ASYMPTOTIC OBSERVERS AS A TOOL FOR MODELLING PROCESS DYNAMICS

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ABSTRACT

This paper deals with the dynamical modelling of processes with a special emphasis on wastewater treatment. Dynamical process modelling is usually derived from mass balance considerations and results in models which contain two types of terms representing the hydrodynamics and transport dynamics, and the conversion due to the involved (bio)chemical reactions involved, respectively. The conversion terms are indeed generally speaking the products of two terms : a yield coefficient and a reaction rate (strictly speaking, the kinetics). The latter usually concentrates a predominant part of the model uncertainty. The bioprocess model building exercise is usually global in the sense that it concerns all the terms involved in the model. In addition to the inherent bioprocess modelling difficulties (model complexity, data scarcity), this makes the interpretation of the model identification results difficult if not questionable. In this paper it is suggested how to use asymptotic observers to model and validate reaction schemes independently of the reaction kinetics. The results will be illustrated with two wastewater treatment processes : an activated sludge process and a detoxification reactor. © 1997 IAWQ. Published by Elsevier Science Ltd

INTRODUCTION

The dynamical modelling of wastewater treatment processes is characterized by two important features. First of all, the models are most often highly complex, they are usually high-order non linear systems incorporating a large number of state variables and parameters. For instance, the IAWQ activated sludge model n°1 (Henze et al, 1986) contains 13 state variables and 19 parameters. Secondly there is, generally, a lack of cheap and reliable sensors for (on-line) measurement of the key state variables, in particular those involved in the model. Despite considerable efforts, on-line sensor technology is still considered to be the weakest part in the real-time process control chain (Harremoës et al, 1993; Vanrolleghem and Verstraete, 1993). Both problems are common to all biotechnological processes, although particularly crucial in wastewater treatment, because of the inherent particularly complex nature of these processes, involving for instance many different microbial populations, and which, furthermore, are often difficult to measure reliably with the available instrumentation. Because of the model complexity and the scarcity of on-line sensors, the model building exercise, prior to any identification, is certainly a key question. Dynamical modelling of bioprocesses (including biological

wastewater treatment processes) is usually derived from mass balance considerations (e.g. Bastin and Dochain, 1990) and results in models containing two types of terms which represent the hydrodynamics and transport dynamics, and the conversion due to the (bio)chemical reactions involved, respectively. The conversion terms are indeed generally speaking the products of two terms : a yield coefficient and a reaction rate (rigourously, the kinetics). The latter usually concentrates a predominant part of the model uncertainty. The model building exercise in bioprocesses is usually global in the sense that it concerns all the terms involved in the model. In addition to the inherent bioprocess modelling difficulties (model complexity, data scarcity), this makes the interpretation of the model identification results difficult if not questionable.

In this paper an approach is suggested on how to use asymptotic observers to model and validate reaction schemes independently of the reaction kinetics. Section 2 will present the general dynamical model for stirred tank bioreactors. It will then be shown how the latter is used to derive the equations of the asymptotic observer, and what are its convergence properties. The final part of Section 2 will introduce the modelling concept and procedure based on the asymptotic observer. The results will be illustrated with two wastewater treatment processes: an activated sludge process (Section 3) and a detoxification reactor (Section 4).

GENERAL DYNAMICAL MODEL AND ASYMPTOTIC OBSERVERS

General Dynamical Model of Stirred Tank Bioreactors

A biotechnological process can be defined as a set of M biochemical reactions involving N components. The reactions most often encountered in bioprocesses are microbial growth (in which the biomass plays the role of an autocatalyst) and enzyme catalysed reactions (in which the biomass can be viewed as a simple catalyst); however many other reactions can also take place, like microorganism death, maintenance, ... These reactions can be formalized into reaction schemes, as it will be illustrated in Sections 3 and 4. The dynamical model of a bioprocess in a stirred tank reactor can be deduced from mass balance considerations and written in the following compact form :

$$\frac{d\xi}{dt} = -D\xi + K\rho + F - Q \tag{1}$$

where ξ is the vector of the bioprocess components $(\dim(\xi) = N)$, D is the dilution rate, K is the yield coefficient matrix $(\dim(K) = N \times M)$, ρ is the reaction rate vector $(\dim(\rho) = M)$, F is the feed rate vector and Q the gaseous outflow rate vector $(\dim(F) = \dim(Q) = N)$. The model (1) has been called the *General Dynamical Model* for stirred tank bioreactors (for further details, see Bastin and Dochain (1990)).

Note that the dynamics of a bioreactor is composed of two terms : $- D\xi + F - Q$ which represents the hydrodynamics and the transport dynamics, and $K\rho$ which represents the conversion. Each conversion term is indeed the product of a yield coefficient (which under ideal conditions may be related to stoichiometry via the matrix K) and of the kinetics (reaction rates) via the vector ρ. The latter term typically concentrates a large part of the model uncertainty. It is generally speaking a function of the process variables. Many kinetic models are proposed in the literature (e.g. Appendix 1 in Bastin and Dochain (1990)), none of them having a strong physical justification.

An essential aspect in the derivation of the general dynamical model of the bioprocess is its reaction network. The notion of reaction network is basically the one considered in chemistry and in chemical engineering, i.e. the schematic representation of the key process (bio)chemical reactions with their respective key reactants and key products. The derivation of the terms in the matrix K is straightforward from the process reaction scheme : indeed each entry k_{ij} of the yield coefficient matrix $K = [k_{ij}]$, i = 1 to N, j = 1 to M is representative of the ith component in the jth reaction : it is negative if the component is a reactant, positive if it is a product, and equal to zero if the component does not intervene in the reaction.

Asymptotic Observers for Stirred Tank Bioreactors

The design of asymptotic observers (Bastin and Dochain, 1990) is based on the (general) dynamical model of the process without the knowledge of the process kinetics ρ being necessary. The derivation of the asymptotic observer equations is based on the following assumptions :

1. M (the number of reactions) components are measured.
2. The feed rates F the gaseous outflow rates Q and the dilution rate D are known either by measurement or by user's choice.
3. The yield coefficient matrix K is known.
4. The reaction rate vector ρ is unknown.
5. The M reactions are irreversible and independent, i.e. rank(K) = R = M

From assumption 1, we can define the following state partition :

$$\xi = [\xi_1, \xi_2]^T \tag{2}$$

where ξ_1 and ξ_2 hold for the measured component concentrations and the unmeasured ones, respectively (with the yield coefficient matrix K_1 corresponding to ξ_1 being full rank). Let us consider the following state transformation :

$$Z = \xi_2 - K_2 K_1^{-1} \xi_1 \tag{3}$$

It follows that the dynamics of Z are independent of the reaction rate ρ :

$$\frac{dZ}{dt} = -DZ + F_2 - Q_2 - K_2 K_1^{-1}(F_1 - Q_1) \tag{4}$$

The equations (3)(4) are the basis for the derivation of the asymptotic observer. The dynamical equations of Z are used to calculate an estimate of Z, which is used, via equation (3) and the data of ξ_1, to derive an estimate of the unmeasured component ξ_2 :

$$\frac{d\hat{Z}}{dt} = -D\hat{Z} + F_2 - Q_2 - K_2 K_1^{-1}(F_1 - Q_1) \tag{5}$$

$$\hat{\xi}_2 = \hat{Z} + K_2 K_1^{-1} \xi_1 \tag{6}$$

The observer (5)(6) is completely independent of the process kinetics and can be implemented without the knowledge of the reaction rates $\rho(\xi)$ being required. The convergence properties can be summarized in the following asymptotically stable dynamical equation of the estimation error :

$$\frac{d(\xi_2 - \hat{\xi}_2)}{dt} = -D(\xi_2 - \hat{\xi}_2) \tag{7}$$

i.e. $(\xi_2 - \hat{\xi}_2)$ will converge asymptotically to zero if D is persistently exciting, i.e. if there exists positive constants δ and β such that $\beta = \int_t^{t+\delta} D(\tau)d\tau$: this simply requires that D is not equal to zero for too long. This condition is clearly easily fulfilled in fedbatch and continuous reactors.

Asymptotic observers

The basic idea of the approach is to use the asymptotic observer not for on-line estimation but for model building, more precisely for modelling the reaction network part of the dynamics *independently of the kinetics*. It is based on the convergence properties of the observer : because of these, we know that the asymptotic observer is able to give a reliable replica of the dynamics of the process components if the reaction scheme is correct (i.e. representative of the key process reactions) and if only the values of the yield coefficients are known (and not the reaction kinetics).

Assume one has a set of experimental data of the concentrations and (when appropriate) gaseous outflow rates of the key process components (whose number is equal to N) as well as of the hydrodynamics (mainly, the flow rates). The procedure is the following.

• Select a plausible reaction network involving the measured components.
• Build the dynamical model in the format of the General Dynamical Model.
• Select M (= number of a priori selected reactions) components and build the asymptotic observer to estimate the N-M remaining components.
• Try to fit the estimated values of the N-M components to their experimental values by selecting appropriate values of the yield coefficients.
• The final step is usual : either the fitting is satisfactory and we stop, or it is not and we go back to the first step (select another reaction scheme candidate, possibly with another set of process components).

ILLUSTRATIVE CASE STUDY # 1 : AN ACTIVATED SLUDGE PROCESS

The activated sludge process is usually operated in two sequential tanks (see Figure 1) : an aerator (in which the degradation of the pollutants S takes place) and a settler (which is used to recycle part of the biomass X to the aerator). The IAWQ model (Henze et al, 1986) proposes a comprehensive set of reactions. Yet a simple and often considered way to look at the aerator operation is to consider a simple microbial growth for carbon removal (see e.g. Marsili-Libelli (1984)).

$$S + C \rightarrow X \tag{8}$$

Mass balances applied to the concentrations of the substrate S, dissolved oxygen C and biomass X (in the aerator and in the settler) give the following set of dynamical equations :

$$\frac{dS}{dt} = -k_1 \mu X + \frac{F_{in}}{V} S_{in} - \frac{F_{in} + F_R}{V} S \tag{9}$$

$$\frac{dC}{dt} = -k_2 \mu X + k_L a(C_S - C) - \frac{F_{in} + F_R}{V} C \tag{10}$$

$$\frac{dX}{dt} = \mu X + \frac{F_R}{V} X_R - \frac{F_{in} + F_R}{V} X \tag{11}$$

$$\frac{dX_R}{dt} = -\frac{F_R + F_W}{V_S} X_R + \frac{F_{in} + F_R}{V_S} X \tag{12}$$

where X_R is the concentration of the recycled biomass (g/l), F_{in}, F_R and F_W are the influent, recycle and waste flow rates (l/h), respectively, and V and V_S the aerator and settler volumes (l). By defining :

$$D_{in} = \frac{F_{in}}{V}, \ D_2 = \frac{F_R}{V}, \ D_1 = D_{in} + D_2, \ D_3 = \frac{F_{in} + F_R}{V_S}, \ D_4 = \frac{F_R + F_W}{V_S} \tag{13}$$

the dynamical equations of the process ($N = 4$, $M = 1$) can be rewritten in the formalism of the general dynamical model (1) with the following definitions :

$$\xi = \begin{bmatrix} S \\ C \\ X \\ X_R \end{bmatrix}, \ K = \begin{bmatrix} -k_1 \\ -k_2 \\ 1 \\ 0 \end{bmatrix}, \ F = \begin{bmatrix} D_{in}S_{in} \\ k_La(C_S-C) \\ 0 \\ 0 \end{bmatrix}, \ D = \begin{bmatrix} D_1 & 0 & 0 & 0 \\ 0 & D_1 & 0 & 0 \\ 0 & 0 & D_1 & -D_2 \\ 0 & 0 & -D_3 & D_4 \end{bmatrix}, \ \rho = \mu X, \ Q = 0 \tag{14}$$

Note that since there is only one reaction, one measurement is enough to evaluate this reaction scheme. Note also that the assumption 2 considered above implies that the transfer coefficient k_La and the oxygen saturation concentration C_S are assumed to be known. If we consider the following state partition :

$$\xi_1 = C, \ \xi_2 = \begin{bmatrix} S \\ X \\ X_R \end{bmatrix} \tag{15}$$

the variables Z are defined as follows :

$$Z = \begin{bmatrix} Z_1 \\ Z_2 \\ Z_3 \end{bmatrix} = \begin{bmatrix} S - k_1 C/k_2 \\ X + C/k_2 \\ X_R \end{bmatrix} \tag{16}$$

and the asymptotic observer takes the following form :

$$\frac{dZ_1}{dt} = -D_1 Z_1 - \frac{k_1}{k_2} k_L a(C_S - C) + D_{in}S_{in} \tag{17}$$

$$\frac{dZ_2}{dt} = -D_1 Z_2 + k_2 k_L a(C_S - C) + D_2 Z_3 \tag{18}$$

$$\frac{dZ_3}{dt} = -D_4 Z_3 + D_3(Z_2 - k_2 C) \tag{19}$$

$$\hat{S} = Z_1 + \frac{k_1}{k_2} C \tag{20}$$

$$\hat{X} = Z_2 - \frac{1}{k_2} C \tag{21}$$
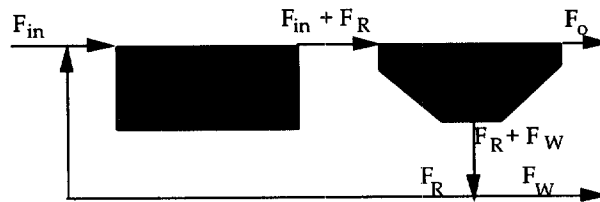
$$\hat{X}_R = Z_3 \tag{22}$$

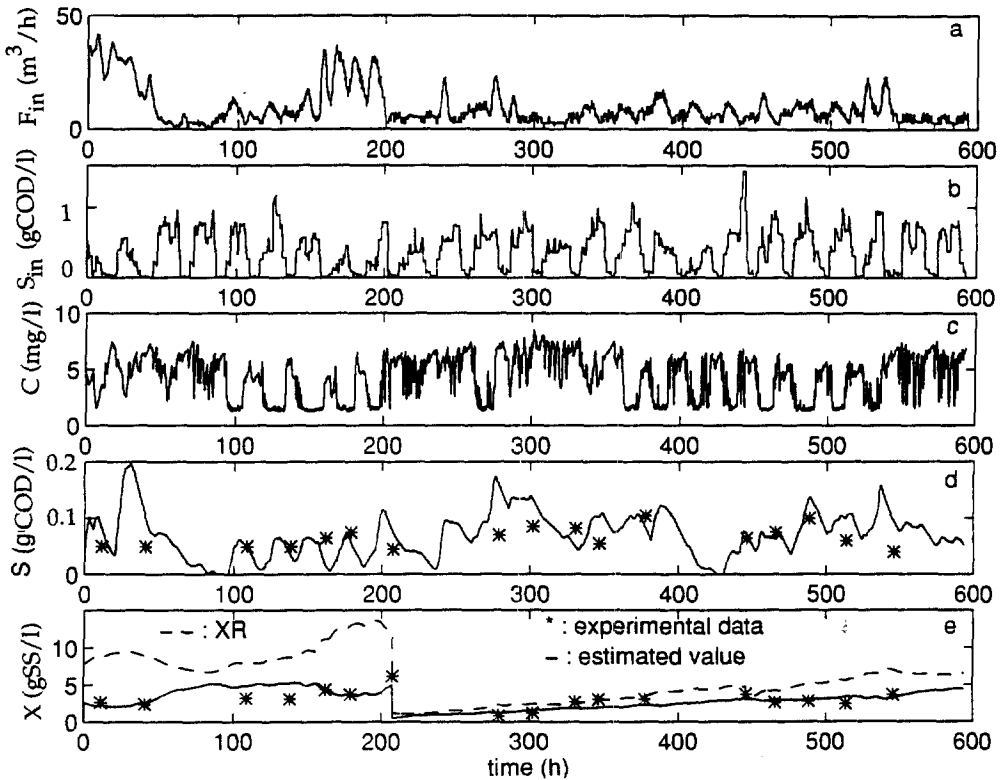**Figure 1.** Schematic view of an activated sludge process

Figure 2. Experimental data and estimation results of the activated sludge process
(Maria Middelares, Gent, Belgium)

Let us now use the above observer for modelling the reaction scheme. Let us consider a wastewater treatment plant where data of oxygen, COD and suspended solids are available. The considered data coming from the Maria Middelares treatment plant (Gent, Belgium) consist of : on-line data of dissolved oxygen and influent COD, some off-line measurements of the COD in the effluent and of the suspended solids in the aerator (yet no precise measurement of the recycle flow rate and only time points (t = 208 h and 449 h) when biomass discontinuous wastage is carried out). The question that we address is the following : can we validate a simple microbial growth reaction scheme for this plant from these data? This is a challenging problem if we consider the measurement constraints. Figure 2 shows the result of the reaction scheme modelling. Figures 2a, 2b and 2c show the data of the influent flow rate F_{in}, the influent substrate concentration S_{in} and the dissolved oxygen C, respectively, while Figures 2d and 2e compare the estimation results given by the asymptotic observer with the off-line data for S and X, respectively. The computed value of X_R is also shown (in dotted lines) in Figure 2d. The recycle flow rate F_R is kept constant at the design value of 8 m³/h. The volumes are : $V = 380$ m³, $V_S = 265$ m³; the determination of C_S and k_La gave the following result : $C_S = 10$ mg/l, $k_La =$ 1.7 h⁻¹. We note that although the reaction scheme is very simple and that some of the data are not very precise, the reaction scheme is fairly well validated. The values of the yield coefficients corresponding to the best fit are : $k_1 = 190$, $k_2 = 400$.

ILLUSTRATIVE CASE STUDY # 2 : A DETOXIFICATION PROCESS

Soil decontamination has become an important matter in wastewater treatment in recent years, resulting for instance in the increasing use and development of biological detoxification processes (Holliger et al, 1988). For instance, polychlorinated aliphatic compounds (Modesto Filho et al (1992), Boucquey et al (1995)), recalcitrant compounds, and halogenated aromatic compounds (Boyd and Shelton, 1984) may be treated by microbial mixed populations in strict anaerobic conditions. In this context, a packed bed reactor has been developed and successfully applied to the anaerobic destruction of a mixture of toxic and recalcitrant molecules (chlorinated aliphatics) on a laboratory scale (Modesto Filho et al (1992), Boucquey et al (1995)).
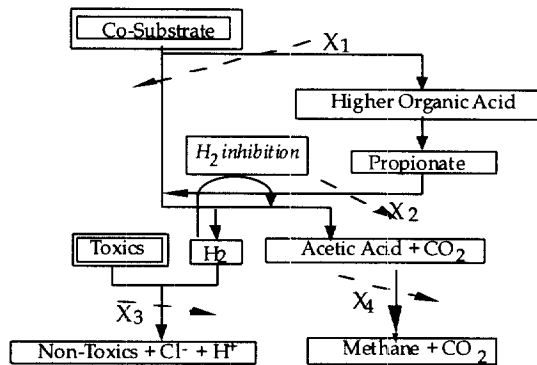

Figure 3. Scheme of the four-reaction model of the anaerobic digestion in a detoxification process

The anaerobic digestion is a complex biochemical network involving different microorganism populations and biochemical reactions. A four-reaction model is often considered to describe it (Mosey, 1983) (see Fig.3). Here again the constraints on the available data for modelling are quite hard : only off-line measurements of hydrogen, acetate, toxics and non-toxics at the reactor output, and of the co-substrate in the influent are available. A plausible reaction network is then :

$$S \rightarrow H_2 + VA_2 \tag{23}$$

$$H_2 + T \rightarrow N \tag{24}$$

where S, H_2, VA_2, T and N represent the co-substrate (ammonium citrate), the hydrogen, the acetate, the toxics and the non-toxics, respectively. Different sets of data corresponding to different experiments are available. Because of the high recirculation rate (usually 18 d^{-1}), the reactor is run under rather homogeneous conditions, and the transport time delay between the reactor input and its output is negligible with regard to the measurement frequency (the lowest measurement frequency is 3-4 days for the acetate). This validates the use of a stirred tank reactor model. Therefore the dynamics of the process in the General Dynamical Model formalism are as follows :

$$\xi = \begin{bmatrix} S \\ VA_2 \\ H_2 \\ T \\ N \end{bmatrix}, K = \begin{bmatrix} -1 & 0 \\ k_1 & 0 \\ k_2 & -k_3 \\ 0 & -k_4 \\ 0 & 1 \end{bmatrix}, F = \begin{bmatrix} DS_{in} \\ 0 \\ 0 \\ DT_{in} \\ DN_{in} \end{bmatrix}, \rho = \begin{bmatrix} \rho_1 \\ \rho_2 \end{bmatrix}, Q = 0 \tag{25}$$

Let us consider the state partition :

$$\xi_1 = \begin{bmatrix} S \\ H_2 \end{bmatrix}, \xi_2 = \begin{bmatrix} VA_2 \\ T \\ N \end{bmatrix} \tag{26}$$
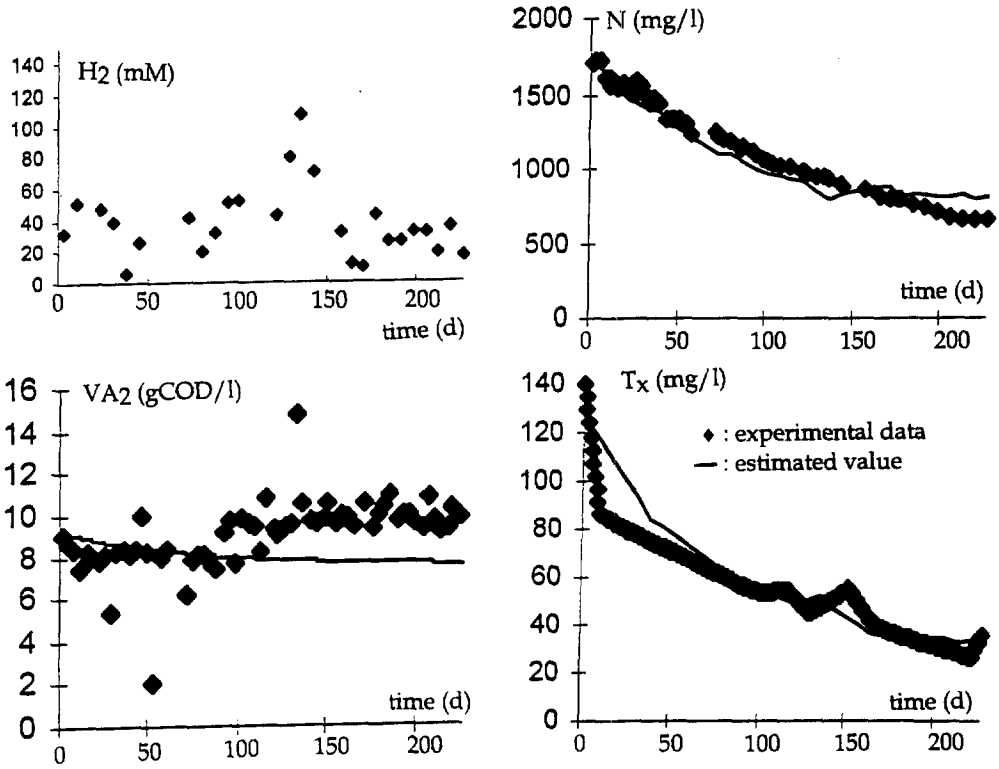

Figure 4. Experimental data and estimation results of the detoxication process
(Bioengineering unit, Louvain-la-Neuve, Belgium)

The asymptotic observer equations follow from the above model and (5)(6) :

$$\frac{d\hat{Z}_1}{dt} = -D\hat{Z}_1 - k_1 DS_{in} \tag{27}$$

$$\frac{d\hat{Z}_2}{dt} = -D\hat{Z}_2 - \frac{k_2 k_4}{k_3} DS_{in} + DT_{in} \tag{28}$$

$$\frac{d\hat{Z}_3}{dt} = -D\hat{Z}_3 + \frac{k_2}{k_3} DS_{in} + DN_{in} \tag{29}$$

$$VA_2 = \hat{Z}_1 + k_1 S \tag{30}$$

$$\hat{T} = \hat{Z}_2 + \frac{k_2 k_4}{k_3} S + \frac{k_4}{k_3} H_2 \tag{31}$$

$$\hat{N} = \hat{Z}_3 - \frac{k_2}{k_3} S - \frac{1}{k_3} H_2 \tag{32}$$

The asymptotic observer-based modelling has been applied on three sets of data with similar results. Since the co-substrate is not measured at the reactor output and COD estimation indicate its complete utilization, its value has been assumed in rough approximation to be negligible. Figure 4 shows one set of results for which $D = 0.014$ d^{-1}, $S_{in} = 0.3$ gCOD/l, $N_{in} = 457$ mg/l. Figure 4a gives the data of H_2 and Figures 4b, 4c and 4d compares the experimental data of VA_2, T and N with their estimates provided by the above asymptotic observer for the following values of the yield coefficients : $k_1 = 25$, $k_2 = 800$, $k_3 = 0.8$, $k_4 = 0.008$. Note here again the fairly good validation of the reaction scheme.

CONCLUSIONS

This paper has dealt with the modelling of reaction schemes of wastewater treatment processes independently of the knowledge of the kinetics. We have shown that the decoupling from the process kinetics is possible via the use of asymptotic observers. The methodology has been illustrated on two process examples (activated sludge process, detoxification process). A complementary aspect of the proposed modelling approach is the estimation of the reaction rates, which we did not consider here for lack of space but for which possible solutions can be found e.g. in Bastin and Dochain (1990, Chotteau (1995).

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