ITSE OBSERVERS FOR BATCH PROCESSES. A WASTEWATER TREATMENT CASE STUDY

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Abstract: This paper deals with the design of observers for batch processes and the tuning of the observer gains with the objective to guarantee fast convergence of the state estimates. The approach followed in the present proposes to use an ITSE (Integral of the Time-weighted Square Error) criterion. The approach is illustrated on a batch process used in wastewater treatment, sequencing batch reactor (SBR).

Keywords: State observer, batch process, ITSE

1. INTRODUCTION

A key question in process control is how to monitor reactant and product concentrations in a reliable and cost effective manner. However, it appears that, in many practical applications, only some of the concentrations of the components involved and critical for quality control are available for on-line measurement. For instance, dissolved oxygen concentration in bioreactors, temperature in non-isothermal reactors and gaseous flow rates are available for on-line measurement while the values of the concentrations of products, reactants and/or biomass are often available via off-line analysis. An interesting alternative which circumvents and exploits the use of a model in conjunction with a limited set of measurements is the use of state observers. The design and application of state observers in (bio)processes has been an active area over the past decades (Doyle, 1997; Dochain, 2003a).

The design and application of state observers and parameter estimators to batch processes poses specific challenging questions, typically related to the time limitation of the batch operation. The question has been largely discussed in (Agrawal and Bonvin, 1989). It is obviously closely related to the control of the process, which is basically a finite-time optimal control problem, as it is nicely explained in (Bonvin *et al*., 2001).

One specific challenge of state observation and parameter estimation in batch processes is to design algorithms that are able to provide reliable estimates very quickly after the beginning of the batch. The problem is that so far the performance of parameter and state estimators are basically analyzed on the basis of the asymptotic behaviour of the related algorithms.

Bonvin and his coworkers (Agrawal and Bonvin, 1989; Agrawal and Bonvin, 1991; DeVallière and Bonvin, 1990) have identified several factors for the limitation of the extended Kalman filter when it is used to estimate both state variables and process parameters. These factors that are closely related to the inherent linearization of the estimator, are the following ones :

1) the bad knowledge about the key reaction parameters (these must be usually estimated, often with poor initial guesses);
2) the large variations of the operating conditions (particularly in batch);
3) the inaccuracy of the initial estimates of the state variables;
4) the imprecise measurement of the amounts of added agents;

5) the sensitivity of the reaction systems to trace certain species (e.g. impurities in polymerisation reactions)

These works suggest that, beyond the proposed improvements, there is a room to develop new tools for the design and analysis of state observers that are better appropriate to the specific features of batch processes. So far the scientific literature seems to very silent to what is often mentioned as a key question in process control today.

An appealing approach, developed in particular in (Bonné and Jorgensen, 2001) and (Bonvin *et al.*, 2001), is the batch to batch improvement of the estimation and control algorithms. In (Bonné and Jorgensen, 2001), the emphasis is put on a model-based iterative learning control. In this approach, Model Predictive Control (MPC) is applied for trajectory tracking on the basis of a dynamical model of the batch process obtained by identification of Finite Impulse response (FIR) models or of AutoRegressive models with eXogenous inputs (ARX). Regularization is used in order to reduce the large dimensionality of the identification. In order to limit the negative effect of regularization (biased estimates), regularization weights are considered. A survey on optimal control in a large sense (the authors prefer the words "dynamic optimization") in batch processes is presented in (Bonvin *et al*., 2001). The batch-to-batch improvement is presented in the context of measurement-based optimization (MBO). MBO can include in particular parameter and state estimation as well as model refinement. Typically, when state and parameter is considered, one of the techniques described before is used. Improvement of the performance of the estimation of state variables and parameter can be obtained by considering for instance the recommendations given by (Agrawal and Bonvin, 1989) and (DeVallière and Bonvin, 1990) and summarized here above.

Beside the batch-to-batch improvement idea, new avenues should be traced in the design of state and parameter estimators. One of the main problem of the design of the presently available techniques is that it is based on *asymptotic* properties of the algorithms. In other words, the key issue usually addressed in the design of state observers and parameter estimators is to guarantee that for a time sufficiently large (tending to infinity!), the estimates will converge to the true values or within a bounded area close to these. But this approach is obviously inappropriate in the context of batch and semi-batch processes where one cannot wait very long before obtaining reliable estimates. The need to have rapidly reliable estimates is a crucial issue in batch and semi-batch operation. One possible suggestion would be to use, in the selection of the design parameters, criteria like the ITSE (Integral of the Time-weighted Square Error) criterion or other criteria that penalize remaining errors after a defined period of time. Such an approach has been followed in the present work. We have considered as a case study the model of sequencing batch reactors (SBR's) used in wastewater treatment, that are in particular under study in the framework the EOLI EC project.

The paper is organized as follows. The next section will introduce the model of the SBR under study. Then the observer equations and the ITSE observer parameter calibration procedure are introduced. Finally the ITSE observer performance are illustrated via simulation results.

2. PROCESS DESCRIPTION

The aerobic treatment of domestic and industrial wastewaters by activated sludge is a common process, but the characteristics of many industrial discharges often cause operational problems in continuous flow systems. Therefore, discontinuous processes, as sequencing batch reactors (SBR's), will be considered in this project because, in terms of investment and operation costs, process stability, and operation reliability, they are better than the conventional continuous activated sludge process. In dairy plants, SBR could be applied to raw wastewater with low organic load and intermittent production of wastewater or as post treatment after an anaerobic process when the organic load is high. When the flow rate of wastewater is continuous it is possible to use more than one SBR or a variation of SBR with continuous inflow of wastewater and intermittent outflow. Different carbon/nitrogen ratio and different type of carbon to be removed are obtained in each case. SBR is a promising system to treat these effluents. It is cheaper than other aerobic systems, it allows carbon removal and denitrification in the same reactor, and also phosphorus removal. A typical SBR process cycle with aerobic and anoxic phases to achieve nitrification and denitrification is composed by filling, mixing-aeration, sedimentation, draining and idle phases. In the following SBR model, we concentrate on the two successive batch steps : the anoxic phase followed by the aerobic phase. The model refers explicitly to these two phases. For the present process, one denitrification step and one step nitrification are considered in the anoxic and aerobic phases, respectively. Therefore the reaction scheme considered here is the following.

Anoxic phase

Denitrification : $S_C + S_{NO} \rightarrow X_h + N_2$
Ammonification : $S_N \rightarrow S_{NH}$

Aerobic phase

Nitrification : $S_O + S_{NH} \rightarrow X_a + S_{NO}$
C-removal : $S_C + S_O \rightarrow X_h$
Ammonification : $S_N \rightarrow S_{NH}$

The dynamics of the process are given by the following mass balance equations.

Anoxic phase

$$\frac{dX_h}{dt} = \mu_{hN} X_h \tag{1}$$

$$\frac{dS_C}{dt} = -k_1\,\mu_{hN}\,X_h \tag{2}$$

$$\frac{dS_{NO}}{dt} = -k_2\,\mu_{hN}\,X_h \tag{3}$$

$$\frac{dS_{NH}}{dt} = k_3\,r_N \tag{4}$$

$$\frac{dS_N}{dt} = -r_N \tag{5}$$

Aerobic phase

$$\frac{dX_h}{dt} = \mu_h\,X_h \tag{6}$$

$$\frac{dX_a}{dt} = \mu_a\,X_a \tag{7}$$

$$\frac{dS_C}{dt} = -k_4\,\mu_h\,X_h \tag{8}$$

$$\frac{dS_O}{dt} = -k_5\,\mu_h\;X_h - k_6\,\mu_a\,X_a + k_L\,a\,(S_{O\max} - S_O) \tag{9}$$

$$\frac{dS_{NO}}{dt} = k_7\,\mu_a\,X_a \tag{10}$$

$$\frac{dS_{NH}}{dt} = k_3\,r_N - k_8\;\mu_a\,X_a \tag{11}$$

$$\frac{dS_N}{dt} = -r_N \tag{12}$$

Where S_c, S_{NH}, S_{NO}, S_N, S_O, X_h and X_a are the biodegradable substrate concentration (carbon, mgCOD/L), the ammonia nitrogen concentration (mgN/L), the nitrate and nitrite concentration (mgN/L), the soluble organic nitrogen (mgN/L), the concentration of the dissolved oxygen (DO) in the water (mg/L) and the concentration of the digester biomasses (heterotrophs and autotrophs)(mgVSS/L), respectively.

And $k_1 = \frac{1}{Y_{hN}}$; $k_2 = \frac{1-Y_{HN}}{2.86\,Y_{HN}}$; $k_4 = \frac{1}{Y_h}$;
$k_5 = \frac{1-Y_h}{Y_h}$; $k_6 = \frac{\beta_1}{Y_a}$; $k_7 = \frac{\beta_2}{Y_a}$; $k_8 = \frac{1}{Y_a}$

With their values identified in the framework of the EC EOLI project (Betancur et al, 2003) and the following kinetic expressions:

$$\mu_{hN} = \mu_{hN\max}\;\frac{S_C - S_{C\min}}{K_{C1} + S_C - S_{C\min}}\;\frac{S_{NO}}{K_{NO} + S_{NO}} \tag{13}$$

$$r_N = \mu_0\,(S_N - S_{N\min}) \tag{14}$$

$$\mu_h = \mu_{h\max}\;\frac{S_C - S_{C\min}}{K_{Ch} + S_C - S_{C\min}}\;\frac{S_O}{K_{Oh} + S_O} \tag{15}$$

$$\mu_a = \mu_{a\max}\;\frac{S_{NH}}{K_{NHa} + S_{NH}}\;\frac{S_O}{K_{Oa} + S_O} \tag{16}$$

3. ITSE OBSERVER

If we consider the following state space model of order n:

$$\frac{dx}{dt} = f\,(x,u) \tag{17}$$

where the measured variables y are related to the state variables x and the inputs u by:

$$y = h(x,u) \tag{18}$$

the general structure of a state observer can be written as:

$$\frac{d\hat{x}}{dt} = f\,(\hat{x},u) + K(\hat{x})\,(y - \hat{y}) \tag{19}$$

where $\hat{x}$ and $\hat{y}$ are the on-line estimates of x and y given by:

$$\hat{y} = h(\hat{x}) \tag{20}$$

with $K(\hat{x})$ the observer gain.

It is well known that the design of classical observers consists of choosing an appropriate gain, $K(\hat{x})$, such that the error dynamics has some desired properties (Dochain, 2003a). In the case of the extended Luenberger observer (ELO), the objective is to select $K(\hat{x})$ such that the linearised error dynamics around the process dynamics observation error e ($e = x - \hat{x}$) is asymptotically stable.

On the other hand the problem of choosing the appropriate gain $K(\hat{x})$ for ITSE observers becomes an optimisation problem. It consists on finding $K(\hat{x})$ that minimizes the following objective function J:

$$J = \int_0^T t\,e^2(t)\,dt \tag{21}$$

With T being an appropriate window of time. In this way the design of the observer includes minimization of the observation error together with better convergence rates.

3.1 Simulation Results

First of all the ITSE observer was tested for a simple CSTR process with Monod kinetics (Dochain, 2003b).

The model dynamics is described by the following equations:

$$\frac{dS}{dt} = -k_1\,\mu\,X + D\,S_{in} - DS \tag{22}$$

$$\frac{dX}{dt} = \mu\,X - D\,X \tag{23}$$

With k_1, μ, D and S_{in} being the yield coefficient, the specific growth rate (h^{-1}), the dilution rate (h^{-1}) and the influent substrate concentration (gL^{-1}) respectively.

$\mu = \frac{\mu_{max} S}{K_S + S}$ being a Monod kinetics with μ_{max} the maximum specific growth rate (h^{-1}) and K_S the saturation constant (gL^{-1}).

The observer equations become:

$$\frac{d\hat{S}}{dt} = -k_1 \mu_{max} \frac{\hat{S}}{K_S + \hat{S}} \hat{X} + D S_{in} - D\hat{S} + K_1 (S - \hat{S}) \quad (24)$$

$$\frac{d\hat{X}}{dt} = \mu_{max} \frac{\hat{S}}{K_S + \hat{S}} \hat{X} - D\hat{X} + K_2 (S - \hat{S}) \quad (25)$$

Considering the value of the parameters included in (Dochain 2003a) and the following initial values X(0)=1 (gL^{-1}), $\hat{X}(0)$= 5 (gL^{-1}), S(0)=30 (gL^{-1}) and $\hat{S}(0)$=50 (gL^{-1}) the ITSE observer performance can be seen in Figure 1

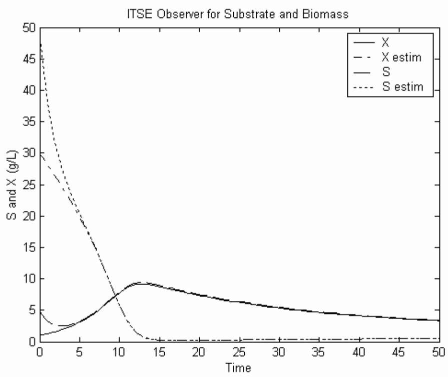


Fig 1. ITSE observer for biomass (X) and substrate (S) concentrations for a simple CSTR process

The ITSE performance was then compared with an ELO observer with gains K_1 and K_2 selected as indicated in (Dochain, 2003b) with $\lambda_1 = \lambda_2 = -0.1$ being the selected poles of the error dynamics (see Figure 2).

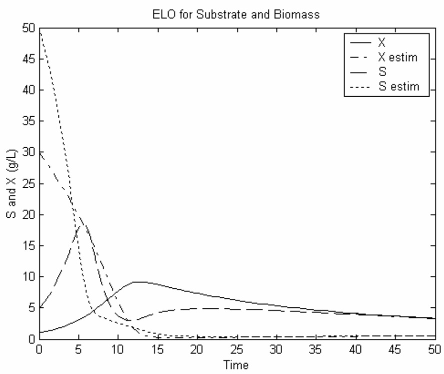


Fig. 2. Extended Luenberger Observer for biomass (X) and substrate (S) concentrations for a simple CSTR process

It can be noticed that the ITSE observer performs better than ELO with very good convergence properties.

4. APPLICATION TO THE WASTEWATER TREATMENT PROCESS

In order to illustrate the performance of the ITSE observer in the SBR with perturbed initial conditions, we first proceed with the anoxic phase.

4.1 *ITSE Observer for the Anoxic Phase*

In a first step and taking into account that the system of equations (1)-(2)-(3) is not observable with only one measurement (S_{NO}) (the observability matrix constructed from the Jacobian of system (1)-(2)-(3) is of rank 2), we started by developing an asymptotic observer for S_c as follows :

Let $$Z = \frac{-k_2}{k_1} S_C + S_{NO} \quad (26)$$

Then the asymptotic observer which is independent from the specific kinetics is written as follows :

$$\frac{d\hat{Z}}{dt} = 0 \quad \text{and} \quad \hat{S}_C = \frac{-k_1}{k_2}(\hat{Z} - S_{NO}) \quad (27)$$

Then, by considering the already determined $\hat{S}_C$ in a second step, we developed the following observer :

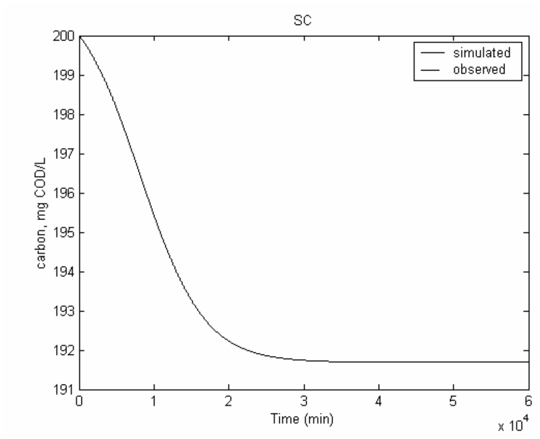
$$\frac{d\hat{X}_h}{dt} = \hat{\mu}_{hN} \hat{X}_h + K_1 (\hat{S}_{NO} - S_{NO}) \quad (28)$$

$$\frac{d\hat{S}_{NO}}{dt} = -k_2 \hat{\mu}_{hN} \hat{X}_h + K_2 (\hat{S}_{NO} - S_{NO}) \quad (29)$$

with

$$\hat{\mu}_{hN} = \mu_{hN\max} \frac{\hat{S}_C - S_{C\min}}{K_{C1} + \hat{S}_C - S_{C\min}} \frac{\hat{S}_{NO}}{K_{NO} + \hat{S}_{NO}} \quad (30)$$

Considering the parameter values of the EOLI project (Betancur et al, 2003) and the following initial values: $X_h(0)$=1; $\hat{X}_h(0)$= 1.2; $S_C(0)$= $S_C(0)$= 200 (carbon, mg COD/L); $S_{NO}(0)$= $\hat{S}_{NO}(0)$ =0.5 (mg N/L) which correspond to a 20% error in the initial observed value of X_h . The ITSE observer performs as shown in Figure 3.



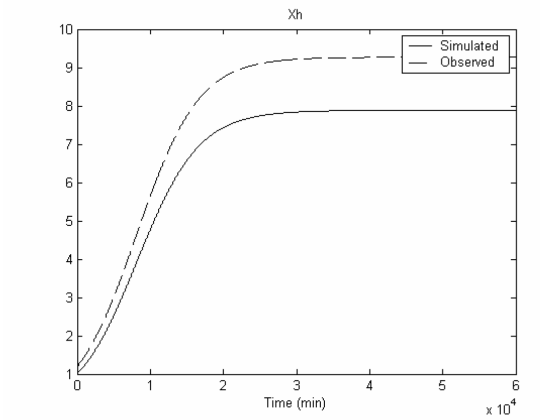


Fig. 3. ITSE Observer for S_c and X_h during the anoxic phase of the wastewater treatment process with a 20% error in the initial condition of X_h

As it can be seen in Figure 3, the ITSE is biased for X_h observation. In fact it happens that X_h can be poorly observed from S_{NO} measurements. The observability test shows that the observability matrix constructed from the Jacobian of system equations (1) and (3) is of rank 2 if and only if $\mu_{hN} >> 0$ which is not at all the case. This is also the reason why the equivalent ELO performs in a very unstable way. It can be proved that the gain K_1 of the ELO has μ_{hN} in a denominator.

4.*2 ITSE Observer for the Anoxic and AerobicPhase*

In a first step we begun by developing an asymptotic observer for X_a as follows :

Let $$Z = k_7 X_a - S_{NO} \qquad (31)$$

Then the asymptotic observer which is independent from the specific kinetics is written as follows :

$$\frac{d\hat{Z}}{dt} = 0 \quad \text{and} \quad \hat{X}_a = \frac{1}{k_7}(\hat{Z} + S_{NO}) \qquad (32)$$

By considering the estimated value of $\hat{X}_a$ given by the asymptotic observer, the observer for the other state variables considering that S_O, S_{NO} and S_{NH} are measured variables is given by the following set of equations :

$$\frac{d\hat{S}_N}{dt} = -\hat{r}_N + K_1(\hat{S}_{NH} - S_{NH}) \qquad (33)$$

$$\frac{d\hat{S}_{NH}}{dt} = k_3 \hat{r}_N - k_8 \hat{\mu}_a \hat{X}_a + K_2(\hat{S}_{NH} - \hat{S}_{NH}) \qquad (34)$$

$$\frac{d\hat{X}_h}{dt} = \hat{\mu}_h \hat{X}_h + K_3(\hat{S}_O - S_O) \qquad (35)$$

$$\frac{d\hat{S}_C}{dt} = -k_4 \hat{\mu}_h \hat{X}_h + K_4(\hat{S}_O - S_O) \qquad (36)$$

$$\frac{d\hat{S}_O}{dt} = -k_5 \hat{\mu}_h \hat{X}_h - k_6 \hat{\mu}_a \hat{X}_a + k_L a(S_{O\max} - \hat{S}_O) + K_5(\hat{S}_O - S_O) \qquad (37)$$

a nd the following kinetic expressions:

$$\hat{\mu}_{hN} = \mu_{hN\max} \frac{\hat{S}_C - S_{C\min}}{K_{C1} + \hat{S}_C - S_{C\min}} \frac{\hat{S}_{NO}}{K_{NO} + \hat{S}_{NO}} \qquad (38)$$

$$\hat{r}_N = \mu_0(\hat{S}_N - S_{N\min}) \qquad (39)$$

$$\hat{\mu}_h = \mu_{h\max} \frac{\hat{S}_C - S_{C\min}}{K_{Ch} + \hat{S}_C - S_{C\min}} \frac{\hat{S}_O}{K_{Oh} + \hat{S}_O} \qquad (40)$$

$$\hat{\mu}_a = \mu_{a\max} \frac{\hat{S}_{NH}}{K_{NHa} + \hat{S}_{NH}} \frac{\hat{S}_O}{K_{Oa} + \hat{S}_O} \qquad (41)$$

Taking into account that S_{NO} is a measured variable we shall only consider that:

$$\frac{d\hat{S}_{NO}}{dt} = k_7 \hat{\mu}_a \hat{X}_a \qquad (42)$$

Considering the value of the parameters included in (Betancur et al, 2003) and the following initial values: $X_h(0)=1$; $\hat{X}_h(0)=$ 1.2; $S_C(0)=\hat{S}_C(0)=$ 200; $S_{NO}(0)=\hat{S}_{NO}(0)=0.5$; $S_{NH}(0)=0.1$; $\hat{S}_{NH}(0)=0.12$; $S_N(0)=20$; $\hat{S}_N(0)=24$; $X_a(0)=1$; $\hat{X}_a(0)=1.2$; $S_O(0)=0.010$; $\hat{S}_O(0)=0.012$. The ITSE observer performs as shown in Figure 4.

It is worth noting that the ITSE performs very well even with the important initial errors in some of the observed variables. Another advantage over the ELO is that the observer gains are easy to determine which is not the case for the ELO when the system is of high order as it is the case for the wastewater treatment process.

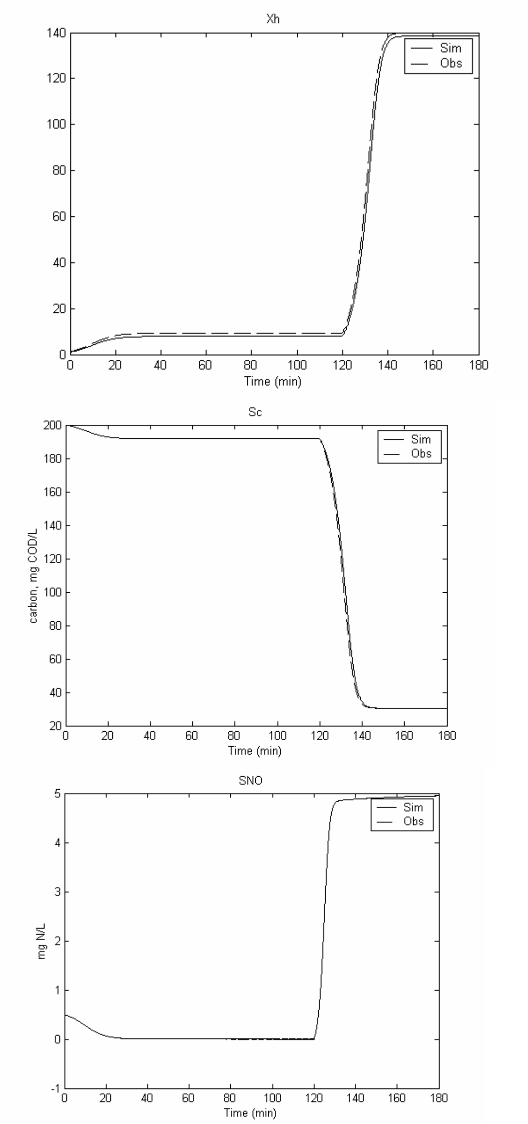


Fig. 4. ITSE Observer for S_c , X_h and S_{NO} during the anoxic and aerobic phase of the wastewater treatment process with a 20% error in the initial condition of $X_{h,}$, S_{NH}, S_N, X_a *and* S_O

5. CONCLUSIONS

In this paper, we have handled the question designing state observers that can possibly account for the limited time duration of batch processes by considering the design of ITSE observers in which the observer gains are computed via an ITSE criterion. The results of the observer have been illustrated first with a simple microbial growth model, then with the model of a SBR process, a process used in wastewater treatment.

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