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Efficient Operation of Urban Wastewater Treatment Plants

Software sensors for state forecasting accompanied with fault residues information and confidence interval on outputs using raw sensor signals Deliverable D4.1

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WP4 is concerned with the design of software sensors, i.e. tools that allow to provide on-line values of key process components that are not accessible for on-line measurement. The developed software sensors are concerned with the on-line estimation of substrate and biomass concentrations from the on-line measurements of dissolved oxygen in presence of uncertainty in the kinetics. Due to the existence of two process types, resulting in two models (EM1 and EM2), two separate studies have been performed, each one concentrating on one specific process type.

1) EM1-based software sensors

The design of the first type of software sensors has been concentrating on the on-line estimation of biomass and substrate concentrations mainly in the context of the toxic compounds treatment plant described by model EM1 under the assumption (in line with the statistical analysis of the model parameters) of poor knowledge of the kinetics parameters of the biomass growth (Haldane model). The approach considered for the EOLI project is a combination of an asymptotic observer with an adaptive observer that provides both state and parameter on-line estimates.

As a matter of illustration, let us consider the EM1 model where the parameter uncertainty is assumed to be concentrated on the parameter μ_0 of the Haldane model. The available on-line measurements are the dissolved oxygen S_O and $S_{O,in}$, the inlet COD concentration $S_{C,in}$ and the inlet flow rate q_{in}.

Since the operation time is intrinsically limited, one major challenge in the software sensor design is to able to act on the convergence rate of the observer so that estimates of the unmeasured biomass and substrate can convergence fast enough to their true experimental values. Asymptotic observers are robust observers with respect to the lack of knowledge about the process kinetics but their convergence rate is fully dependent on the operating conditions (via the inlet flow rate). That's why an alternative is proposed in the EOLI project that combines an asymptotic observer with an adaptive observer. Let us concentrate here on the case where the priority is to obtain a fast estimate of the biomass concentration X.

For the asymptotic observer, we first define the following auxiliary variables :

$$z_1 = S_O + k_2 X$$
$$z_2 = S_O - \frac{k_2}{k_1} S_C$$

Their mass balance equations obtained from model EM1 are equal to :

$$\frac{dz_1}{dt} = \frac{b}{k_2} S_O - \frac{b}{k_2} z_1 + \frac{q_{in}}{V}(S_{O,in} - z_1) + k_L a(S_{Os} - S_O)$$
$$\frac{dz_2}{dt} = \frac{b}{k_2} S_O - \frac{b}{k_2} z_1 + \frac{q_{in}}{V}(S_{O,in} - \frac{k_2}{k_1} S_{C,in} - z_2) + k_L a(S_{Os} - S_O)$$

By inverting the definitions of z_1 and z_2, we obtain estimates from the measurement of the dissolved oxygen S_O and the values of z_1 and z_2 provided by the computation of the above equations :

$$X_e = \frac{z_1 - S_O}{k_2}$$
$$S_{C,e} = S_O - \frac{k_1}{k_2}(S_O - z_2)$$

where S_{Ce} and X_e hold for the estimates of SC and X provided by the asymptotic observer. These above 4 equations are the asymptotic observer of our EOLI observer.

The adaptive observer is based on the assumption that a mean value of μ_0 (denoted $\bar{\mu}_0$) is known. The adaptive observer will therefore provide an estimate of the deviation from this mean (possibly wrong)

value. The design of the observer is based on the mass balance equations of the biomass concentration X and of the dissolved oxygen concentration S_O:

$$\frac{d\hat{X}}{dt} = \bar{\mu}_0(S_{Ce})\hat{X} + \Delta\mu_0(S_{Ce})X_e - \frac{q_{in}}{V}X + C_1(S_O - \hat{S}_O)$$

$$\frac{d\hat{S}_O}{dt} = -k_2\bar{\mu}_0(S_{Ce})\hat{X} - k_2\Delta\mu_0(S_{Ce})X_e - b\hat{X} + \frac{q_{in}}{V}(S_{O,in} - S_O) + k_L a(S_{Os} - S_O) + C_2(S_O - \hat{S}_O)$$

$$\frac{d(\Delta\mu_0)}{dt} = C_3(S_O - \hat{S}_O)$$

In the above equations $\Delta\mu_0$ is the on-line estimate of the deviation of μ_0. Note the estimates of the asymptotic observer are used in the above adaptive observer; they play a key role in the stability analysis of the observer. C_1, C_2 and C_3 are the design parameters, in other words the knobs on which we can act to modify the convergence rate of the estimation of X. A careful mathematical stability analysis shows that they have to be selected as follows :

$$C_1 = -(\lambda_1 + \lambda_2 + \lambda_3) - \frac{q_{in}}{V} + \bar{\mu}_0(S_e)$$

$$C_2 = \frac{\lambda_1\lambda_2\lambda_3}{\bar{\mu}(S_e)X_e(b + k_2 q_{in}/V)}$$

$$C_3 = \frac{\lambda_1\lambda_2\lambda_3}{b + \bar{\mu}_0(S_e)}\left[(\lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_1\lambda_3) + C_2\left(\frac{q_{in}}{V} - \bar{\mu}_0(S_e)\right) - C_3 k_2\bar{\mu}(S_e)X_e\right]$$

In the above equations λ_1, λ_2 and λ_3 are the eigenvalues associated to the adaptive observer. They are indeed the true knobs for selecting the convergence rate. They have to be negative (to guarantee the stability of the adaptive observer). When referring to simple dynamics views, large values of the eigenvalues mean fast convergence. However other dynamical effects (like the zero dynamics) may interfere and deteriorate the convergence in presence of large eigenvalues. Moreover, the presence of noise on the measurement may also limit the values of the eigenvalues. The appropriate selection of the design parameters is therefore is a job that has to be performed carefully, in particular via exhaustive numerical simulations.

Alternative versions of the above EOLI observer can be deduced, e.g. by considering other parameter uncertainty assumptions or for the on-line estimation of the substrate concentration with convergence faster than with the asymptotic observer.

The EOLI observer have been tested in numerical simulation under various conditions. The figure here below illustrates the performance of the EOLI observer in typical operating conditions of the fedbatch process of Mexico. The intial values of the biomass concentration and of the substrate concentration have been set with 10% error with respect to their values. The eignevalues have been set to –5. Note that the adaptive observer is able to converge faster than the asymptotic observer.

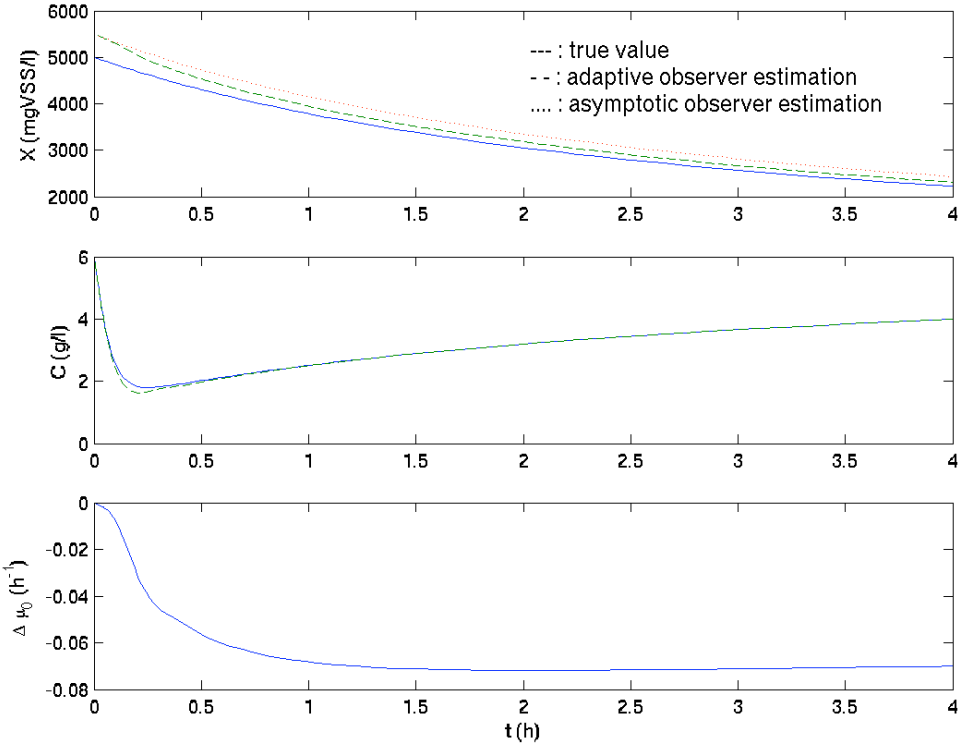


Figure 1. Adaptive observer for EM1

2) EM2-based software sensors

The second type of software sensors are based on the model EM2. Because both the carbon and nitrogen are treated, two specific phases are needed : aerobic (presence of oxygen) and anoxic (no oxygen but nitrite and nitrate). During the anoxic phase, the nitrite+nitrate from the last cycle are transformed into gaseous nitrogen. This step is realized by heterotrophic bacteria who also need soluble organic carbon to grow (Hu et al, 2003)(Jeppsson, 1996). When all the nitrite-nitrate has been removed, one can switch to aerobic mode where the ammonium nitrogen will be transformed into nitrite and nitrate while the remaining soluble carbon will be removed.

From now on, we only concentrate on what happens during the aerobic phase and the following notations are used :

X_1 : Heterotrophic microorganisms. (mg/l)

X_2 : Autotrophic microorganisms (mg/l)

S_1 : Organic carbon. (mg COD /l)

S_2 : Ammonium nitrogen. (mg N-NH4/l)

S_3 : Nitrates/Nitrites nitrogen (mg N-NO3/l+ mg N-NO2/l)

S_4: Dissolved oxygen (mg O2/l)

The reaction scheme of the aerobic phase is as follows :

$$\begin{array}{l} k_1 S_1 + k_4 S_4 \quad \square\square^{\mu_1}\square \quad X_1 \\ k_2 S_2 + k_5 S_4 \quad \square\square^{\mu_2}\square \quad X_2 + k_3 S_3 \end{array} \qquad (1)$$

This synthetic scheme means that S_1 and S_2 are degraded by X_1 and X_2 respectively with the rates μ_1 and μ_2 in the presence of S_4. In other words, the pollutant S_1 serves as a basis for the growth of X_1 while S_2 is transformed into S_3 by X_2.

Considering the above reaction scheme, we can apply the mass balance principle to determine the state space model of the aerobic phase (Bastin et al 1990):

$$\dot{X}_1 = \mu_1(S_1, S_4)X_1 \tag{2}$$

$$\dot{X}_2 = \mu_2(S_1, S_4)X_2 \tag{3}$$

$$\dot{S}_1 = -k_1\mu_1(S_1, S_4)X_1 \tag{4}$$

$$\dot{S}_2 = -k_2\mu_2(S_1, S_4)X_2 \tag{5}$$

$$\dot{S}_3 = k_3\mu_2(S_1, S_4)X_2 \tag{6}$$

$$\dot{S}_4 = -k_4\mu_1(S_1, S_4)X_1 - k_5\mu_2(S_1, S_4)X_2 + K_L a(S_4^{\max} - S_4) \tag{7}$$

with

$$\mu_1 = \mu_{1\max}\frac{S_1 - S_1^*}{K_{S1} + S_1 - S_1^*}S_4; \qquad \mu_2 = \mu_{2\max}\frac{S_2}{K_{S2} + S_2}S_4. \tag{8}$$

As can be seen, the specific growth rates in aerobic phase, μ_1 and μ_2, are proportional to the dissolved oxygen concentration, S_4, in the reactor instead of the classical expression $\frac{S_4}{K_O + S_4}$ proposed in (Henze *et al*., 1987). It is essentially because the available experiments were realized with a non-limiting oxygen concentration, S^* being the average of residual COD in the reactor (Mazouni *et al*., 2004).

It was shown in (Mazouni et al, 2004) that the model is very sensitive to the oxygen transfer coefficient K_La. This parameter is itself very sensitive to environmental conditions such as input air flow rate. When operating in real conditions, it is possible to classify the operating conditions into a finite number of classes depending on the input air flow rate. That way, a limited number of set of process parameters can be identified and, depending on the environmental conditions, the user can predict the future behavior of the process in using the specific model associated with the actual operating conditions. In other words, we use a multi-model approach : the process is not described by only one model but by *n* models, each of them being related to a given range of input air flow rates (a value of K_La).

For the parameter identification, the procedure used is the same than the one proposed in (Mazouni *et al*., 2004). Available experimental data correspond to 6 aerobic SBR cycles where the influent concentrations and the input air flow rate were changed as mentioned in Table 1. Four experiments were performed with an influent concentration of 50 l/min (namely the experiments realized on 27.10.03, 29.10.03, 31.10.03 and 04.11.03). The influent concentration for the experiment No. 06.11.03 is 75 l/min and for experiment No. 12.11.03 is 25 l/min. In the last column in Table 1, the values of oxygen mass transfer coefficients, K_La, that are calculated for each experiment are shown. As can be seen, three types (classes) of experiments could be distinguished, according the value of K_La. The first one consists of four experiments with $K_La=18.75$; the two others listed in the Table 1 consist of one experiment namely 06.11.03 and 12.11.03 with $K_La=23.00$ and $K_La=9.60$ respectively.

The experiments No. 27.10.03, 29.10.03, 31.10.03 are used for parameter identification of process model of the group with $K_La=18.75$. The experiment 04.11.03 is used for cross-validation of this model. The others two groups are presented with an unique experiment for each group. The experiments were carried out in winter periods of the year : three experiments in October, and three in November.

Table 1 Influent concentration and air flow rate for each experimental data used for identification

Exp. No	Air flow (l/min)	COD in (mg/l)	NTK in (mg/l)	K_La (h^{-1})
27.10.03	50	4318.18	168.00	18.75
29.10.03	50	4772.25	183.68	18.75
31.10.03	50	4476.92	204.40	18.75
04.11.03	50	4836.85	319.20	18.75
06.11.03	75	4235.45	260.4	23.00
12.11.03	25	4945.61	285.60	9.60

Remember that the aerobic model consists of six variables and nine parameters. The parameters m_{max1} and m_{max2} are the maximum specific growth rates of X_1 and X_2 (Heterotrophic and Autotrophic microorganisms respectively); K_{s1} and K_{s2} are saturation constants associated with substrates S_1 and S_2 respectively; k_1, k_2 and k_3 are the yield coefficients for degradation of S_1 by X_1 and S_2 by X_2; and for the production of S_3 by X_2 respectively. The coefficients k_4 and k_5 are oxygen yield coefficients associated with X_1 and X_2 respectively while S_4^{max} is the maximal value of dissolved oxygen in the liquid medium.

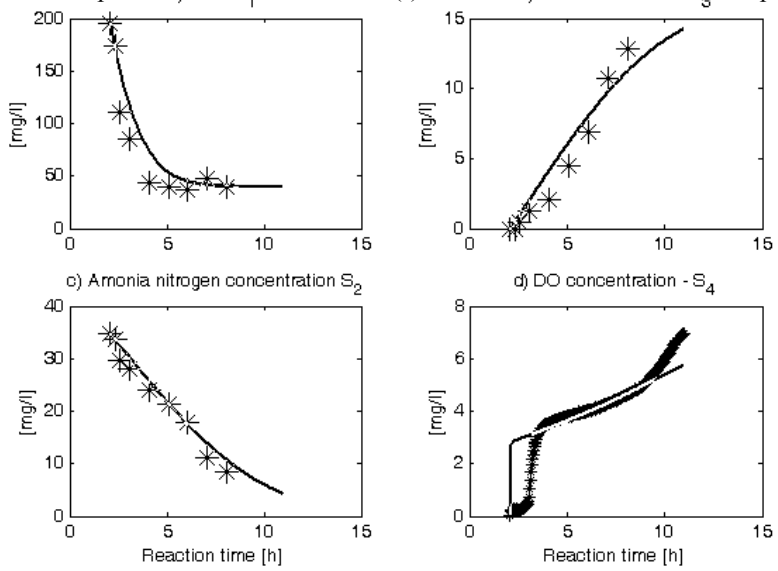
An optimization algorithm that was proposed in (Mazouni *et al*., 2004) is applied for model parameter estimation. The optimization criterion is chosen to obtain the minimal error between experimental data and simulated outputs of the system (2)-(8). The results of parameter estimation are shown in Table 2. As can be seen, different sets of parameter values are obtained for each class of experiments depending on the value of K_La. Model parameter values of the group with $K_La=18.75$ are obtained as medium values of three experiments and cross-validated with the data of the fourth one. The model parameters are shown in the Table 2.

Table 2 Estimated parameters for aerobic model

Exp. N	μ_{1max}	μ_{2max}	K_{S1}	K_{S2}	k_1	k_2	k_3	k_4	k_5
27.10.03	0.014	0.023	192.7	93.3	5.81	0.55	0.25	0.35	8.96
29.10.03	0.023	0.016	107.9	91.8	1.99	0.76	0.32	2.43	7.25
31.10.03	0.031	0.013	112.3	101.7	2.34	0.71	0.27	2.43	7.33
model	0.023	0.017	137.6	95.6	3.38	0.67	0.28	1.74	7.85
06.11.03	0.027	0.012	109.2	111.9	2.63	0.64	0.30	1.99	6.99
12.11.03	0.031	0.013	98.2	101.3	4.67	0.90	0.28	1.40	6.02

In Figures 3 (a,b,c and d), the model for experiments with $K_La=18.75$ is cross-validated with data from the experiment No. 04.11.03 (not listed in Table 2). The model parameters are obtained as medium values of parameters of the other experiments of the same group that are used for model identification.

Fig.4. Model parameter cross-validation. (-)model and (*) experimen



Hereabove we have derived three models for three different values of input air flow rates. The model parameters have been estimated. It should be noticed that these models could be used to derive observers of diverse classes. However, biological processes exhibit uncertain behaviours and our objective is to design a system able to monitor S_1 and S_3 from the on-line measurements of S_2 and S_4 – independently of the reaction kinetics - which, with no doubt, are the terms that are the most affected by uncertainty.

Introducing the auxiliary variables :

$$\begin{cases} Z_1 = S_2 + \dfrac{k_2}{k_3} S_3 \\ Z_2 = S_4 - \dfrac{k_4}{k_1} S_1 + \dfrac{k_5}{k_3} S_2 \end{cases} \tag{10}$$

allows us to consider the following dynamical sub-model :

$$\begin{cases} \dfrac{dZ_1}{dt} = 0 \\ \dfrac{dZ_2}{dt} = K_L a (S_4^{\max} - S_4) \end{cases} \tag{11}$$

Assuming that S_2 and S_4 are measured on-line and that $Z_1(0)= Z_{10}$ and $Z_2(0)= Z_{20}$ are known, the system (10)-(11) can be used to get an on-line estimation of S_1 and S_3 as :

$$\begin{cases} \hat{S}_1 = \dfrac{k_5 k_1}{k_2 k_4}(Z_1 - S_2) - \dfrac{k_1}{k_4}(Z_2 - S_4) \\ \hat{S}_3 = \dfrac{k_3}{k_2}(Z_1 - S_2) \end{cases} \tag{12}$$

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