , i = 1,..,4, $\mu_{i,max}$, i = 1,..,3, K_{NO3}, K_{NO2}, K_{Xa1} and K_{Xa2}), whose numerical values have to be inferred from experimental data.

Based on the assumption of constant (but unknown) relative errors on the measurement data, the following output-error criterion is defined:

$$J = \sum_{k=1}^{15}\sum_{i=1}^{3}\sum_{l=1}^{8}\left(\ln(y_{i,mes}(z_l, t_k)) - \ln(y_{i,mod}(z_l, t_k))\right)^2 \qquad (11)$$

where:

- constant relative errors on the measurements $y_{i,mes}$ are equivalent to constant absolute errors on the logarithms of the measurements $\ln(y_{i,mes})$,
- 15 sample times, at each of which 3 component concentrations (S_C, S_{NO3} and S_{NO2}) in 8 different spatial locations are measured, representing a total of 360 data points.

The output-error criterion (11) is minimized with respect to the unknown model parameters using a Levenberg-Marquardt algorithm. Positivity constraints on the parameters are imposed through a logarithmic transformation.

The model prediction is compared to the measured signals (direct and cross-validation); see for instance Fig. 2, which shows the spatial concentration profile of nitrite, at a particular sample time. The model agreement is satisfactory.

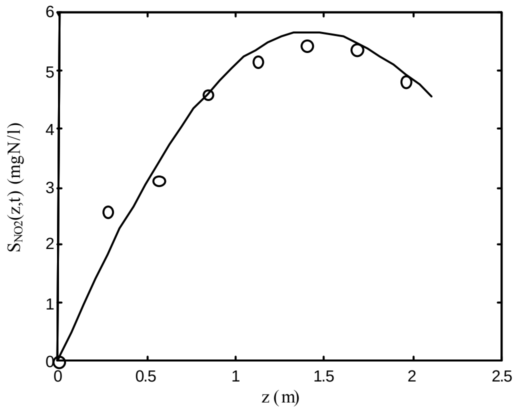

Fig. 2: Spatial nitrite concentration profile (direct validation - solid line: model prediction, circles: measured values).

4. STATE ESTIMATION

The long transient phases observed in real-life operations can be explained by biomass growth and inactivation processes, i.e. the global rate at which biomass develops determines the overall dynamics of the biofilter. The uniformity of the biomass distribution inside the porous bed is also a primary determinant of the biofilter performance in face of large variations of the feed conditions. For process monitoring, it would therefore be interesting to visualize the biomass concentration profiles on-line. However, these profiles are difficult to measure in practice, and it is required to resort to state estimation techniques. With regard to the modeling uncertainties, particularly of the reaction kinetics, it is appealing to design an asymptotic observer (Bastin and Dochain, 1990), which is the first solution considered in the following.

4.1. Asymptotic observers

The mass balance PDEs (7-10) can be reformulated in a more compact form as follows

$$\frac{\partial \xi}{\partial t} = -\mathbf{v}\frac{\partial \xi}{\partial z} + \mathbf{K}\boldsymbol{\varphi} \qquad (12)$$

or

$$\frac{\partial}{\partial t}\begin{bmatrix}\xi_f \\ \xi_s\end{bmatrix} = \begin{bmatrix}-v\cdot\frac{\partial \xi_f}{\partial z} \\ 0\end{bmatrix} + \begin{bmatrix}\mathbf{K}_f \\ \mathbf{K}_s\end{bmatrix}\cdot\boldsymbol{\varphi} \qquad (13)$$

where $\mathbf{v}$ is the velocity vector, $\mathbf{K}$ is the pseudo-stoichiometry matrix, $\boldsymbol{\varphi} = \boldsymbol{\mu}X_a$ is the reaction rate vector, and the state $\xi = [S_{NO3} \quad S_{NO2} \quad S_C \quad X_a]^T$ is decomposed into the components in solution in the fluid phase $\xi_f = [S_{NO3} \quad S_{NO2} \quad S_C]^T$, which can be measured on-line in a few locations along the reactor axis, and the component anchored on the solid phase $\xi_s = [X_a]$, which is not measured.

Following (Bastin and Dochain, 1990; Dochain and Vanrolleghem, 2001), the procedure to develop an asymptotic observer is to partition ξ into two subvectors ξ_a and ξ_b, $\xi = [\xi_a \quad \xi_b]^T$, such that the corresponding partition of the pseudo-stoichiometry matrix $\mathbf{K} = [\mathbf{K}_a \quad \mathbf{K}_b]^T$ with

$$\mathbf{K} = \begin{bmatrix} -\nu_2/\alpha_1 & 0 & 0 \\ \nu_2/\alpha_2 & -\nu_4/\alpha_2 & 0 \\ -\nu_1 & -\nu_3 & 0 \\ 1 & 1 & -1 \end{bmatrix} \qquad (14)$$

is of full row rank. Here, rank ($\mathbf{K}$) = M = 3 (M is the number of independent reactions in the reaction scheme), so that rank ($\mathbf{K}_a$) should be 3.

This condition excludes the commonly used partition into measured and non measured components, i.e. $\xi_a = \xi_f$ and $\xi_b = \xi_s$, as rank ($\mathbf{K}_a$) = 2 only. Hence, the following partition is selected

$$\xi_a = \begin{bmatrix} \xi_{af} \\ \xi_{as} \end{bmatrix} = \begin{bmatrix} S_{NO_3} \\ S_{NO_2} \\ X_a \end{bmatrix} \quad \text{and} \quad \xi_b = [S_C] \qquad (15)$$

which leads to a full row rank submatrix $\mathbf{K}_a$.

It is then possible to define a new state vector $\mathbf{z}$ by

$$\mathbf{z} = \mathbf{A}_0 \xi_a + \xi_b = [\mathbf{A}_{0f} \quad \mathbf{A}_{0s}] \begin{bmatrix} \xi_{af} \\ \xi_{as} \end{bmatrix} + \xi_b \qquad (16)$$

where the matrix $\mathbf{A}_0$ is the unique solution of

$$\mathbf{A}_0 \mathbf{K}_a + \mathbf{K}_b = 0 \qquad (17)$$

The evolution of $\mathbf{z}$ is given by

$$\frac{\partial \mathbf{z}}{\partial t} = \mathbf{A}_{0f} \cdot \frac{\partial \xi_{af}}{\partial t} + \mathbf{A}_{0s} \cdot \frac{\partial \xi_{as}}{\partial t} + \frac{\partial \xi_b}{\partial t} \qquad (18)$$

Substituting the time derivatives by their expressions (13), the equations of the asymptotic observer, from which the reaction kinetics are eliminated, are obtained

$$\frac{\partial \hat{\mathbf{z}}}{\partial t} = -v \cdot \left(\mathbf{A}_{0f} \cdot \frac{\partial \xi_{af}}{\partial z} + \frac{\partial \xi_b}{\partial z} \right) \qquad (19)$$

$$\hat{\xi}_{as} = \mathbf{A}_{0s}^{-1} \cdot \left(\hat{\mathbf{z}} - \mathbf{A}_{0f} \cdot \xi_{af} - \xi_b \right) \qquad (20)$$

For this observer to be completely defined, the inverse $\mathbf{A}_{0s}^{-1}$ (which, in the particular case under consideration, is a scalar) is required. This information can be obtained by solving equation (17), which gives $\mathbf{A}_{0s} = 0$!

The asymptotic observer is therefore not applicable with the model structure (13) since the partition of the state vector leads either to a submatrix $\mathbf{K}_a$ which is not full row rank or to a null matrix $\mathbf{A}_{0s}$. The only way round would be to simplify the model and to abandon the equation describing the biomass inactivation process (as was the case in the work of Bourrel *et al.*, 2000), which we know is not acceptable.

4.2. Receding-horizon observers

As the concentration measurements are rare and corrupted by noises, the concept of full-horizon observer (Bogaerts and Hanus, 2001), which uses all the measurement information available up to the current time, is extended to the distributed parameter model of the biofilter.

The *prediction step* (between samples $t_k < t < t_{k+1}$) corresponds to the solution of the model PDEs (12)

$$\frac{\partial \hat{\xi}}{\partial t} = -\mathbf{v} \frac{\partial \hat{\xi}}{\partial z} + \mathbf{K} \boldsymbol{\varphi}(\hat{\xi}) \qquad 0 \le t < t_{k+1} \qquad (21)$$

subject to initial conditions

$$\hat{\xi}(0) = \hat{\xi}_{0/k} \qquad (22)$$

and boundary conditions corresponding to the inlet concentrations.

The *correction step* (at sampling times) corresponds to the following optimization problem:

$$\hat{\xi}_{0/k} = \underset{\xi_0}{\text{Arg min}} \, J_k(\xi_0) \qquad (23)$$

with $J_k(\xi_0)$ given by

$$\frac{1}{2} \sum_{j=1}^{k} (\mathbf{y}_{mes}(t_j) - \mathbf{y}_{mod}(t_j))^T \mathbf{Q}(t_j)^{-1} (\mathbf{y}_{mes}(t_j) - \mathbf{y}_{mod}(t_j)) \qquad (24)$$

$$J_k(\xi_0) = \frac{1}{2} \sum_{j=1}^{k} (\mathbf{y}_{mes}(t_j) - \mathbf{y}_{mod}(t_j))^T \mathbf{Q}(t_j)^{-1} (\mathbf{y}_{mes}(t_j) - \mathbf{y}_{mod}(t_j))$$

where $\mathbf{y}_{mes}$ represents the vector of measurements (nitrate, nitrite and ethanol concentrations in 8 locations along the biofilter axis), $\mathbf{y}_{mod}$ the corresponding model prediction, and **Q** the covariance matrix of the measurement errors.

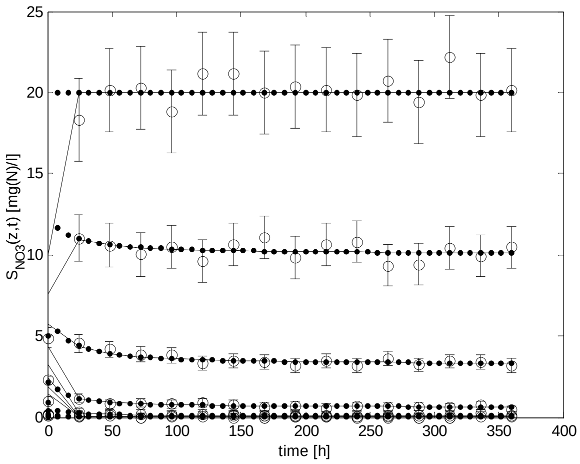

Fig. 3: Temporal evolution of the real (dots) and estimated (solid lines) nitrate concentrations in the 8 measurement locations, and concentration measurements (circles) together with their 99% confidence intervals.

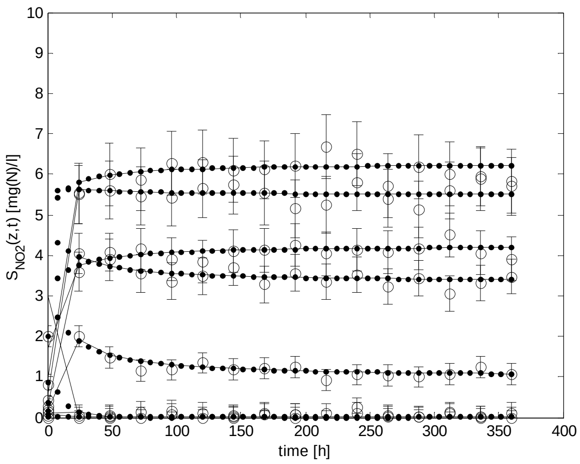

Fig. 4: Temporal evolution of the real (dots) and estimated (solid lines) nitrite concentrations in the 8 measurement locations, and concentration measurements (circles) together with their 99% confidence intervals.

In order to reduce the dimensionality of the optimization problem (27-28), the vector of initial conditions $\hat{\xi}_{0/k}$ is expressed as a set of exponential profiles, i.e.

$$\hat{\xi}_{0,i}(z)=\alpha_i \cdot \exp(-\beta_i \cdot z) \qquad (25)$$

(i = S_{ON3}, S_{ON2}, S_C, X_a) which leads to the on-line determination of 8 parameters.

The observer is first tested in simulation. The biofilter model is used to generate simulation data, which are corrupted by noise. Figures (3-4) compare the temporal evolution of the real and estimated concentrations in the 8 measurement locations distributed along the biofilter axis, as well as the measured concentrations together with their 99% confidence intervals. Figure (5) compares the biomass estimates with their real values (which are not measured), whereas figure (6) illustrates the time evolution of the corresponding spatial profiles.

As it is apparent from figures (3-6), the performance of the full-horizon observer is very satisfactory. Experimental application confirms this observation, as depicted in figures (7-8) which show the initial nitrite concentration profiles (initial measured profile and initial exponential guess) and the same profiles after 404 hours. The convergence of the observer is satisfactory, despite the modeling errors and the measurement noise. The observer performance cannot however be fully tested, as biomass measurements are not available.

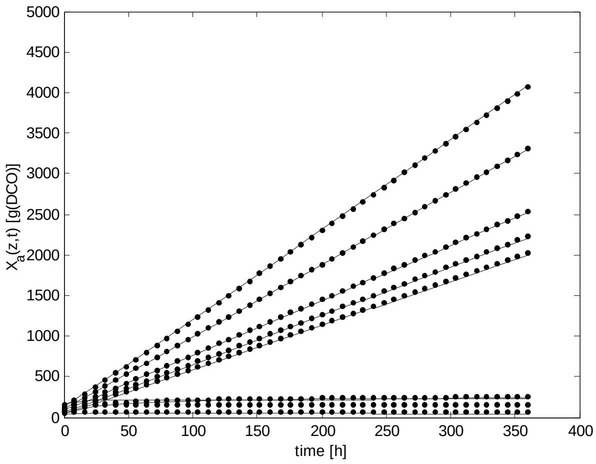

Fig. 5: Temporal evolution of the biomass concentration estimates (solid lines) and of the real, non measured, concentrations (dots).

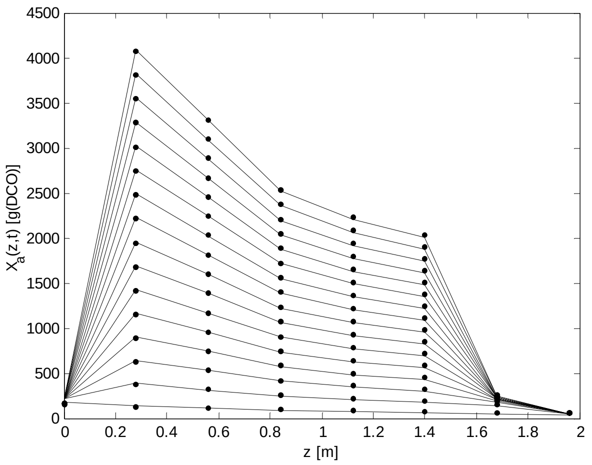

Fig. 6: Temporal evolution of the biomass spatial profiles (solid lines) and of the real, non measured, concentrations (dots).

5. CONCLUSION

In this paper, a distributed parameter model of a fixed-bed biofilter used for nitrogen removal in municipal wastewater treatment is derived. The unknown model parameters are estimated from experimental data collected over a period of several months. The main contribution of this modeling study is to show that the long transient phases observed in real-life operations can be explained by biomass growth and inactivation processes, i.e. the global rate at which biomass develops determines the overall dynamics of the biofilter.

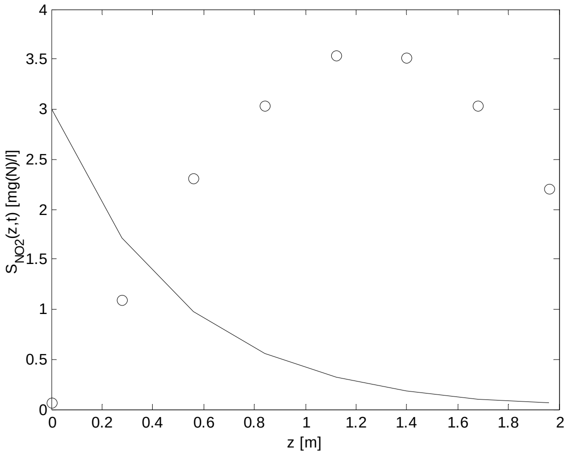

Fig. 7: Initial measured profile (circles) and exponential initial condition (solid line) of nitrite concentration.

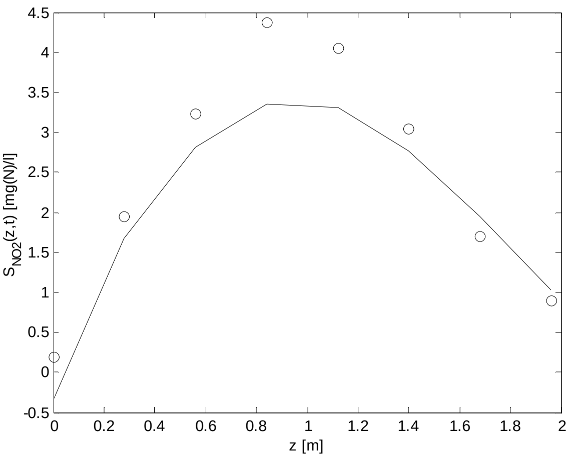

Fig. 8: measured profile (circles) and estimate (solid line) of nitrite concentration after 404 hours.

As the biomass distribution cannot be measured in practice, it is appealing to design a software sensor (or state observer) to reconstruct this information on-line. To this end, two options are considered: (a) an asymptotic observer, and (b) an exponential observer.

The asymptotic observer does not rely on the knowledge of the reaction kinetics, which is a decisive advantage with regard to the model uncertainties. However, the asymptotic observer appears unsuitable for the considered model structure, and an exponential observer, e.g. an extended Kalman filter or an extended Luenberger observer, is the only feasible solution. In this latter class of observers, receding-horizon (or full-horizon, when measurements are rare and corrupted by noises) observer provide a very simple, yet rigorous, solution to the nonlinear state estimation problem in distributed parameter systems with stochastic disturbances.

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