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Simultaneous States and Parameters Estimation of an Ozonation Reactor Based on Dynamic Neural Network

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Abstract

This paper deals with the simultaneous states and parameters estimation of an ozonation reactor using a dynamic neural network and the least squares method. We use a dynamic model derived from mass balance considerations. We propose a continuous time algorithm which includes two parallel procedures: state estimation using a Dynamic Neural Network (DNN) and parameters identification based on Least Squares Method (LSM). A set of numerical simulations has been carried out in order to illustrate the performance of this algorithm.

1. Introduction

The design and control of ozonation reactors have always been the challenging tasks mostly because of the inadequacy of on-line sensors with

[0]AMS (MOS) 2001 Subject classifications:
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fast sampling rate and small time delay (since ozone is the most quick oxidant), and the complex nonlinear strongly interactive behavior of ozonation reactions. The only available measurements concern the concentration of ozone in the gaseous phase of the reactor. To overcome the present limitations of sensors technology (for example, sensors for concentrations measurement are not available or are very expensive since special chromatography devices are required, etc.), a differential neural network is used for state estimation (compound concentrations) [7] [4] [23] [9] [11]. As in many engineering problems, we are concerned with the simultaneous states and parameters estimation for nonlinear systems.

In this paper we propose a continuous time algorithm which includes two parallel procedures: state estimation using a *Differential Neural Network* (DNN) and, parameters identification based on *Least Squares Method* (LSM).

Several studies have been dedicated to the use neural networks techniques for constructing states observers for nonlinear systems. In [3] a nonlinear observer, based on the ideas given in [5], is combined with a feedforward neural network, which is used to solve a matrix equation. In [8] a nonlinear observer is used to estimate the nonlinearities of an input signal. As far as we know, the first observer for nonlinear systems using dynamic neural networks was presented in [10]. The stability of this observer with on-line adaptation of neural network weights is analyzed, but several restrictive assumptions are made: the nonlinear plant must contain a known linear part and a strictly positive real (*SPR*) condition must be fulfilled. In [17] a robust neuro-observer with time delay term and adjusted weights in the hidden layer is presented.

In this paper a Differential Neuro-Observer (DNO) is used for the estimation of the compound concentrations (states). Based on the DNO outputs, the chemical reaction rates are identified using the continuous version of the Least Squares Method (LSM) with a projection procedure. The theoretical analysis of this DNO is carried out using Lyapunov-like technique.

Several simulation results have been carried out in order to illustrate

the feasibility and the efficiency of the presented approach.

The *remainder* of this paper is organized as follows. The model of the considered ozonation reactor as well as the problem formulation are presented in the next section. Section 3 deals with observability condition for the partial (but more practice) case of $N = 3$ compounds mixture. The neuro-observer with the corresponding learning law for the weight matrix is described in Section 4. The estimation of the reaction rate constants is discussed in Section 5. Numerical simulations are given in section 6. Section 7 concludes this paper.

2. Process Modelling and Problem Formulation

2.1. Reactor Model and Measurable Variables

Ozone-liquid systems are extensively used in different industrial environmental processes such as wastewater, river and drinking water treatment, etc. The main aim of the ozonation treatment ("purification") is the quick and effective elimination of hydrocarbon contaminants (paraffins, olefins and aromatic compounds) from the given liquid mixture (for example, water) [1] [19]). Such processes are usually carried out in ozonation reactors under specific temperature and pressure.

The ozonation reactor, considered here, represents a semi-batch reactor where the ozone feed enters the bottom as shown in Fig. 1. Several parallel ozonation reactions take place in the reactor [6]:

$$O_3 + A_i \xrightarrow{k_i} B_i \left(i = \overline{1, N}\right)$$

where O_3 is ozone, A_i is one of the organic compounds and B_i is the corresponding ozonation product.

The monotonic decreasing elimination curves for different organic compounds (c_t^i is the current concentration of the compound A_i) are shown in Fig. 2.

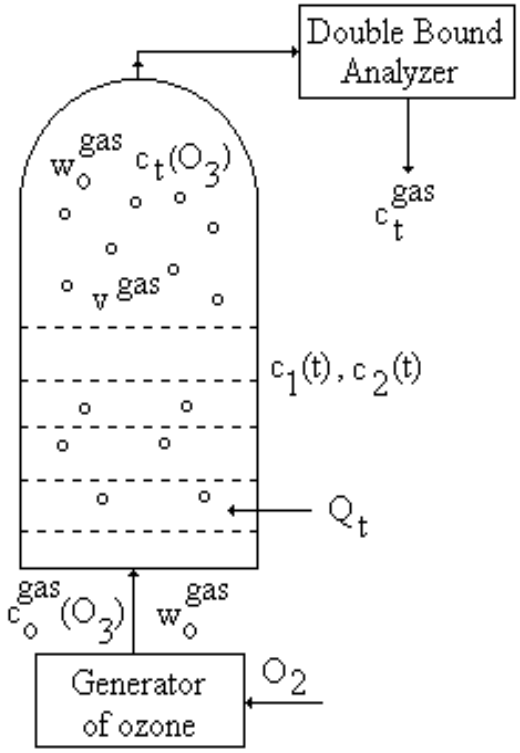

Figure 1: Schematic diagram of the ozonization reactor.

The ozonation process can be stopped at time τ if the "contaminant level" for all contaminants does not exceed a given value, namely d, that is,

$$\tau := \max_{i=\overline{1,N}} \left\{ t_i : c^i_{t_i} = d \right\} \tag{1}$$

The mathematical model of these processes, developed in [18], is actively applied to ozonation reactor design [20], the efficiency optimization and the prediction of their actual performance [21], operation and maintenance, ensuring safety, and development of control strategies [2] [13].

The model of the considered semi-batch ozonation reactor is described

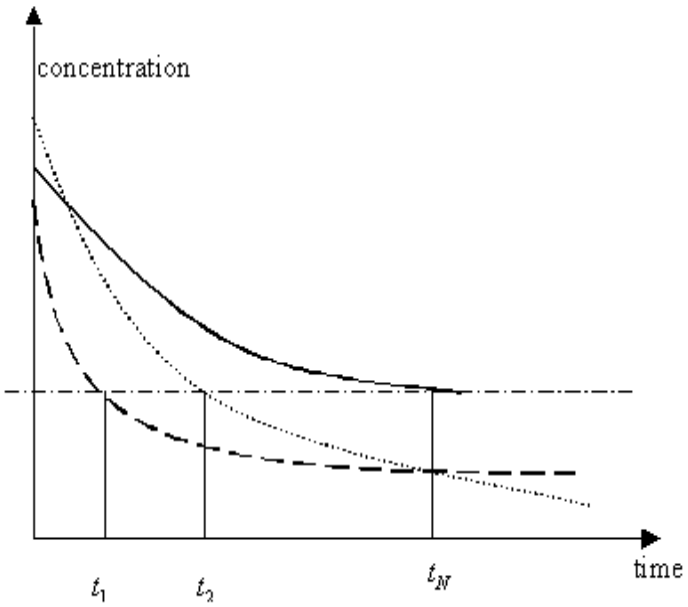

Figure 2: Concentration of different organic compounds.

in what follows.

2.1.1. Ozone Mass Balance

The mass balance consideration (with respect to ozone) leads to the following model [18] given in the integral form:

$$\begin{gathered}\int_{\tau=0}^{t} w^{gas} c_t^{in} d\tau = \int_{\tau=0}^{t} w^{gas} c_t^{out} d\tau + c_t^{out} v^{gas} + Q_t + v^{liq} \sum_{i=1}^{N} (c_0^i - c_t^i) \\ c_t^{in} := c_0^{gas} = const,\ c_t^{out} := c_t^{gas}\end{gathered} \tag{2}$$

or, in the equivalent differential form,

$$\frac{d}{dt} c_t^{out} := \frac{1}{v^{gas}} \left\{ w^{gas} \left[c_t^{in} - c_t^{out} : \right] - \frac{d}{dt} \left[Q_t + v^{liq} \sum_{i=1}^{N} \left(c_0^i - c_t^i \right) \right] \right\} \tag{3}$$

where c_t^i $(mole/l)$ is the i^{th} organic compound concentration at time $t \geq 0$, $i = 1, ..., N$, N is the number of different organic compounds dissolved in the liquid phase of the given ozonation reactor, $c_t^{out} := c_t^{gas}$ $(mole/l)$ is the gas (moles) which do not react with organic compounds dissolved in the solvent and can be *directly measured* in the outlet of the ozonation reactor, w^{gas} (l/s) is the gas consumption assumed to be constant, v^{gas} (l) is the volume of the gas phase which is assumed to be constant, Q_t $(mole)$ is the dissolved ozone, and v^{liq} (l) is the volume of the liquid phase. It is assumed to be constant.

2.1.2. Ozone Dissolution Process

The differential equation associated with the ozone dissolution process is is given by:

$$\frac{d}{dt}\left[Q_t + v^{liq}\sum_{i=1}^{N}\left(c_0^i - c_t^i\right)\right] = K_{sat}[Q_{\max} - Q_t] \tag{4}$$

where K_{sat} (s^{-1}) is the ozone volumetric mass transfer coefficient, and $Q_{\max} = \alpha c_t^{out} v^{liq}(mole)$ is the maximum of ozone being in the saturated $(t \to \infty)$ liquid phase under the given conditions. The parameter α deduced from the Henry constant.

2.2. Organic Compounds Reactions with Ozone

The differential equations describing the bimolecular chemical reactions for each organic compound are [21]:

$$\frac{d}{dt}c_t^i = -k_i c_t^i Q_t / v^{liq} \quad (i = 1, ..., N) \tag{5}$$

where k_i $(ls^{-1}mol^{-1})$ is the rate constant of the ozonation reaction related to the i^{th} organic compound.

2.3. Problem Setting

Before the problem formulation, let us introduce two "auxiliar" processes $\hat{Q}_t$ and y_t, which may be constracted based on the measurable process c_t^{gas}.

Substitution of (4) into (3) leads to

$$Q_t = Q_{\max} + K_{sat}^{-1} v^{gas} \frac{d}{dt} c_t^{out} - K_{sat}^{-1} w^{gas} \left[c_t^{in} - c_t^{out} \right]$$

Based on Euler approximation, we derive

$$\frac{d}{dt} c_t^{out} \simeq h^{-1} \left(c_t^{out} - c_{t-h}^{out} \right), h > 0 \tag{6}$$

Q_t can be estimated as follows

$$\begin{aligned} Q_t &= \hat{Q}_t + v^{liq} \xi_t \\ \hat{Q}_t &:= Q_{\max} + K_{sat}^{-1} v^{gas} h^{-1} \left(c_t^{out} - c_{t-h}^{out} \right) - K_{sat}^{-1} w^{gas} \left(c_t^{in} - c_t^{out} \right) \end{aligned} \tag{7}$$

where ξ_t is the unmeasured dynamics related to the approximation (6). ξ_t is given by

$$\xi_t := \left(Q_t - \hat{Q}_t \right) / v^{liq} = K_{sat}^{-1} v^{gas} \left[\frac{d}{dt} c_t^{out} - h^{-1} \left(c_t^{out} - c_{t-h}^{out} \right) \right] / v^{liq} \tag{8}$$

The integration of (4) directly leads to the following expression:

$$S_t := \sum_{i=1}^{N} c_t^i = \sum_{i=1}^{N} c_0^i + \frac{1}{v^{liq}} \left(Q_t - Q_0 \right) - \frac{1}{v^{liq}} \int_{s=0}^{t} K_{sat} [Q_{\max} - Q_s] ds \tag{9}$$

In view of (7), (9) can be written as follows

$$S_t = y_t + \xi_t \tag{10}$$

where y_t is given by

$$\begin{aligned} y_t := \sum_{i=1}^{N} c_0^i + \left(\hat{Q}_t - Q_0 \right) / v^{liq} - \left[c_t^{in} - c_t^{out} \right] v^{gas} / v^{liq} \\ - w^{gas} / v^{liq} \int_{s=0}^{t} \left[c_s^{in} - c_s^{out} \right] ds \end{aligned} \tag{11}$$

So, the processes y_t and $\hat{Q}_t$, related to the considered ozonation reactor and constructed based only on the available measurements of c_t^{out}, satisfy

$$\begin{cases} Q_t = \hat{Q}_t + v^{liq}\xi_t \\ \xi_t = y_t - S_t \end{cases} \tag{12}$$

The problem which we are dealing with can be formulated as follows: based on the available data $\{c_t^{out}\}$ (and, hence, on $\hat{Q}_t$ and y_t) construct the estimates $\hat{c}_t^i$ of the state vector c_t^i as well as the estimates $\hat{k}_{i,t}$ of unknown parameters $k_i\,(1,...,N)$ and derive their accuracy bounds.

As already mentioned, reliable sensors for concentrations measurement are not available or are very expensive, an efficient estimation procedure (based only on $\{c_t^{out}\}$) can contribute significantly to the improvement of the reactor monitoring and control. The model of this process is given by

$$\begin{cases} \frac{d}{dt}c_t^i = -k_i c_t^i \left(\hat{Q}_t/v^{liq} + \xi_t\right) \quad (i = 1,...,N) \\ y_t = \sum\limits_{i=1}^{N} c_t^i - \xi_t \end{cases} \tag{13}$$

and represents the basis for on-line estimation of the current compound concentrations c_t^i and the identification of the rate constants k_i.

3. Observability Condition

First, to understand whether or not the output signal y_t contains enough information to estimate the components c_t^i $(i = 1,...,N)$, try to obtain, so-called, *"observability condition"*. To do that, consider now the same problem, assuming that c_t^{out} as well as $\frac{d}{dt}c_t^{out}$ are available, that is, put $\xi_t = 0$. It implies that Q_t is available too and the considered process model can be rewritten as follows:

$$\begin{cases} \frac{d}{dt}c_t^i = f_t^i\,(c_t^i) := -k_i c_t^i Q_t/v^{liq} \quad (i = 1,...,N) \\ y_t = \sum\limits_{i=1}^{N} c_t^i \end{cases} \tag{14}$$

where c_t^i and y_t are the states and output of the corresponding dynamic system whose model is given by (14).

Consider the case $N = 3$ which covers a lot of practical situations. The calculation of the *Lie* derivatives of the time-functions $\dot{y}_t$ and $\ddot{y}_t$ along the trajectories of this system leads to

$$\begin{bmatrix} y_t \\ \dot{y}_t \\ \ddot{y}_t \end{bmatrix} = \mathcal{O}_t \begin{bmatrix} c_t^1 \\ c_t^2 \\ c_t^3 \end{bmatrix}$$

where $\mathcal{O}_t$ is the observability matrix given by

$$\mathcal{O}_t = \begin{bmatrix} 1 & 1 & 1 \\ -\tilde{k}_1 Q_t & -\tilde{k}_2 Q_t & -\tilde{k}_3 Q_t \\ \tilde{k}_1\left(\tilde{k}_1 Q_t^2 - \dot{Q}_t\right) & \tilde{k}_2\left(\tilde{k}_2 Q_t^2 - \dot{Q}_t\right) & \tilde{k}_1\left(\tilde{k}_2 Q_t^2 - \dot{Q}_t\right) \end{bmatrix} \quad (15)$$
$$\tilde{k}_i := k_i / v^{liq} \quad (i = 1, ..., N = 3)$$

The states c_t^i of the system (14) are globally observable if and only if

$$\begin{aligned} \det \mathcal{O}_t = Q_t \Big[& \tilde{k}_1\left(\tilde{k}_1 Q_t^2 - \dot{Q}_t\right)\left(\tilde{k}_2 - \tilde{k}_3\right) + \tilde{k}_2\left(\tilde{k}_2 Q_t^2 - \dot{Q}_t\right)\left(\tilde{k}_3 - \tilde{k}_1\right) \\ & + \tilde{k}_1\left(\tilde{k}_2 Q_t^2 - \dot{Q}_t\right)\left(\tilde{k}_1 - \tilde{k}_2\right)\Big] \\ = Q_t^3 \Big[& \tilde{k}_1^2\left(\tilde{k}_2 - \tilde{k}_3\right) + \tilde{k}_2^2\left(\tilde{k}_3 - \tilde{k}_1\right) + \tilde{k}_3^2\left(\tilde{k}_1 - \tilde{k}_2\right)\Big] \neq 0 \end{aligned}$$

That is, the process y_t contains the sufficient information to estimate the states c_t^i if Q_t is not equal to zero and all reaction rates are different:

$$(Q_t \neq 0) \wedge (k_2 \neq k_3) \wedge (k_1 \neq k_2) \wedge (k_1 \neq k_3) \quad (16)$$

4. Neuro-Observer

4.1. Neuro-Observer Structure

According to [22] [14] [15], consider the dynamic neuro-observer given by

$$\begin{cases} \frac{d}{dt}\widehat{x}_t = A\widehat{x}_t + W_t\sigma(\widehat{x}_t) + K\left[y_t - \widehat{y}_t\right] \\ \hat{y}_t = C^T\widehat{x}_t, \qquad C^T = (1, ..., 1) \in \mathcal{R}^n \end{cases} \quad (17)$$

where $\widehat{x}_t \in \mathcal{R}^n$ is the state of the observer interpreted as the current estimate of the state vector $c_t = \left(c_t^1, ..., c_t^N\right)^\intercal$, $A \in \mathcal{R}^{n\times n}$ is a matrix to be selected, $\sigma : \mathcal{R}^n \to \mathcal{R}^k$ a smooth vector field usually represented by the sigmoid of the form

$$\sigma_i(x) = \frac{a_i}{1 + e^{-b_i^\intercal x}} - c_i \tag{18}$$

$W_t \in \mathcal{R}^{n\times k}$ is the weight matrix to be adjusted by a learning procedure, y_t is given by (11) and K is the observer gain matrix to be selected. The parameters a_i, b_i and c_i are assumed to be *a priori* given or selected during the experiment by *"try-to-test'* method. The sigmoid vector functions $\sigma(\cdot)$, commonly used in neural networks as the activation function, satisfy the Lipshitz condition $\left(\forall x^{'}, x^{''} \in \mathcal{R}^n\right)$

$$\widetilde{\sigma} := \sigma\left(x^{'}\right) - \sigma\left(x^{''}\right)$$
$$\widetilde{\sigma}^T \Lambda_{_\sigma} \widetilde{\sigma} \leq \left(x^{'} - x^{''}\right)^\intercal D_\sigma \left(x^{'} - x^{''}\right)$$

where $\Lambda_{_\sigma} = \Lambda_{_\sigma}^\intercal > 0$, $D_\sigma = D_\sigma^\intercal > 0$ are known normalizing matrices. The structure of the neuro-observer is shown in Fig. 3.

4.2. Basic Assumptions

A1: The pair (A, C) is detectable, that is, there exists a matrix K such that the combined matrix $\mathcal{A} := A - KC^\intercal$ is stable (Hurwitz).

A2: There exist a gain matrix K, strictly positive defined matrices $\bar{Q}$, Λ_1, $\Lambda_{_\varphi}$ and a positive $\delta > 0$ such that the matrix Riccati equation

$$Ric := P\mathcal{A} + \mathcal{A}^\intercal P + P\mathcal{R}P + \mathcal{Q} = 0 \tag{19}$$

with

$$\mathcal{A} := A - KC^T \text{ - a stable matrix}$$
$$\mathcal{R} := \Lambda_1^{-1} + \Lambda_{_\varphi}^{-1} + W^* \Lambda_{_\sigma}^{-1} W^{*\intercal}$$
$$W^* = W_0 \text{ - an initial weitght matrix}$$
$$\mathcal{Q} := D_{_\sigma} + \bar{Q} + \delta I$$

has a positive definite solution P.

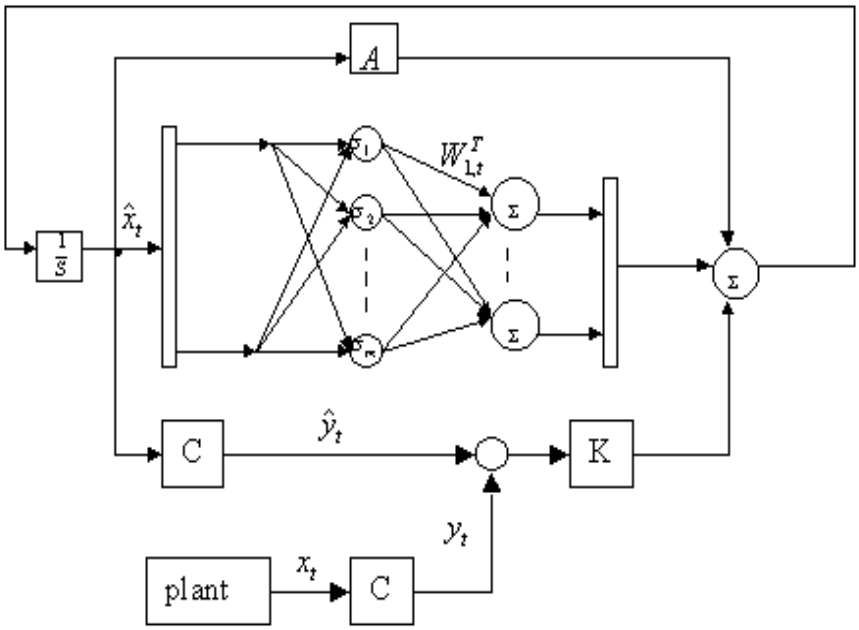

Figure 3: Neuro-observer structure.

4.3. Learning Law

Let the weight matrix W_t be adjusted as follows:

$$\begin{aligned}\dot{W}_t =& DP\left(N_\delta^{-1}\right)^\intercal \left(2\left(C^+\right)^\intercal e_t\right. \\ &\left. - \left[\left(C^+\right)^\intercal \Lambda_\xi^{-1} C^+ + \delta I\right]^\intercal N_\delta^{-1} P\left(W_t - W^*\right)\sigma\left(\widehat{x}_t\right)\right)\sigma^\intercal\left(\widehat{x}_t\right)\end{aligned} \tag{20}$$

where e_t is the output observation error given by

$$e_t := y_t - C^T\widehat{x}_t$$

$$N_\delta := CC^+ + \delta I, \quad \delta > 0, \quad C^+ = C^\intercal / \|C\|^2 = C^\intercal / N$$

and Λ_ξ any positive definite matrix satisfying $\xi_t^\intercal \Lambda_\xi \xi_t \leq 1$ (ξ_t is defined by (12)). In practice, Λ_ξ can selected as $\Lambda_\xi = \lambda I$ where λ is a small enough positive scalar.

4.4. Upper Bound for Estimation Error

Theorem 4.1. If, under assumptions **A1-A2**, the updating law is given by (20), then the averaged observation error satisfies the following performance:

$$\begin{gathered}\overline{\lim_{T\to\infty}}\frac{1}{T}\int_0^T \Delta_t^T \bar{Q}\Delta_t dt \le \overline{\eta} := \overline{\lim_{T\to\infty}}\frac{1}{T}\int_0^T \eta_t dt \\ \eta_t := \xi_t^{\intercal}\left(K^{\intercal}\Lambda_1^{-1}K + \Lambda_{\xi}\right)\xi_t + \varphi_t^{\intercal}\Lambda_{\varphi}\varphi_t \\ \varphi_t := \left[W^*\sigma\left(c_t\right) + Ac_t - f_t\left(c_t\right)\right]\end{gathered} \tag{21}$$

Proof. From (12) and (17), it follows

$$\begin{gathered}\dot{\Delta}_t = A\widehat{x}_t + W_t\sigma\left(\widehat{x}_t\right) + K\left[y_t - C^T\widehat{x}_t\right] - f_t\left(c_t\right) \\ = \left(A - KC^T\right)\Delta_t - K\xi_t + \tilde{W}_t\sigma\left(\widehat{x}_t\right) \\ +W^*\left[\sigma\left(\widehat{x}_t\right) - \sigma\left(c_t\right)\right] + \left[W^*\sigma\left(c_t\right) + Ac_t - f_t\left(c_t\right)\right]\end{gathered} \tag{22}$$

where $\tilde{W}_t := W_t - W^*$. Consider the Lyapunov function given by

$$V_t := V\left(\Delta_t, \tilde{W}_t\right) := \Delta_t^{\intercal}P\Delta_t + \frac{1}{2}tr\left\{\tilde{W}_t^{\intercal}D^{-1}\tilde{W}_t\right\},\ D = D^{\intercal} > 0 \tag{23}$$

which derivative, calculated over the trajectories of (22), satisfies

$$\dot{V}_t = \dot{V}\left(\Delta_t, \tilde{W}_t\right) = 2\Delta_t^{\intercal}P\dot{\Delta}_t + tr\left\{\left(\frac{d}{dt}\tilde{W}_t^{\intercal}\right)D^{-1}\tilde{W}_t\right\} \tag{24}$$

The substitution of (22) into (24) implies:

1)

$$2\Delta_t^{\intercal}P\left(A - KC^T\right)\Delta_t = \Delta_t^{\intercal}\left[P\left(A - KC^T\right) + \left(A - KC^T\right)^{\intercal}P\right]\Delta_t \tag{25}$$

2)

$$-2\Delta_t^{\intercal}PK\xi_t \le \Delta_t^{\intercal}P\Lambda_1^{-1}P\Delta_t + \xi_t^{\intercal}K^{\intercal}\Lambda_1^{-1}K\xi_t \tag{26}$$

(here the inequality

$$X^{\intercal}Y + Y^{\intercal}X \le X^{\intercal}\Lambda^{-1}X + Y^{\intercal}\Lambda Y \tag{27}$$

which is valid for any $X, Y \in \mathcal{R}^{n\times m}$ and any $\Lambda = \Lambda^{\intercal} \in \mathcal{R}^{n\times n}$, is applied).

3) by (27) it follows

$$\begin{aligned}
2\Delta_t^T P\tilde{W}_t\sigma\left(\widehat{x}_t\right) =& 2\left(-e_t^{\intercal}C^+N_{\delta}^{-1} - \xi_t^{\intercal}C^+N_{\delta}^{-1} + \delta\Delta_t^{\intercal}N_{\delta}^{-1}\right)P\tilde{W}_t\sigma\left(\widehat{x}_t\right)\\
=& -tr\left\{2\sigma\left(\widehat{x}_t\right)e_t^{\intercal}C^+N_{\delta}^{-1}P\tilde{W}_t\right\}\\
&-2\xi_t^{\intercal}C^+N_{\delta}^{-1}P\tilde{W}_t\sigma\left(\widehat{x}_t\right) + 2\delta\Delta_t^{\intercal}N_{\delta}^{-1}P\tilde{W}_t\sigma\left(\widehat{x}_t\right)\\
\leq& -tr\left\{2\sigma\left(\widehat{x}_t\right)e_t^{\intercal}C^+N\delta^{-1}P\tilde{W}_t\right\}\\
&+\sigma^{\intercal}\left(\widehat{x}_t\right)\tilde{W}_t^{\intercal}P\left(N_{\delta}^{-1}\right)^{\intercal}\left(C^+\right)^{\intercal}\Lambda_{\xi}^{-1}C^+N_{\delta}^{-1}P\tilde{W}_t\sigma\left(\widehat{x}_t\right)\\
&+\xi_t^{\intercal}\Lambda_{\xi}\xi_t + \delta\Delta_t^{\intercal}\Delta_t + \delta\sigma^{\intercal}\left(\widehat{x}_t\right)\tilde{W}_t^{\intercal}P\left(N_{\delta}^{-1}\right)^{\intercal}N_{\delta}^{-1}P\tilde{W}_t\sigma\left(\widehat{x}_t\right)\\
=& tr\left\{\sigma\left(\widehat{x}_t\right)\left[-2e_t^{\intercal}C^+ + \sigma^{\intercal}\left(\widehat{x}_t\right)\tilde{W}_t^{\intercal}P\left(N_{\delta}^{-1}\right)^{\intercal}\right.\right.\\
&\left.\left.\times\left[\left(C^+\right)^{\intercal}\Lambda_{\xi}^{-1}C^+ + \delta I\right]\right]N_{\delta}^{-1}P\tilde{W}_t\right\} + \xi_t^{\intercal}\Lambda_{\xi}\xi_t + \delta\Delta_t^{\intercal}\Delta_t
\end{aligned}$$

since

$$e_t := y_t - C^T\widehat{x}_t = -C^{\intercal}\Delta_t - \xi_t$$

$$\Delta_t^{\intercal}C = -e_t^{\intercal} - \xi_t^{\intercal}$$

and

$$\begin{aligned}
\Delta_t^{\intercal} &= \Delta_t^{\intercal}N_{\delta}N_{\delta}^{-1} = \Delta_t^{\intercal}\left(CC^+ + \delta I\right)N_{\delta}^{-1}\\
&= -e_t^{\intercal}C^+N_{\delta}^{-1} - \xi_t^{\intercal}C^+N^{-1} + \delta\Delta_t^{\intercal}N_{\delta}^{-1}
\end{aligned}$$

$$N_{\delta} := CC^+ + \delta I,\ \delta > 0$$

(C^+ represents the pseudo-inverse of C).

4) by the property of the sigmoid function, we derive

$$\begin{aligned}
2\Delta_t^{\intercal}PW^*\left[\sigma\left(\widehat{x}_t\right) - \sigma\left(c_t\right)\right] &\leq \Delta_t^{\intercal}PW^*\Lambda_{\sigma}^{-1}W^{*\intercal}P\Delta_t\\
&+\left[\sigma\left(\widehat{x}_t\right) - \sigma\left(c_t\right)\right]^{\intercal}\Lambda_{\sigma}\left[\sigma\left(\widehat{x}_t\right) - \sigma\left(c_t\right)\right]\\
&\leq \Delta_t^{\intercal}\left(PW^*\Lambda_{\sigma}^{-1}W^{*\intercal}P + D_{\sigma}\right)\Delta_t
\end{aligned}$$

5) for the term $\varphi_t := \left[W^*\sigma\left(c_t\right) + Ac_t - f_t\left(c_t\right)\right]$, tending to zero in view of (5), it follows:

$$2\Delta_t^{\intercal}P\varphi_t \leq \Delta_t^{\intercal}P\Lambda_{\varphi}^{-1}P\Delta_t + \varphi_t^{\intercal}\Lambda_{\varphi}\varphi_t$$

Adding and substracting the term $\Delta_t^\intercal \bar{Q} \Delta_t$ ($\bar{Q} = \bar{Q}^\intercal > 0$) from the right-hand side of (24), we obtain:

$$\dot{V}_t \leq \Delta_t^\intercal Ric \Delta_t + tr\left[L_t + \tfrac{d}{dt}\left(\widetilde{W}_t\right)^\intercal D^{-1}\right] - \Delta_t^\intercal \bar{Q} \Delta_t + \eta_t$$

where

$$L_t := \sigma\left(\widehat{x}_t\right)\left[-2e_t^\intercal C^+ + \sigma^\intercal\left(\widehat{x}_t\right)\tilde{W}_t^\intercal P\left(N_\delta^{-1}\right)^\intercal\left[\left(C^+\right)^\intercal \Lambda_\xi^{-1} C^+ + \delta I\right]\right] N_\delta^{-1} P$$

$$\eta_t := \xi_t^\intercal\left(K^\intercal \Lambda_1^{-1} K + \Lambda_\xi\right)\xi_t + \varphi_t^\intercal \Lambda_\varphi \varphi_t$$

By **A2** and by the updating law (20), it follows that $Ric = 0$ and $DL_t^\intercal = -\frac{d}{dt}\widetilde{W}_t$, that implies

$$\dot{V}_t \leq -\Delta_t^\intercal \bar{Q} \Delta_t + \eta_t \tag{28}$$

Integrating (28) over the interval $[0, T]$, and dividing both side by T, we finally obtain

$$T^{-1}\left(V_T - V_0\right) \leq -T^{-1}\int_{s=0}^{T} \Delta_s^\intercal \bar{Q} \Delta_s ds + T^{-1}\int_{s=0}^{T} \eta_s ds$$

that leads to the following estimate:

$$\begin{aligned} T^{-1}\int_{s=0}^{T} \Delta_s^\intercal \bar{Q} \Delta_s ds &\leq T^{-1}\int_{s=0}^{T} \eta_s ds - T^{-1}\left(V_T - V_0\right) \\ &\leq T^{-1}\int_{s=0}^{T} \eta_s ds + T^{-1} V_0 \end{aligned}$$

Theorem is proven.

A remark is in order at this point.

Remark 4.2. The upper bound $\overline{\eta}$ for the averaged quadratic estimation error can be done less than any $\varepsilon > 0$ since $\varphi_t \to 0$ by (5) and ξ_t can be done small enough by the selection of the time-interval h in the approximation (6).

The main concern of the next section is the estimation of the parameters (reaction rate constants).

5. Identification of the Reaction Rate Constants

From the previous sections, it follows that the neuro-observer (17) can be used to identify (estimate) the chemical reaction rates (14). Observe that $\widehat{x}_t = \widehat{c}_t$ as well as $d\widehat{x}_t/dt$ are given by the neuro-observer. In these conditions, we are ready to define the *LS*-estimates $\hat{k}_i(t)$ as the following optimization problem:

$$\left(\hat{k}_1(t), ..., \hat{k}_N(t)\right) := \arg\min_{k_i} \int_{s=0}^{t} \sum_{i=1}^{N} \left(\frac{d\widehat{x}_s^i}{ds} + k_i \widehat{x}_s^i \hat{Q}_s v_{liq}^{-1}\right)^2 ds \tag{29}$$

whose solution satisfies (with $o(\eta)$-approximation) the following differential equation:

$$\begin{gathered}
\tfrac{d}{dt}\tilde{K}_t = \left(\tfrac{d}{dt}\widehat{x}_t - \widehat{K}_t \widehat{x} \hat{Q}_t / v^{liq}\right) \widehat{x}_t^T \Gamma_t \hat{Q}_t / v^{liq} \\
\dot{\Gamma}_t = -\Gamma_t \widehat{x}_t \widehat{x}_t^T \Gamma_t \left(\hat{Q}_t / v^{liq}\right)^2, \quad \Gamma_0 = \eta^{-1} I \\
\tilde{K}_t := diag\left(\tilde{k}_{1,t}, ..., \tilde{k}_{N,t}\right) \\
\hat{K}_t = \begin{bmatrix}
\hat{k}_{1,t} = \left[\tilde{k}_{1,t}\right]_+ & 0 & \cdot & 0 \\
0 & \cdot & 0 & 0 \\
0 & 0 & \cdot & 0 \\
0 & \cdot & 0 & \hat{k}_{N,t}\left[\tilde{k}_{N,t}\right]_+
\end{bmatrix}
\end{gathered} \tag{30}$$

where η is a small enough positive constant and the function $[\cdot]_+$ is defined as follows

$$[z]_+ := \begin{cases} z & \text{if} \quad z \geq 0 \\ 0 & \text{if} \quad z < 0 \end{cases} \tag{31}$$

From an initial condition $\widehat{K}_0$, we calculate the diagonal elements of $\widehat{K}_t$ on-line, using $\hat{Q}_t$ and $\widehat{x}_t$ generated by (7) and (17), respectively.

Remark 5.1. This algorithm generates the continuous-time Least Squares estimates with a special projection procedure (31).

The next section presents the simulation results.

6. Simulation Results

The simulation experiments described in this section are intended to illustrate the main results presented previously. The estimation algorithms described and analyzed in this paper are easy to code since they have few adjustable (design) parameters: the matrices A, $\Lambda_1, \Lambda_{_\varphi}, W^*, \Lambda_{_\sigma}, K, D$ and the scalars δ and η.

6.1. Experiment 1 (Medium Rate Process)

This experiment has been carried out using the following values for the parameters associated with the ozonation reactor (3),(5):

$c_o^1 = 1 \times 10^{-5}$	$c_o^2 = 1 \times 10^{-5}$	$Q_o = 10^{-8}$	$c_o^{in} = 1 \times 10^{-6}$
$k_1 = 10^5$	$k_2 = 10^4$	$K_{sat} = 0.2$	$Q_{\max} = 1.68 \times 10^{-8}$
$v_{liq} = 8 \times 10^{-3}$	$v_{gas} = 6 \times 10^{-3}$	$w_{gas} = 1.94 \times 10^{-3}$	

- First, we check the identification ability of the neural network for this chemical system.

If the system is observable, we may construct a dynamical neural network to estimate $c_t^1$and c_t^2. The neural network is the same as in (17) ($n = 4$). The experiments reported herein have been carried out for the following values

$$A = diag[-2, -2, -2, -2],\ \sigma(\widehat{x}_i) = 2/\left(1 + e^{-2\widehat{x}_i}\right) - 0.5$$
$$K = [3, 3]^T,\ \widehat{x}_0 = [10^{-5}, 10^{-5}]$$

The algorithm was designed with the following parameters $\overline{\eta} = 2$, $Q_0 = I_4$, $\Lambda_1^{-1} = 2I_4$, $\Lambda_\xi = 0.1I$

$$\overline{W}_1 = \begin{bmatrix} 3 & 0.1 & 0.1 & 0.1 \\ 0.1 & 3 & 0.1 & 0.1 \\ 0.1 & 0.1 & 3 & 0.1 \\ 0.1 & 0.1 & 0.1 & 3 \end{bmatrix} \text{ and } D_\sigma = \begin{bmatrix} 1 & 0.1 & 0.1 & 0.1 \\ 0.1 & 1 & 0.1 & 0.1 \\ 0.1 & 0.1 & 1 & 0.1 \\ 0.1 & 0.1 & 0.1 & 1 \end{bmatrix}.$$

These design parameters gave good results. For the Riccati equation (19), we obtain the following solution:

$$P = \begin{bmatrix} 0.3477 & 0.01 & 0.01 & 0.01 \\ 0.01 & 0.3477 & 0.01 & 0.01 \\ 0.01 & 0.01 & 0.3477 & 0.01 \\ 0.01 & 0.01 & 0.01 & 0.3477 \end{bmatrix}.$$

$W_{1,t}$ is updated according to the procedure (20) with $D = dI$, $d = 5$.

The initial weights have been selected as follows:

$$W_{1,0} = \begin{bmatrix} 10^{-5} & 10^{-6} & 0 & 0 \\ 10^{-6} & 10^{-5} & 0 & 0 \\ 0 & 0 & 10^{-5} & 10^{-5} \\ 0 & 0 & 10^{-5} & 10^{-5} \end{bmatrix}.$$

The time evolution of the weights are shown in Fig. 4.

The identification results are shown in Figs. 5-7.

These figures represent the evolution of c_t^1, c_t^2, Q_t, c_t^{out} and $W_{1,t}$. They highlight the performance of the identification procedure. For example, the concentration c_t^1 tends to zero after approximately 65 iterations.

- Second, we check the neuro-observer ability to estimate the states of the ozonation reactor.

If c_t^{out} is only measurable, we use the model (14). Because k_1 and k_2 are also unknown, we need to construct first a neuro-observer to estimate c_t^1 and c_t^2. The neural observer is the same as in (17) ($n = 2$). The design parameters have been selected as follows:

$$A = diag[-2, -2], C = [1, 1], N = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix},$$

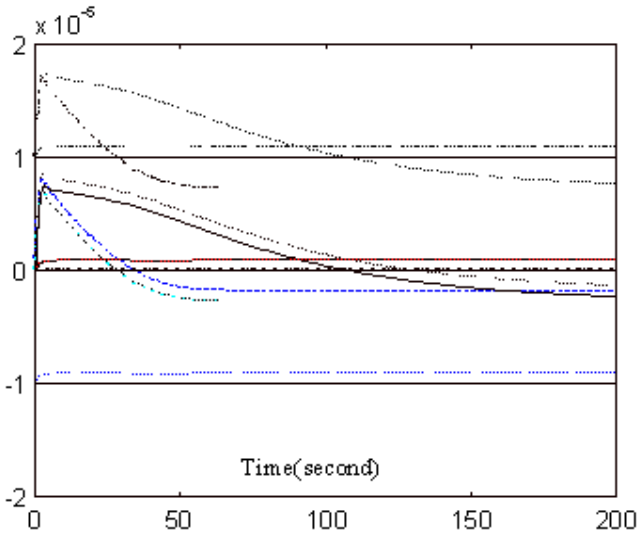

Figure 4: Evolution of $W_{1,t}$.

$$\sigma(\widehat{x}_i) = 2/\left(1+e^{-2\widehat{x}_i}\right) - \frac{1}{2}, \widehat{x}_0 = \left[10^{-5}, 10^{-5}\right], \ K = [3,3]^T,$$

$$\overline{W}_1 = \begin{bmatrix} 3 & 0.1 \\ 0.1 & 3 \end{bmatrix}, \Lambda_1^{-1} = 2I_2, Q_0 = I_2, D_\sigma = \begin{bmatrix} 1 & 0.1 \\ 0.1 & 1 \end{bmatrix}, \ \delta = 0.1.$$

Observe that $\mathcal{A} = A - KC$ is stable. The solution of the Riccati equation (19) is

$$P = \begin{bmatrix} 0.3614 & 0.01 \\ 0.01 & 0.3614 \end{bmatrix}.$$

$W_{1,t}$ is updated as in (20) with

$$\widetilde{W}_{1,0} = 0, \ W_{1,0} = \begin{bmatrix} 7.25 \times 10^{-6} & -1.09 \times 10^{-6} \\ -1.75 \times 10^{-6} & 7.91 \times 10^{-6} \end{bmatrix}$$

The observer results are shown in Fig. 8. The continuous lines represent the estimations. The estimations $\hat{c}_t^1$ and $\hat{c}_t^2$ of the states c_t^1 and c_t^2

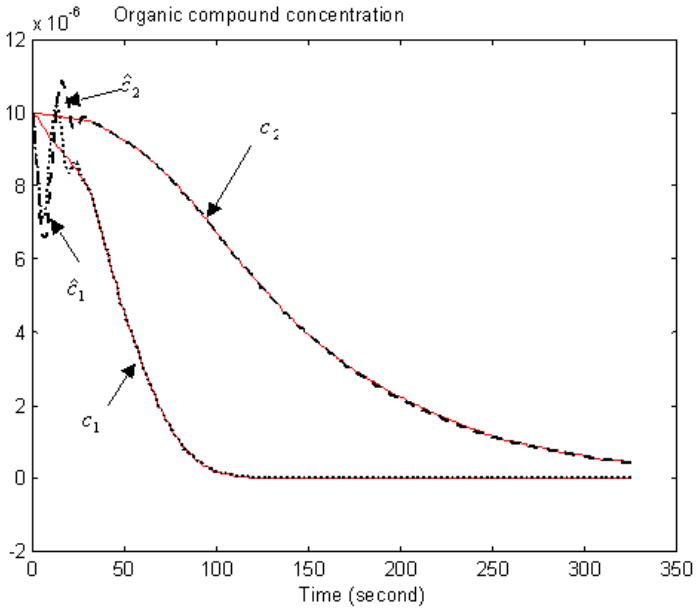

Figure 5: Identification: evolution of $c_t^1$and c_t^2.

given by the neuro-observer are in close agreement with the simulation data carried out from the dynamic model of the ozonation reactor.

These simulation results show the efficiency of the approach presented in this paper. The neuro-observer is able to give good estimates of the non measurable states of the considered chemical reactor. Owing to its ability to give a good estimates of the states, the neuro-observer can be used for other applications.

- Third, we check the least squares estimation ability to estimate the reaction rate constants for this chemical system. Based on (30), we use the estimations $\hat{c}_t^1$, $\hat{c}_t^2$ and $\hat{Q}_t$ to identify (estimate) the reaction rate constants k_1 and k_2. The design parameters are selected as follows:

$$\eta = 10^{16}, \widehat{K}_0 = \begin{bmatrix} 0.1 & 0 \\ 0 & 0.1 \end{bmatrix}.$$

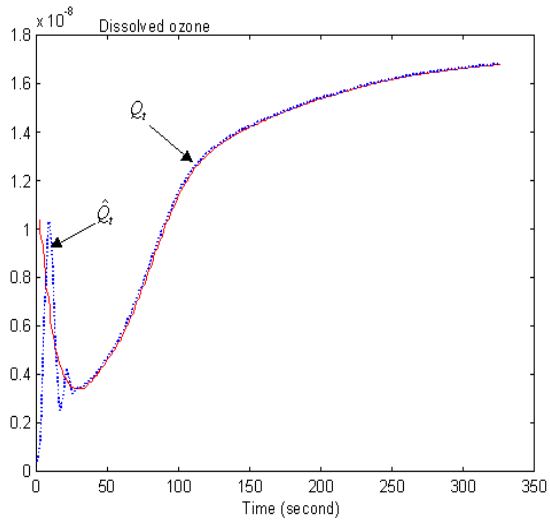

Figure 6: Identification: evolution of Q_t.

The estimation results are depicted in Fig. 9. The estimated constants k_1 and k_2 converge after approximately 1000 iterations. Notice that these constants are the key feature of the dynamic behaviour of the reactor. This figure shows that it is easy to estimate the constants k_1 and k_2 without computational burden.

6.2. Experiment 2 (High Rate Process)

Now consider the same reactor with

$$k_1 = 10^6, \quad k_2 = 10^5$$

(the other parameters remain unchanged). As before , we use the same neuro-observer and the LS- method. The simulation results are shown in Figs. 7-10. These figures indicate, respectively, how c_t^1, c_t^2, $W_{1,t}$, $\hat{k}_1$, and $\hat{k}_2$ evolve with stage (iteration) number.

The constants k_1 and k_2 are well estimated.

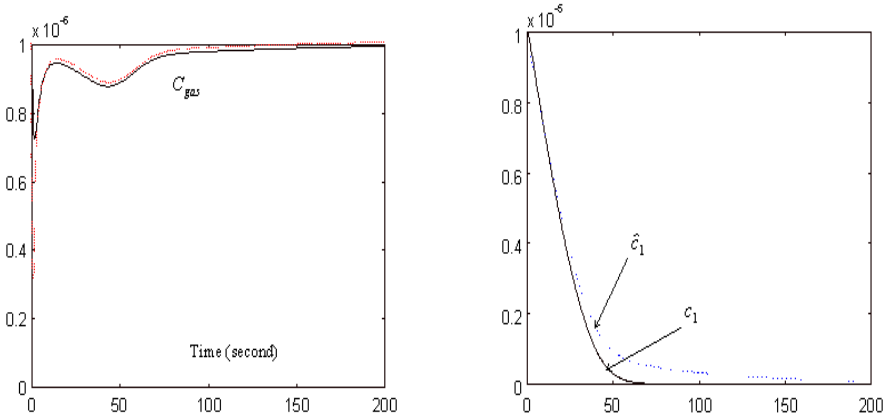

Figure 7: Identification: evolution of c_t^{out}. Neuro observer for the concentration c_t^1.

Since the considered system (ozonation reactor) is asymptotically stable, the presented observer is meaningful only when the convergence of the state estimation error to the guaranteed tolerance zone is faster than the dynamics of the process. The numerical experiments show that the dynamics of the neuro-observer are faster than those associated with the ozonation reactor.

7. Conclusions

A DNN-observer and a continuous least squares algorithm with a projection procedure have been presented for the simultaneous states and parameters estimation of an ozonation reactor. The analysis of the estimation error for this neuro-observer has been carried out. Several simulation results illustrate the perfomance and the feasibility of this estimation algorithm. The algorithm presented in this paper is used

- when the concentration sensors are not available or are very expensive;
- for the implementation of state-feedback controllers;

- etc.

The estimation algorithm, described and analyzed in this paper, can find potential applications in many industries such as chemical, mineral, etc.

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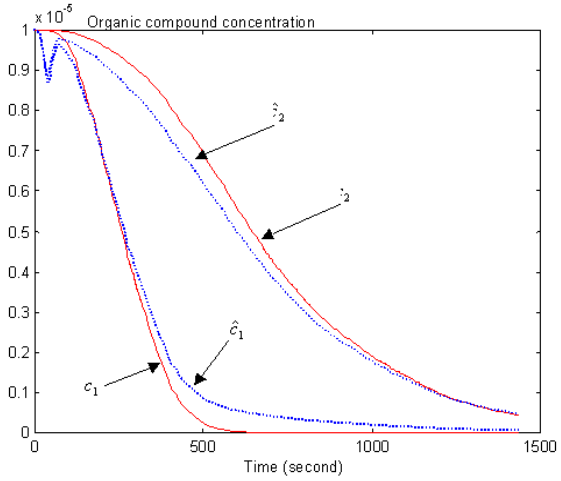


Figure 8: Neuro observer for the concentrations c_t^1 and c_t^2.

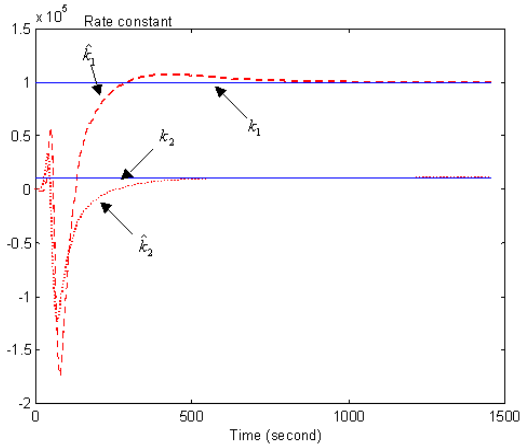


Figure 9: Estimations of k_1 and k_2.

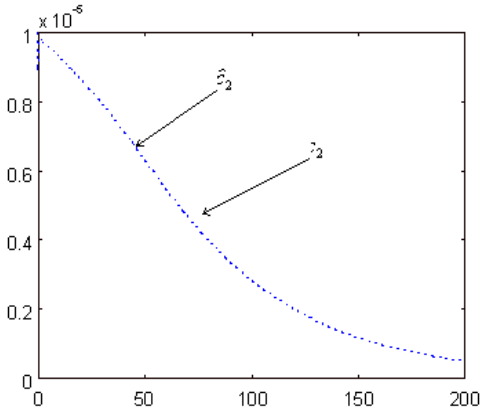
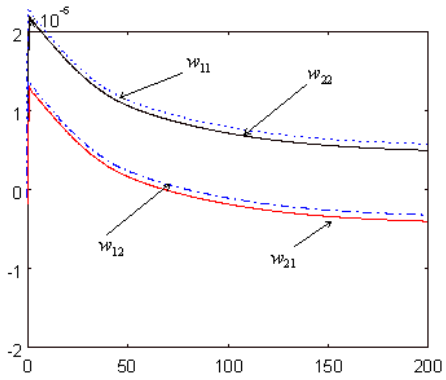
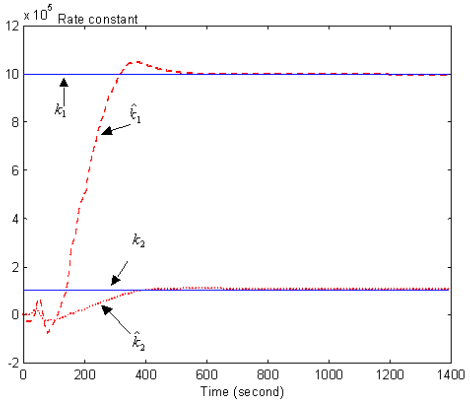


Figure 10: Identification: evolution of c_t^{out}.



The evolution of $W_{1,t}$.



The Estimations of k_1 and k_2.