15th Triennial World Congress, Barcelona, Spain

STATE AND DISTURBANCE ESTIMATION FOR AN ALTERNATING ACTIVATED SLUDGE PROCESS

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Abstract: An application of the extended Kalman filter for a nonlinear model of an activated sludge process (ASP), working in an alternating aerobic-anoxic phase medium, is proposed. The filter is used to estimate both the states and non-stationary disturbances, to better evaluate changes in operating conditions. It is to be pointed out that, according to the structure of the reduced nonlinear system, the observer is a two-alternated-observer scheme. Filtering results are shown by using both experimental data and simulations. *Copyright © 2002 IFAC*

Keywords: Extended Kalman filter, estimation, unknown input observation, model reduction, wastewater treatment.

1. INTRODUCTION

Wastewater treatment processes are known as very complex systems, involving different time-scaled dynamics and unknown input disturbances. As in most of real systems, control strategies are quite limited due to the lack of on-line performant and low cost instrumentation. Dealing with this problem requires the attention to preliminary steps as process modelling, model reduction and observation. This paper addresses the problem of reconstructing unmeasurable state variables and/or unknown inputs for a single reactor ASP.

Different kinds of models describing the sludge process can be found in the literature. Holmberg (1982) has proposed an empirical model for specific analysis, design and control purposes. For carbon and nitrogen removal the standard industrial is the Activated Sludge Model (ASM) No. 1 developed by the task group of the recently renamed International Association on Water Quality (IAWQ) (Henze *et al.*, 1987), which includes thirteen state variables and more than fifteen parameters. Complex mathematical models as ASM No.1 are difficult to handle for estimation/control purposes. Hence, simplified models are more exploitable, always respecting a compromise between model complexity and model precision based upon ulterior goals in control design.

In previous works, several nonlinear reduced models have been presented (Jeppson, 1995; Julien *et al.*, 1999; Zhao and Kümmel, 1995). In this article we use a reduced nonlinear model developed by (Gómez-Quintero *et al.*, 2000) involving four state differential equations and thirteen parameters. The reduction strategy applied to obtain this model has taken into account some biochemical considerations and grouping of parameters. The reduced-order model matches specific characteristics for a laboratory pilot plant.

This paper concerns the application of an extended Kalman filter (EKF) to observe the unmeasurable variables and one of the most sensitive unknown inputs of the system, the influent nitrogen concentration. This filtering procedure is simple to apply and does not involve any numerical effort which makes it suitable for on-line observation. In previous works the problem of state and parameter estimation in an alternating ASP by using an EKF has been considered for a single aerobic-anoxic model (Zhao and Kümmel, 1995; Lukasse *et al.*, 1999). We propose a two-alternated-observer scheme, which takes into account changes in model structure associated to the switching from aerobic to anoxic phases in the reactor.

2. THE EXTENDED KALMAN FILTER

State estimation in biological processes has been studied since about three decades for several specific applications (see a survey in (Soroush, 1998)) and big efforts to develop reliable observers for nonlinear systems have been done. Basically, they can be classified on two groups : those that are extensions of the Kalman filter and the Luenberger observer (Jazwinski, 1970; Zeitz, 1987), and those derivated from the nonlinear control theory (Krener and Isidori, 1983) but which can only be applied to restricted classes of nonlinear processes (Farza *et al.*, 1999; Gauthier and Kupka, 1994).

The EKF has been applied successfully to many chemical and biochemical processes despite the linear first-order approximation involved in the approach (Bastin and Dochain, 1990; Aubrun *et al.*, 2001). However, a few applications of this algorithm to an alternating ASP are available in the literature (Zhao and Kümmel, 1995; Lukasse *et al.*, 1999).

The EKF is used here both to estimate the state vector of the nonlinear system and to identify time-varying disturbances considered as time-varying parameters. The disturbances can be modelled as stochastic variables which are included as new states needed to eliminate bias in the state estimates when the system operates under non-ideal conditions. For this purpose, let us consider the nonlinear continuous-time system with discrete-time observation of the form:

$$\begin{aligned} \dot{x}^d(t) &= f^d(x^d, x^s, t) + w^d(t), \; x^d(0) \\ \dot{x}^s(t) &= \varepsilon + w^s(t), \; \varepsilon \to 0, \quad\quad x^s(0) \\ y_k &= h(x_k^d, x_k^s, k) + v_k \end{aligned} \tag{1}$$

where y is the vector of measured outputs, $x = [x^d \; x^s]'$ represents the complete vector of internal states, with x^d the modelled deterministic part and x^s the stochastic part involving time-varying model parameters and/or disturbances. $w = [w^d \; w^s]'$ and v are Gaussian white noise zero mean and covariance matrices $Q(t)$ and R_k, respectively. t is the time variable and k corresponds to the iteration at time t_k. The algorithm is based on the steps of (Queinnec *et al.*, 1999):

- Prediction of the state and the output estimates at time $k+1$ by numerical integration of (1) between $t = t_k$ and $t = t_{k+1}$.
- Linearized approximation of f and h around the state estimate at time $k+1$, i.e., Jacobian matrices of system (1) :

$$F = \begin{bmatrix} \dfrac{\partial f}{\partial x^d} & \dfrac{\partial f}{\partial x^s} \\ 0 & 0 \end{bmatrix}, \quad H = \begin{bmatrix} \dfrac{\partial h}{\partial x^d} & \dfrac{\partial h}{\partial x^s} \end{bmatrix}$$

- Prediction of the positive semi-definite covariance matrix P at time $k+1$ by numerical integration of the filter differential Riccati equation.
- Determination of the observation gain, and readjustment of the state estimate and covariance matrix at time $k+1$.

The noise covariance matrices $Q(0)$ and R_0 as the initial value of Riccati matrix solution P_0 are tuning parameters to be chosen conveniently in order to avoid poor and biased estimates of the nonlinear system.

3. MODEL DESCRIPTION

The approach developed in this paper is based on the nonlinear model given in (Gómez-Quintero *et al.*, 2000) and is briefly presented in this section.

The ASM describes the elimination process of nitrogen and carbon by alternating aerobic and anoxic phases. It has been adapted to a specific wastewater treatment process by Julien *et al.* (Julien *et al.*, 1999).

Then, the following strategy for model reduction was applied: first, certains approximations were done by observing the time evolution of some of the ASM variables and their influence in process kinetics in order to reduce the number of differential equations; second, a grouping of some of the original parameters with those generated by the lattest simplifications where done, resulting in a reduction of the new model parameters. Among the whole set of parameters, some of them have kept their physical meaning while some others have to be identified.

The four dynamics described by this reduced nonlinear model are the concentrations of: readily biodegradable substrate S_S, nitrate S_{NO_3}, ammonia S_{NH_4} and dissolved oxygen S_{O_2}. These four state variables are considered as the most important for our case study. The reduced nonlinear model is given by the following set of equations :

$$\begin{aligned}
\dot{S}_S \;&= DS_{Sin} + D_c S_{Sc} - (D + D_c)S_S \\
&-\alpha_1 \frac{1}{Y_H} S_S \Big(\frac{S_{O_2}}{S_{O_2} + K_{O_2H}} + \frac{S_{NO_3}}{S_{NO_3} + K_{NO_3}} \frac{K_{O_2H}}{S_{O_2} + K_{O_2H}} \Big) \\
&+\alpha_4 \Big(\frac{S_{O_2}}{S_{O_2} + K_{O_2H}} + \eta_{NO_3h} \frac{S_{NO_3}}{S_{NO_3} + K_{NO_3}} \frac{K_{O_2H}}{S_{O_2} + K_{O_2H}} \Big) \\
\dot{S}_{NO_3} &= -(D + D_c)S_{NO_3} \\
&-\alpha_1 \frac{1 - Y_H}{2.86 Y_H} S_S \frac{S_{NO_3}}{S_{NO_3} + K_{NO_3}} \frac{K_{O_2H}}{S_{O_2} + K_{O_2H}} \\
&+\alpha_2 \frac{S_{NH_4}}{S_{NH_4} + K_{NH_4AUT}} \frac{S_{O_2}}{S_{O_2} + K_{O_2AUT}} \\
\dot{S}_{NH_4} &= DS_{NH_4in} - (D + D_c)S_{NH_4} \\
&-\alpha_1 i_{NBM} S_S \Big(\frac{S_{O_2}}{S_{O_2} + K_{O_2H}} + \frac{S_{NO_3}}{S_{NO_3} + K_{NO_3}} \frac{K_{O_2H}}{S_{O_2} + K_{O_2H}} \Big) \\
&-\alpha_2 \frac{S_{NH_4}}{S_{NH_4} + K_{NH_4AUT}} \frac{S_{O_2}}{S_{O_2} + K_{O_2AUT}} + \alpha_3 \\
\dot{S}_{O_2} \;&= -(D + D_c)S_{O_2} + k_L a (S_{O_2sat} - S_{O_2}) \\
&-\alpha_1 \frac{1 - Y_H}{Y_H} S_S \frac{S_{O_2}}{S_{O_2} + K_{O_2H}} \\
&-4.57 \alpha_2 \frac{S_{NH_4}}{S_{NH_4} + K_{NH_4AUT}} \frac{S_{O_2}}{S_{O_2} + K_{O_2AUT}}
\end{aligned} \tag{2}$$

where the terms $\alpha_{i,i=1,\ldots,4}$ are parameters specific to the reduced order model. D and D_c are the wastewater inflow and the carbonaceous matter flow respectively. Physical constants and yields values are those which had been identified for the ASM model (Julien *et al.*, 1999).

Remark 3.1. During aerobic phase, the dissolved oxygen concentration (S_{O_2}) is assumed to be high enough to avoid inhibition in biological growth reactions. Model dynamics are represented by a fourth-order equation system (2). Once the oxygen transfert rate is settled to zero ($k_La = 0$, no oxygen is supplied to the aeration tank) the dissolved oxygen remaining in the reactor is consumed by the biomass and S_{O_2} becomes equal to zero (this is the beginning of the anoxic phase). The fourth differential equation associated to oxygen dynamics becomes irrelevant and the terms related to S_{O_2} dissapear from the remaining equations in (2). Thus, the model is simplified and reduced to a third-order system. This mathematical fact should be taken into account for the filter design.

For identification purpose, we generally dispose of off-line measurements of dissolved oxygen, ammonia and nitrate concentrations. In this study, two sets of data have been used to test the filter.

The first one is composed of experimental data. Measurements of S_{NO_3}, S_{NH_4} and S_{O_2} have been obtained in a laboratory pilot plant, at a 20 min. sampling period during two periods of six hours. Parameters α_i may be determined by calculation from their mathematical expression and ASM parameters. They have also been identified on the first period of six hours, while the second period, obtained a few days latter has been kept for validation and filtering. The inflow rate has been increased by 75% of the initial value, at time t = 3 hours, for the second period. Calculated and identified parameters α_i are shown in Table 1 and the reduced-order model simulations are plotted on Figure 1. The reference model plotted in this figure is an adaptation of the ASM No.1 proposed by Julien *et al.* (Julien *et al.*, 1999). More details about the reduced-order model performances and parameter values can be found in (Gómez-Quintero *et al.*, 2000).

	pilot plant data		GPSX data
Parameter	Calculated Values	Identified Values	Identified Values
α_1 $(1/d)$	95.81	62.59	46.91
α_2 $(g/m^3/d)$	197.65	187.37	276.73
α_3 $(g/m^3/d)$	78.88	52.63	87.64
α_4 $(g/m^3/d)$	1516.1	987.2	1546.8

Table 1. Values of parameters α_i

The second set of data is provided by a numerical simulation of an ASP run on the GPSX software. Simulation settings correspond to a realistic plant configuration. Data from states S_{NO_3}, S_{NH_4} and S_{O_2} are used at a 20 min. sampling period, during 96 hours. Influent characteristics are changed every 24 hours. Operating conditions on the first 24 hours have been settled as the initial conditions for the reduced-order model. The identification of parameters $\alpha_{i,i=1,\ldots,4}$ has been done by using the first six-hours interval of numerical values. Results are also listed on Table 1.

For filtering purpose, we have only considered the dissolved oxygen and the nitrate concentration at a 20 min. sampling period as the available on-line measurements, which is coherent with the real measurements limitations of our pilot plant.

4. REDUCED MODEL FILTERING

Considering that our objective is a full-order observer design, the deterministic state vector to be estimated by the EKF has variables S_S, S_{NO_3}, S_{NH_4} and S_{O_2} as components. The choice of the stochastic states has been assisted by considering the results from a sensitivity study of the reduced-order model to parameters and influent characteristics. These additional states should help the model to match the real process under unexpected changes on operating conditions and/or disturbances.

In the one hand, model parameters inherited from the ASM No. 1 (e.g. Y_H, K_{NO_3}) are assumed to preserve standard values found in literature (Henze *et al.*, 1987). Parameters $\alpha_{i,i=1,\ldots,4}$ can be identified *a priori* or re-identified on-line from a set of measurements. Thus, they are not a priority to be added as stochastic states. On the other hand, the nonlinear model has shown to be very sensitive to changes performed on influent settings (i.e. variations on the influent biodegradable substrate concentration $S_{S_{in}}$ and ammonia concentration S_{NH_4in}). Any knowledge about these concentrations is currently not available on-line, they are even hardly measured at all. Ammonia input concentration is the most influential, so it is a good choice as stochastic state.

With this set of states (S_S, S_{NO_3}, S_{NH_4}, S_{O_2}, S_{NH_4in}) our attention is then addressed to the available on-line measurements to determine if the system meets the observability requirements for filtering design.

4.1 *State observability*

For nonlinear systems the notion of observability is reduced to test the local observability of the system. This theory is not reviewed here, a complete description can be found in (Soroush, 1997).

Attempting to match the realistic operating environment for this class of processes only measurements of nitrate (y_1) and dissolved oxygen (y_2) are considered. Under this assumption, the system with extended state vector (S_S, S_{NO_3}, S_{NH_4}, S_{O_2}, S_{NH_4in}) is locally observable. During the anoxic phase, it has been said that the nonlinear system becomes a third-order system as the dissolved oxygen concentration is zero. Although the unique system output is the nitrate concentration, the extended system with decreased state vector (S_S, S_{NO_3}, S_{NH_4}, S_{NH_4in}) still remains locally observable. So, an EKF can be designed.

4.2 *The two-alternated-filter implementation*

Let us remember that the dynamics of the ASP described by the nonlinear model (2) evolve through two periods, aerobic phase and anoxic phase, plus an intermediate phase between the stop of the aeration and the begining of the anoxic period. Both of aerobic and anoxic phases are periodically sequenced on the bioreactor to accomplish carbon and nitrogen removal.

During the aerobic phase, the dissolved oxygen is present on biomass reactions. S_{O_2} is not zero, our extended model is fifth degree. Tuning matrices for the EKF are of proper dimensions : P and Q are symetric nonsingular matrices of dimension five. Measurements of two variables are available (S_{NO_3}, S_{O_2}) so the output noise covariance matrix R has dimension two.

Once the alternance to the anoxic phase is done (k_La=0, there is no dissolved oxygen in the bioreactor), the oxygen dynamics equation is no more useful and the extended model becomes of fourth degree. Only nitrate concentration measurements are available during this period. This implies that our filter design is also modified. All design matrices become of the right dimensions by losing the row/column associated to the dissolved oxygen. Riccati's equation solution P is also adjusted in this manner.

Nevertheless, when the anoxic period is finished and a new aerobic phase happens, modifications on filtering scheme should be done to re-extend our system from the fourth degree to the fifth degree. Extension of covariances matrices R and Q is direct. A new Riccati's matrix solution P of dimension five is formed by all the terms of the reduced fourth-dimension matrix P and the row/column associated to the dissolved oxygen concentration is reinitialized with the corresponding P_0 values (P_0 is a diagonal matrix meaning that without *a priori* knowledge, no error covariances in state estimates are considered). Differents procedures to reinitialize these terms were tested but numerical simulations have shown more adequate results for the chosen option. This can be justified by the fact that considering no errors covariances related to the dissolved oxygen concentration is less compromising than assuming any value whatever (no knowlegde is available from the lattest anoxic phase), or better than assigning covariances values related to the previous aerobic period (lattest values correspond to the end of the aerobic phase when the whole system dynamics are quite different from those of the beginning).

4.3 *Observer stability*

Some comments have to be done relative to the stability of the two-alternated-observer structure developed in this paper. The observed system may be viewed as an hybrid system which switches between three successive states: aerobic phase, transient aerobic phase without aeration and anoxic phase.

The stability of such an hybrid system may be guaranteed through Lyapunov theory. In the present case, the Kalman filtering approach implicitely guarantees the exitence of a Lyapunov matrice common to both subsystems at the switching instant, and, then, the stability of the whole system.

4.4 *Simulation results*

Numerical simulations of the EKF have been done with the experimental set of data used for model validation and the simulated set of data described in the previous section. Initial values for diagonal tuning matrices R and Q were selected considering the expected errors between real process and operating conditions but were adjusted after repeated simulations until finding a satisfactory filter performance (good convergence speed and noise attenuation). The elements of the diagonal matrix P_0 have also been adjusted to represent the variances of initialization errors in the state estimates.

For the experimental data, the chosen tuning matrices are $Q = diag[0.05, 10^{-3}, 10^{-3}, 10^{-3}, 0.5]$, $R = diag[4.10^{-2}, 4.10^{-2}]$ and $P_0 = diag[2, 0.5, 10^{-2}, 0.5, 10]$. Results are illustrated on figure 2. The initial concentrations are assumed unknown. Adjusts made by the filter when a measurement is available can be easily observed on the figure. Dynamics of the continuous Riccati equation are fast which does not inhibit the filter's response speed. State estimates are satisfactory, in particular those for S_{NH_4} and S_{NH_4in}. Data of ammonia concentration is only used as a graphical reference to evaluate the filter performance. Inflow ammonia estimate agrees with experimental values (its measured value has been 62.8 $g.m^{-3}$). The estimate of the readily biodegradable substrate concentration varies between 9 - 16 $g.m^{-3}$ which corresponds to a reasonable fluctuation interval under these practical operating conditions. Simulations with different initial conditions were done. Specifically, a minimum of knowledge about nitrogen concentration values should be added to ensure a good state estimation.

Figure 3 shows the performance of the EKF for the second set of data (only one aerobic/anoxic cycle is shown). The diagonal tuning matrices for this case are $Q = diag[0.02, 10^{-4}, 10^{-4}, 10^{-4}, 0.05]$, $R =$

$diag[10^{-4},\ 10^{-4}]$ and $P_0 = diag[0.1, 10^{-3}, 10^{-3}, 10^{-3}, 0.1]$. Ammonia concentration is estimated succesfully along the whole simulation (here also, ammonia data are plotted only as graphical reference). The biodegradable substrate estimate also remains realistic for this second case. The influent ammonia estimate is adjusted on-line by the filter to compensate model mismatches with respect to the initial settings. The estimated values for this state variable may certainly correspond to realistic values of $S_{NH_4 in}$. In fact, they are not so far from those fixed by the simulation : 35, 17.5, 26.25 and 43.75 $g.m^{-3}$ from the first to the fourth day respectively. These differences can be explained by the effects of the numerous simplifications on ASM dynamics that cannot be entirely reconstituted by the nonlinear model.

5. CONCLUSION

A nonlinear estimation approach by extended Kalman filtering has been applied to a complex biochemical process, i.e. an activated sludge reduced model with alternating aerobic and anoxic phases.

This method has shown to be satisfactory to estimate the state variables when disturbances are included as additional stochastic states. Utility of these additional states is avoiding model mismatches under certain ranges of changes in operating conditions. It has been discussed the importance of a good choice of stochastic states on the basis of the most influential terms for the model and the knowledge of the most frequent experimental variations.

It is known that covariance matrices have to be well settled for good performance of the EKF. As no particular method is available, a suitable set of values has been obtained only by repeated simulations which may imply a considerable effort by the designer.

Initial states estimates should be partially known from process characteristics (not an exact knowledge is required but an approximated one) to improve algorithm's convergence speed. Off-line measurements can ensure the availability of some useful information for our case study.

Acknowledgements: The authors wish to thank the *Laboratoire d'Ingénierie des Procédés de l'Environnement (LIPE)* of INSA, Toulouse, France, for providing the experimental data and GPSX simulations.

6. REFERENCES

Aubrun, C., D. Theilliol, J. Harmand and J.P. Steyer (2001). Software sensor design for COD estimation in an anaerobic fluidized bed reactor. *Water Sci. and Tech.* **43**, 115–120.

Bastin, G. and D. Dochain (1990). *On-line Estimation and Adaptive Control of Bioreactors*. Elsevier Science Publishers B.V.. Amsterdam (Pays Bas).

Farza, M., H. Hammouri, C. Jallut and J. Lieto (1999). State observation of a nonlinear system : Application to (bio)chemical processes. *AiChE J.* **45**, 93–106.

Gauthier, J.P. and A.K. Kupka (1994). Observability and observers for nonlinear systems. *SIAM J. Control and Optim.* **32**, 975–994.

Gómez-Quintero, C., I. Queinnec and J.P. Babary (2000). A reduced nonlinear model of an activated sludge process. *Int. Symp. on Advanced Control of Chemical Processes* pp. 1037–1042.

Henze, M., C.P. Leslie Grady Jr, W. Gujer, G.v.R. Marais and T. Matsuo (1987). Activated sludge model No. 1. I.A.W.Q. Sci. and Tech. Report No.1. London, U.K.

Holmberg, A. (1982). Modelling of the activated sludge process for micro-processor-based state estimation and control. *Water Research* **16**, 1233–1246.

Jazwinski, A.H. (1970). *Stochastic processes and filtering theory*. New York: Academic Press.

Jeppson, U. (1995). A simplified control-oriented model of the activated sludge process. *Mathematical Modelling of Systems* **1**(1), 3–16.

Julien, S., P. Lessard and J.P. Babary (1999). A reduced-order model for control of a single reactor activated sludge process. *Math. and Comp. Mod. of Dyn. Syst.* **5**(3), 337–350.

Krener, A.J. and A. Isidori (1983). Linearization by output injection and nonlinear observers. *Systems & Control Letters* **3**, 47.

Lukasse, L.J.S., K.J. Keesman and G. van Straten (1999). A recursively identified model for short-term predictions of nh_4/no_3-concentrations in alternating activated sludge processes. *J. Proc. Control* **9**(1), 87–100.

Queinnec, I., D. Léonard and C. Ben-Youssef (1999). State observation for fedbatch control of phenol degradation by *ralstonia eutropha*. In: *Proc. European Control Conference*. Karlsruhe, Germany.

Soroush, M. (1997). Nonlinear state-observer design with application to reactors. *Chemical Engineering Science* **52**(3), 387–404.

Soroush, M. (1998). *Optimisation : theory and applications*. Wiley Eastern Limited. New Delhi (India).

Zeitz, M. (1987). The extended luenberger observer for nonlinear systems. *Systems & Control Letters* **9**, 149.

Zhao, H. and M. Kümmel (1995). State and parameter estimation for phosphorus removal in an alternating activated sludge process. *J. Proc. Control* **5**(5), 341–351.

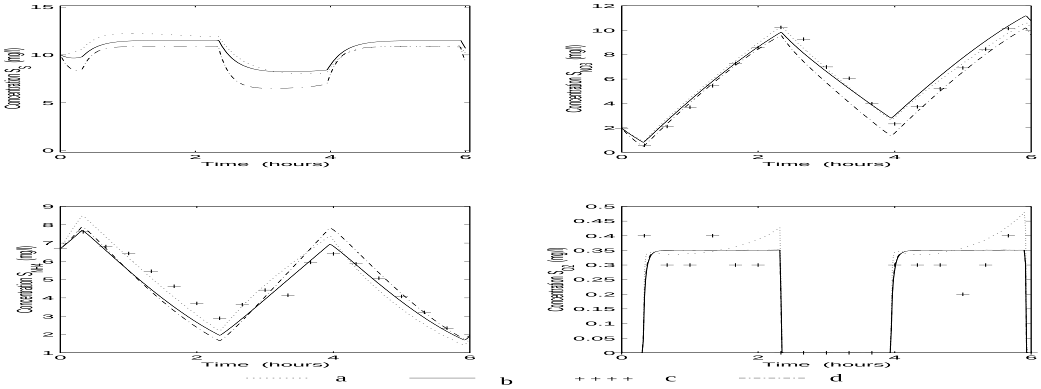

Fig. 1. Experiment 1. Model identification: reference model, **a**; reduced-order model with identified parameters, **b**; experimental data, **c**; reduced-order model with calculated parameters, **d**.

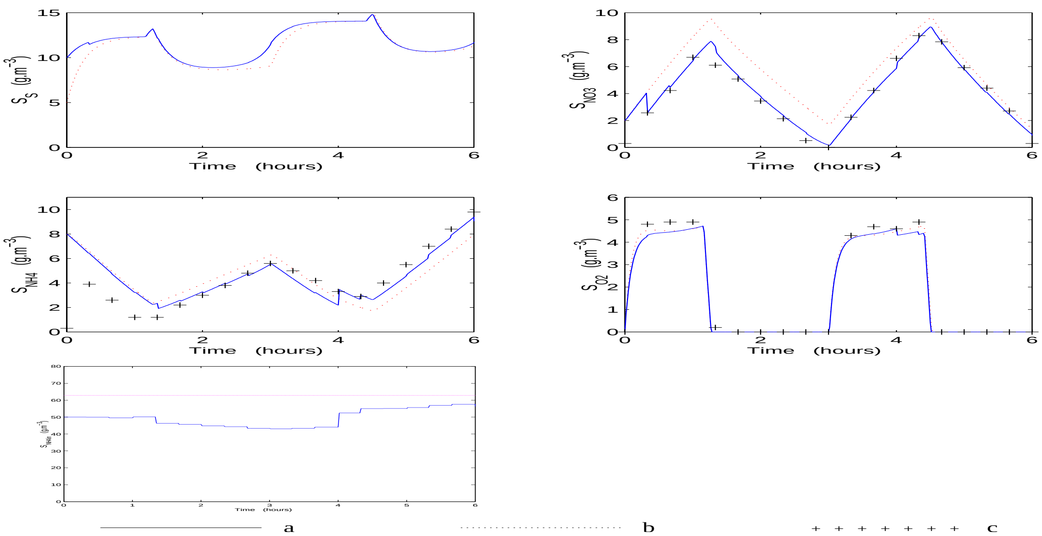

Fig. 2. Experiment 2. State estimation with EKF: estimates, **a**; nonlinear model, **b**; measurements, **c**.

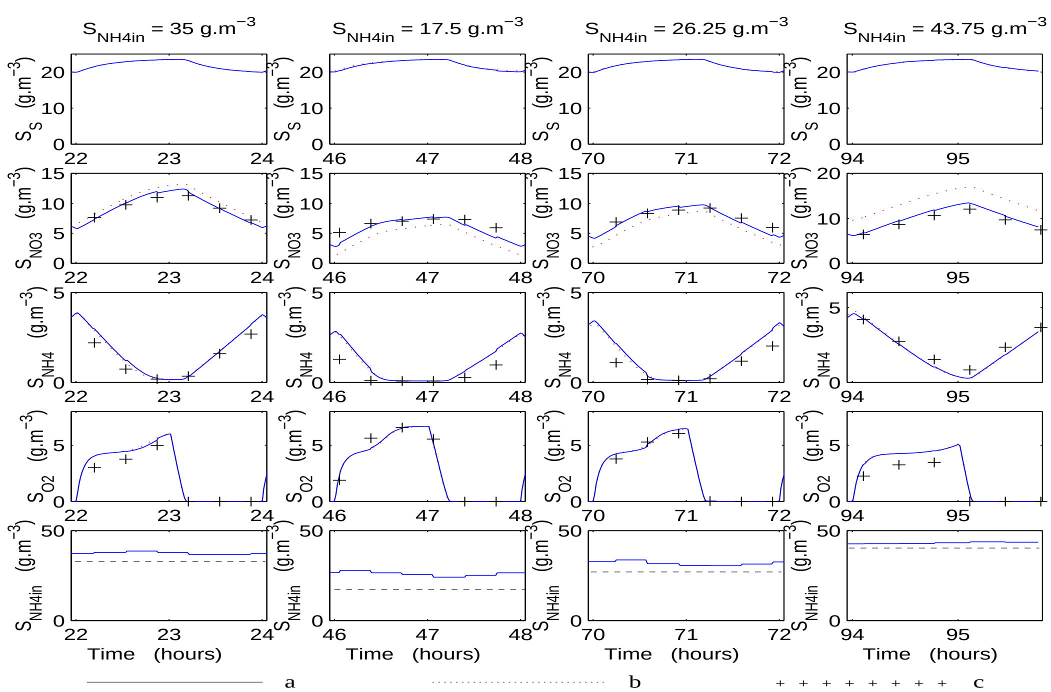

Fig. 3. GPSX data. State estimation with EKF: estimates, **a**; nonlinear model, **b**; measurements, **c**.