STATE ESTIMATION IN FREE-RADICAL POLYMERIZATION REACTORS USING A NONLINEAR INTERCONNECTED HIGH GAIN OBSERVER

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ABSTRACT

In this paper, a new robust nonlinear observer is proposed for the reconstruction of the whole process state variables in a simulated polymerization reactor. It presents an interconnected high gain observer to perform the estimation. This observer has robust performance in the presence of measurement noise and model uncertainty. The global stability of the observer is analytically treated using the Lyapunov theory in order to show the conditions under which exponential convergence can be achieved. Finally, we present a numerical simulation to illustrate the effectiveness of the suggested approach.

Keywords: State estimation, interconnected observer, global stability, robustness, polymerization reactor

1. INTRODUCTION

The major obstacles in the application of computer control algorithms for polymerization reactor is the difficulty of finding adequate and reliable sensors for the on-line measurements of process key variables such as reactant and product concentrations. Sensors in the field of chemical processes are still very expensive and their maintenance is usually time consuming. One way to avoid these problems is to use estimation strategies.

State estimation methods have been initiated in the 1960s. The Kalman filter and the Luenberger observer were the first ones to be introduced ([13]; [20], [21]). The extensions of these two methods, known as extended Kalman filter (EKF) and extended Luenberger observer ([1]-[3]; [5]; [6]; [12]; [16]; [17]; [19]; [23]; [25]-[27]; [29]; [32];). However, several studies show the inadequacy of these methods for highly non-linear processes ([11]; [14]; [17]; [24]; [35]; [36]), because these methods use linear approximation of the nonlinear process model ([34]; [38]). Gauthier et al. ([9];[10]) stated a canonical form and necessary and sufficient observability conditions for a class of nonlinear systems that are linear with respect to inputs. Farza et al. ([7];[8]) developed a simple nonlinear observer for on-line estimation of the reaction rates in chemical and biochemical reactors. The principal advantage of this observer lies in the simplicity of its design and implementation.

Another procedure related to the construction of observers for nonlinear processes, is geometric differential methods [15]. The main idea is to find some state transformation that represents the original system as a linear equation plus a nonlinear term, which is a function of the system output.

A detailed discussion on many of the available state estimation techniques applicable to a broad class of nonlinear systems is provided by Mouyon [22]. Another comprehensive evaluation of various nonlinear observers was presented by Wang et al. [37].

The main objective of this paper is to design an interconnected high gain observer. The global stability of the observer is analytically treated using the Lyapunov theory in order to show the conditions under which exponential convergence can be achieved. The performance of the methodology proposed is illustrated taking as case study a CSTR polymerization reactor, where the main variables (initiator, monomer and growing polymer concentration) are estimated using continuous measurements of temperature, the total molar concentration of dead polymer and the total molar concentration of monomer units present as polymer.

The work is organized as follows. In Section 2, we present the dynamical model under consideration. The design of the corresponding nonlinear observer is presented in section 3. In section 4, the computer simulations were developed to illustrate the performance of the proposed nonlinear observer. Finally, we will close the paper with some concluding remarks.

2. DYNAMICAL MODEL OF THE FREE-RADICAL POLYMERIZATION REACTORS

Polymerization reactors are highly nonlinear processes characterized by multiple steady states, exotic dynamics, and potential reactor runaway ([30]; [33]).

In this paper we consider continuous stirred tank reactors in which free-radical polymerization takes place. The reaction mechanism of free-radical polymerization reactions is well understood and first-principles mathematical models of free-radical polymerization reactors are available in the polymerization literature [33].

Using the equal-reactivity hypothesis and the quasi-steady-state assumption for all radical species, and ignoring the reaction of chain transfer to the polymer, a mathematical model of the class of CSTR free-radical polymerization reactors has the form [30]:

$$\dot{C}_I = -k_I C_I + \frac{F_I C_{I_0} - F C_I}{V} \quad (1)$$

$$\dot{C}_m = -k_p C_m C_{gp} + \frac{F_m C_{m_0} - F C_m}{V} \quad (2)$$

$$\dot{T} = \frac{(-\Delta H)}{\rho C_p} k_p C_m C_{gp} - \frac{UA}{\rho C_p V}\left(T - T_j\right) + \frac{F(T_0 - T)}{V} \quad (3)$$

$$C_{gp} = \sqrt{\frac{2 f^* C_I k_I}{k_t}} \quad (4)$$

with:

$$k_r = A_r e^{-E_r/RT}, \quad r = p, I, t, tc$$

$$F = F_I + F_m + F_s$$

where C_i, C_m, T and C_{gp} represent the concentration of initiator, concentration of monomer, reactor temperature and concentration of growing polymer, respectively. The initiator is azobisisobutyronitrile (AIBN) dissolved in benzene, while the monomer is styrene and the solvent is benzene.

In order to complete the model, following Schmidt and Ray [33], two polymer chain moment equations are added to the mass and energy balances [30]:

$$\dot{\lambda}_0 = -0.5 k_{tc} C_{gp}^2 - \frac{F}{V}\lambda_0 \quad (5)$$

$$\dot{\lambda}_1 = k_p C_m C_{gp} - \frac{F}{V}\lambda_1 \quad (6)$$

where λ_0 is the total molar concentration of dead polymer and λ_1 is the total molar concentration of monomer units present as polymer.

Equations (1-6) can be written in the following dimensionless form [30]:

$$\dot{x}_1 = q_I u_1 - Q x_1 - \phi_I k_I(x_3) x_1 \quad (7)$$

$$\dot{x}_2 = q_m x_{2f} - Q x_2 - \phi_p k_p(x_3) x_2 x_4 \quad (8)$$

$$\dot{x}_3 = Q\left(x_{3f} - x_3\right) + \beta \phi_p k_p(x_3)\, x_2 x_4 - \delta(x_3 - u_2) \quad (9)$$

$$x_4 = \sqrt{\frac{2 f^* \phi_I k_I(x_3)}{\phi_t k_t(x_3)} x_1} \quad (10)$$

$$\dot{x}_5 = 0.5 \phi_t k_t(x_3) x_4^2 - x_5 \quad (11)$$

$$\dot{x}_6 = \phi_p k_p(x_3) x_2 x_4 - x_6 \quad (12)$$

where:

$$k_p(x_3) = \exp\left(\frac{\gamma_p x_3}{\gamma_p + x_3}\right),\ k_I(x_3) = \exp\left(\frac{\gamma_I \gamma_p x_3}{\gamma_p + x_3}\right),$$

$$k_t(x_3) = \exp\left(\frac{\gamma_t \gamma_p x_3}{\gamma_p + x_3}\right)$$

and $Q = q_I + q_m + q_s$

It can be shown that equation (11) becomes:

$$\dot{x}_5 = f^* \phi_I k_I(x_3) x_1 - x_5 \quad (13)$$

The values of the parameters used in the above equations are given in Table 1.

Parameter	value
q_I	0.11429
q_m	0.4
q_s	0.48571
x_{2f}	1.0
x_{3f}	0.0
β	13.17936
f^*	0.6
ϕ_I	0.01688
ϕ_p	2.19560×10^{7}
ϕ_t	9.6583×10^{12}
γ_I	4.18808
γ_p	10.77879
γ_t	0.23699
δ	0.74074

Table 1. Dimensionless parameters values of polymerization model.

Input variables for the observer are dimensionless initiator feed concentration (u_1) and dimensionless jacket temperature (u_2). Measured outputs in dimensionless form are temperature (x_3), the total molar concentration of dead polymer (x_5) and the total molar concentration of monomer units present as polymer (x_6). With this choice of output variables the system is completely observable. This finding is in agreement with the literature on observability in polymerization reactor systems ([28]; [31]; [35]).

3. OBSERVER SYNTHESIS

3.1. PRINCIPLE

There is no systematic method to design an observer for a given nonlinear control system, but several designs are available according to the specific characteristics of the considered nonlinear system. In particular the nonlinear system considered can be seen as an interconnection between several subsystems, where each of these subsystems satisfies some required conditions for an observer to be computable [4].

The idea of the interconnected observer is to design an observer for the whole nonlinear system considered, starting from the separate synthesis of observers for each subsystem with the following assumption: the states of the other subsystems are available for each observer.

Certain assumptions then make it possible to prove the convergence of the whole observers.

Class of systems considered. Each nonlinear subsystem obtained is put in the following form:

$$\begin{cases} \dot{X} = A(u,y)X + g(u,y,X) \\ \quad y = CX \end{cases} \tag{14}$$

with $X \in \mathbb{R}^n$, $u \in \mathbb{R}^m$ and $y \in \mathbb{R}^p$.

3.2. APPLICATION TO THE FREE-RADICAL POLYMERIZATION REACTORS

Input variables for the observer are dimensionless initiator feed concentration (u_1) and dimensionless jacket.

The free radical polymerization model can be rewritten in the form of three interconnected subsystems:

$$\begin{bmatrix} \dot{x}_3 \\ \dot{x}_4 \end{bmatrix} = \begin{bmatrix} -Q & 0 \\ 0 & -0.5Q \end{bmatrix}\begin{bmatrix} x_3 \\ x_4 \end{bmatrix} + \begin{bmatrix} Qx_{3f} + \beta\phi_p k_p(x_3)x_2x_4 \\ 0.5[\frac{x_4}{x_1}q_I u_1 - \phi_I k_I(x_3)x_4 + \frac{\gamma_p^2(\gamma_t-\gamma_I)x_4}{(\gamma_p+x_3)^2}(Q(x_{3f}-x_3) -\delta(x_3-u_2) + \beta\phi_p k_p(x_3)x_2x_4 - \delta(x_3-u_2)] \end{bmatrix} \tag{15}$$

$$\begin{bmatrix} \dot{x}_5 \\ \dot{x}_1 \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ 0 & -Q \end{bmatrix}\begin{bmatrix} x_5 \\ x_1 \end{bmatrix} + \begin{bmatrix} f^*\phi_I k_I(x_3)x_1 \\ q_I u_1 - \phi_I k_I(x_3)x_1 \end{bmatrix} \tag{16}$$

$$\begin{bmatrix} \dot{x}_6 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ 0 & -Q \end{bmatrix}\begin{bmatrix} x_6 \\ x_2 \end{bmatrix} + \begin{bmatrix} \phi_p k_p(x_3)x_2x_4 \\ q_m x_{2f} - \phi_p k_p(x_3)x_4x_2 \end{bmatrix} \tag{17}$$

The three subsystems (15), (16) and (17) can be represented in compact form as follows:

$$\begin{cases} \dot{X}_1 = A_1X_1 + g_1(u,y,X_1,X_3) \\ \quad y_1 = CX_1 \end{cases} \tag{18}$$

$$\begin{cases} \dot{X}_2 = A_2X_2 + g_2(u,y,X_1,X_2) \\ \quad y_2 = CX_2 \end{cases} \tag{19}$$

$$\begin{cases} \dot{X}_3 = A_3X_3 + g_3(u,y,X_1,X_3) \\ \quad y_3 = CX_3 \end{cases} \tag{20}$$

where:

$$A_1 = \begin{bmatrix} -Q & 0 \\ 0 & -0.5Q \end{bmatrix}, \quad A_2 = \begin{bmatrix} -1 & 0 \\ 0 & -Q \end{bmatrix},$$

$$A_3 = \begin{bmatrix} -1 & 0 \\ 0 & -Q \end{bmatrix}$$

$$g_1(u,y,X_1,X_3) = \begin{bmatrix} Qx_{3f} + \beta\phi_p k_p(x_3)x_2x_4 \\ 0.5[\frac{x_4}{x_1}q_I u_1 - \phi_I k_I(x_3)x_4 + \frac{\gamma_p^2(\gamma_t-\gamma_I)x_4}{(\gamma_p+x_3)^2}(Q(x_{3f}-x_3) -\delta(x_3-u_2) + \beta\phi_p k_p(x_3)x_2x_4 - \delta(x_3-u_2)] \end{bmatrix}$$

$$g_2(u,y,X_1,X_2) = \begin{bmatrix} f^*\phi_I k_I(x_3)x_1 \\ q_I u_1 - \phi_I k_I(x_3)x_1 \end{bmatrix},$$

$$g_3(u,y,X_1,X_3) = \begin{bmatrix} \phi_p k_p(x_3)x_2x_4 \\ q_m x_{2f} - \phi_p k_p(x_3)x_4x_2 \end{bmatrix}$$

$C = [1 \quad 0]$, $X_1 = [x_3 \quad x_4]^T$, $X_2 = [x_5 \quad x_1]^T$, $X_3 = [x_6 \quad x_2]^T$

Our goal is to design three interconnected observers for the subsystems (18), (19) and (20) to reconstruct the concentration of initiator, monomer and growing polymer. Consequently, we pose the following assumption:

A.1. The variables (u,y,X_3) and (u,y,X_1) are considered as known signals for the subsystems (18), (19) and (20) respectively. We denote $\upsilon_1 \overset{\Delta}{=} [u \;\; y \;\; X_3]^T$ and $\upsilon_2 \overset{\Delta}{=} [u \;\; y \;\; X_1]^T$

Then the three subsystems (18), (19) and (20) become:

$$\begin{cases} \dot{X}_1 = A_1X_1 + g_1(\upsilon_1,X_1) \\ \quad y_1 = CX_1 \end{cases} \tag{21}$$

$$\begin{cases} \dot{X}_2 = A_2X_2 + g_2(\upsilon_2,X_2) \\ \quad y_2 = CX_2 \end{cases} \tag{22}$$

$$\begin{cases} \dot{X}_3 = A_3X_3 + g_3(\upsilon_2,X_3) \\ \quad y_3 = CX_3 \end{cases} \tag{23}$$

A.2. υ_1 and υ_2 are bounded and supposed to be regularly persistent to guarantee the observability property of the subsystems (21), (22) and (23) respectively.

A.3. The function $g_1(u,y,X_1,X_3)$ is globally Lipschitz with respect to (X_3) uniformly with respect to the inputs (u,y,X_1).

A.4. The function $g_2(u,y,X_1,X_2)$ is globally Lipschitz with respect to (X_1) uniformly with respect to the inputs (u,y,X_2).

A.5. The function $g_3(u,y,X_1,X_3)$ is globally Lipschitz with respect to (X_1) uniformly with respect to the inputs (u,y,X_3).

Under the above assumptions, the nonlinear interconnected observers for the subsystems (18), (19) and (20) are given by:

$$\begin{cases} \dot{\hat{X}}_1 = A_1\hat{X}_1 + g_1(u,y,\hat{X}_1,\hat{X}_3) + S_{\theta_1}^{-1}C^TC(X_1-\hat{X}_1) \\ \theta_1 S_{\theta_1} + A_1^T S_{\theta_1} + S_{\theta_1}A_1 - C^TC = 0 \\ \hat{y}_1 = C\hat{X}_1 \end{cases} \quad (24)$$

$$\begin{cases} \dot{\hat{X}}_2 = A_2\hat{X}_2 + g_2(u,y,\hat{X}_2) + S_{\theta_2}^{-1}C^TC(X_2-\hat{X}_2) \\ \theta_2 S_{\theta_2} + A_2^T S_{\theta_2} + S_{\theta_2}A_2 - C^TC = 0 \\ \hat{y}_2 = C\hat{X}_2 \end{cases} \quad (25)$$

$$\begin{cases} \dot{\hat{X}}_3 = A_3\hat{X}_3 + g_3(u,y,\hat{X}_1,\hat{X}_3) + S_{\theta_3}^{-1}C^TC(X_3-\hat{X}_3) \\ \theta_3 S_{\theta_3} + A_3^T S_{\theta_3} + S_{\theta_3}A_3 - C^TC = 0 \\ \hat{y}_3 = C\hat{X}_3 \end{cases} \quad (26)$$

where:

$$g_1(u,y,\hat{X}_1,\hat{X}_3) = \begin{bmatrix} Qx_{3f} + \beta\phi_p k_p(\hat{x}_3)\hat{x}_2\hat{x}_4 \\ 0.5[\frac{\hat{x}_4}{\hat{x}_1}q_I u_1 - \phi_I k_I(\hat{x}_3)\hat{x}_4 + \frac{\gamma_p^2(\gamma_t-\gamma_I)\hat{x}_4}{(\gamma_p+\hat{x}_3)^2}(Q(x_{3f}-\hat{x}_3) \\ -\delta(\hat{x}_3-u_2) \\ +\beta\phi_p k_p(\hat{x}_3)\hat{x}_2\hat{x}_4 - \delta(\hat{x}_3-u_2)] \end{bmatrix}$$

$$g_2(u,y,\hat{X}_1,\hat{X}_2) = \begin{bmatrix} f^*\phi_I k_I(\hat{x}_3)\hat{x}_1 \\ q_I u_1 - \phi_I k_I(\hat{x}_3)\hat{x}_1 \end{bmatrix},$$

$$g_3(u,y,\hat{X}_1,\hat{X}_3) = \begin{bmatrix} \phi_p k_p(\hat{x}_3)\hat{x}_2\hat{x}_4 \\ q_m x_{2f} - \phi_p k_p(\hat{x}_3)\hat{x}_4\hat{x}_2 \end{bmatrix}$$

$C = [1 \quad 0]$, $\hat{X}_1 = [\hat{x}_3 \quad \hat{x}_4]^T$, $\hat{X}_2 = [\hat{x}_5 \quad \hat{x}_1]^T$, $\hat{X}_3 = [\hat{x}_6 \quad \hat{x}_2]^T$

In order to prove the estimation error convergence of the three observers, we present the stability analysis of the three observers based on Lyapunov theory.

3.3. GLOBAL STABILITY ANALYSIS WITH PARAMETERS UNCERTAINTY

Define the estimation errors as:

$e_1 = X_1 - \hat{X}_1$, $e_2 = X_2 - \hat{X}_2$, $e_3 = X_3 - \hat{X}_3$

We then have:

$$\dot{e}_1 = [A_1 - S_{\theta_1}^{-1}C^TC]e_1 + g_1(u,y,X_1,X_3) - g_1(u,y,\hat{X}_1,\hat{X}_3) \quad (27)$$

$$\dot{e}_2 = [A_2 - S_{\theta_2}^{-1}C^TC]e_2 + g_2(u,y,X_1,X_2) - g_2(u,y,\hat{X}_1,\hat{X}_2) \quad (28)$$

$$\dot{e}_3 = [A_3 - S_{\theta_3}^{-1}C^TC]e_3 + g_3(u,y,X_1,X_3) - g_3(u,y,\hat{X}_1,\hat{X}_3) \quad (29)$$

Now, let us consider that in the process model there is some dynamics uncertainty, the equations (27)-(29) become:

$$\dot{e}_1 = [A_1 - S_{\theta_1}^{-1}C^TC]e_1 + g_1(u,y,X_1,X_3) - g_1(u,y,\hat{X}_1,\hat{X}_3) + \Delta A_1 X_1 + \Delta g_1(u,y,X_1,X_3) \quad (30)$$

$$\dot{e}_2 = [A_2 - S_{\theta_2}^{-1}C^TC]e_2 + g_2(u,y,X_1,X_2) - g_2(u,y,\hat{X}_1,\hat{X}_2) + \Delta A_2 X_2 + \Delta g_2(u,y,X_1,X_2) \quad (31)$$

$$\dot{e}_3 = [A_3 - S_{\theta_3}^{-1}C^TC]e_3 + g_3(u,y,X_1,X_3) - g_3(u,y,\hat{X}_1,\hat{X}_3) + \Delta A_3 X_3 + \Delta g_3(u,y,X_1,X_3) \quad (32)$$

where ΔA_i and Δg_i $(i = 1,2,3)$ are the unknown parts of the process dynamics.

A.6. Suppose that:

$\|\Delta A_i\| \leq \rho_i$, $i = 1,2,3$

$\|\Delta g_1(u,y,X_1,X_3)\| \leq \mu_1$

$\|\Delta g_2(u,y,X_1,X_2)\| \leq \mu_2$

$\|\Delta g_3(u,y,X_1,X_3)\| \leq \mu_3$

This assumption is justified by the fact that the process parameters are bounded and are known with a certain precision and also by the fact that the states variables are bounded.

Theorem:

If assumptions A1-A6 are satisfied, then the system (24)-(26) is an exponential observer for system (18) - (20) for appropriate choice of θ_1, θ_2 and θ_3.

Proof:

Define $V(e) = \sum_{i=1}^{3} V_i(e_i)$ as the Lyapunov candidate function.

where $V_i(e_i) = e_i^T S_{\theta_i} e_i$. Then its time derivative is:

$$\dot{V}_i = \frac{\partial V_i}{\partial X} = \frac{\partial V_i}{\partial e_i} \times \frac{\partial e_i}{\partial X}$$

$$\dot{V}_i = 2e_i^T S_{\theta_i}[(A_i - S_{\theta_i}^{-1}C^TC)e_i + g_i(u,y,X) - g_i(u,y,\hat{X}) + \Delta A_i X_i + \Delta g_i(u,y,X)]$$

$$\dot{V}_i = 2e_i^T S_{\theta_i} A_i e_i - 2e_i^T C^TCe_i + 2e_i^T S_{\theta_i}[g_i(u,y,X) - g_i(u,y,\hat{X})] + 2e_i^T S_{\theta_i}[\Delta A_i X_i + \Delta g_i(u,y,X)]$$

$$\dot{V}_i = e_i^T(-\theta_i S_{\theta_i} - C^TC)e_i - 2e_i^T C^TCe_i + 2e_i^T S_{\theta_i}[g_i(u,y,X) - g_i(u,y,\hat{X})] + 2e_i^T S_{\theta_i}[\Delta A_i X_i + \Delta g_i(u,y,X)]$$

$$\dot{V}_i = -\theta_i e_i^T S_{\theta_i} e_i - 3e_i^T C^TCe_i + 2e_i^T S_{\theta_i}[g_i(u,y,X) - g_i(u,y,\hat{X})] + 2e_i^T S_{\theta_i}[\Delta A_i X_i + \Delta g_i(u,y,X)]$$

$$\dot{V}_i \leq -\theta_i V_i + 2\|e_i\|\|S_{\theta_i}\| \|g_i(u,y,X) - g_i(u,y,\hat{X})\|$$

$$+2\|e_i\|\|S_{\theta_i}\|\|\Delta A_i\|\|X_i\|$$
$$+2\|e_i\|\|S_{\theta_i}\|\|\Delta g_i(u,y,X)\|$$

By using the Lipschitz condition of assumptions A.2-A.6, we have:

$$\|S_{\theta_i}\| \le \eta_{max}(S_{\theta_i})$$
$$\|g_i(u,y,X) - g_i(u,y,\hat{X})\| \le \zeta_i \|e_i\|$$
$$\|X_i\| \le \sigma_i$$
$$\|\Delta A_i\| \le \rho_i$$
$$\|\Delta g_i(u,y,X)\| \le \mu_i$$

where η_{max} denote the largest eigenvalue of S_{θ_i}. $\zeta_i, \sigma_i, \rho_i$ and μ_i denote, respectively, the Lipschitz constants of $g_i(u,y,X)$, X_i, ΔA_i and $\Delta g_i(u,y,X)$

Then, we obtain:

$$\dot{V}_i \le -\theta_i V_i + 2\eta_{max}(S_{\theta_i})\zeta_i \|e_i\|^2$$
$$+2\eta_{max}(S_{\theta_i})\rho_i\sigma_i\|e_i\|^2 + 2\eta_{max}(S_{\theta_i})\mu_i\|e_i\|^2$$
$$\dot{V}_i \le -\theta_i V_i + 2\eta_{max}(S_{\theta_i})(\zeta_i + \rho_i\sigma_i + \mu_i)\|e_i\|^2$$
$$\dot{V}_i \le -\theta_i V_i + 2\frac{\eta_{max}(S_{\theta_i})}{\eta_{min}(S_{\theta_i})}(\zeta_i + \rho_i\sigma_i + \mu_i)V_i$$

where η_{min} is the minimum eigenvalue of matrix S_{θ_i}

since: $\|e_i\|^2 \le \frac{1}{\eta_{min}(S_{\theta_i})} V_1$

$$\dot{V}_i \le -(\theta_i - \Omega_i)V_i$$

with $\Omega_i = (\zeta_i + \rho_i\sigma_i + \mu_i)$

Hence, it results that:

$$\dot{V} \le -\sum_{i=1}^{3}(\theta_i - \Omega_i)V_i$$

Now choose $\theta_i > \Omega_i$. This completes the proof of Theorem.

4. SIMULATION RESULTS

Simulations, using MATLAB Software Package, have been carried out to verify the effectiveness of the proposed method.

A block diagram of the observer system is shown in Figure 1.

The values of the model parameters used in simulation are given in Table 1. The process was excited through u_1 and u_2 ($u_1 = 0.06769$, $u_2 = 1.2788$).

The states initial conditions were set to:

$$x(0) = [1.4967 \times 10^{-6}\,;\ 0.0345\ ;\ 0.65326\ ;$$
$$1.6593 \times 10^{-9}\,;\ 5.7484 \times 10^{-6}\,; 0.00115]^T,$$
$$\hat{X}_1(0) = [2.4937 \times 10^{-9}\,;\ 0.75326]^T,$$
$$\hat{X}_2(0) = [0.7484 \times 10^{-6}; 5.4967 \times 10^{-3}]^T$$
$$\hat{X}_3(0) = [0.0315\,; 0.545]^T$$

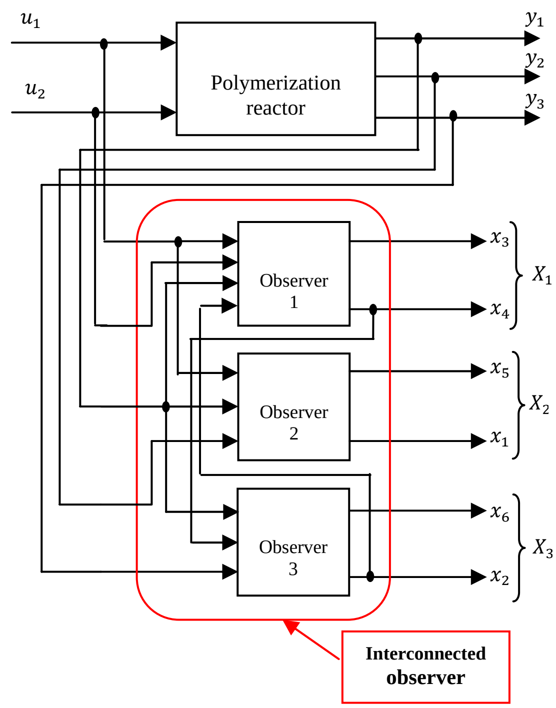

Figure 1. Nonlinear observer block diagram

The estimation results obtained are depicted in Figures 2–7.

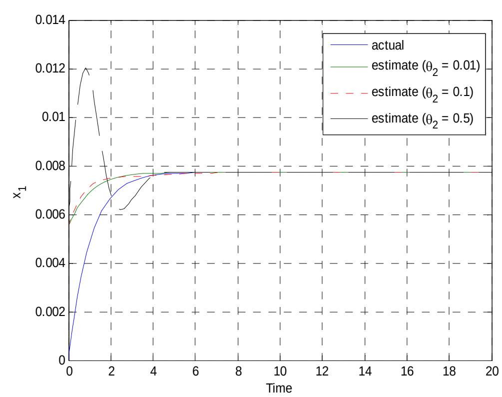

Figure 2. Real and estimated dimensionless initiator concentration.

The influence of the convergence parameter θ on the speed of convergence is clearly shown in these figures:

- A high value of θ decreases the observer time convergence, but also it leads to a high oscillation.
- A low value of θ reduces the oscillations, but it increases the observer time convergence.

In fact, it is right to choose an optimal value of θ which fulfill the desired performances.

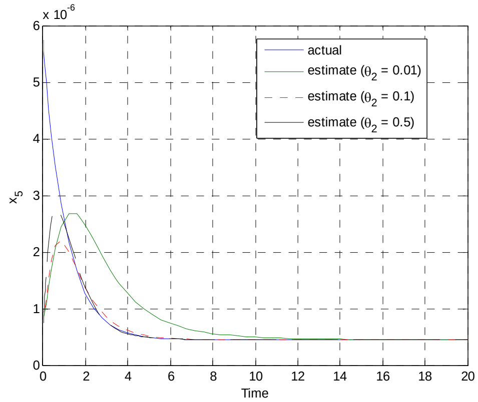

Figure 3. Real and estimated dimensionless dead polymer concentration

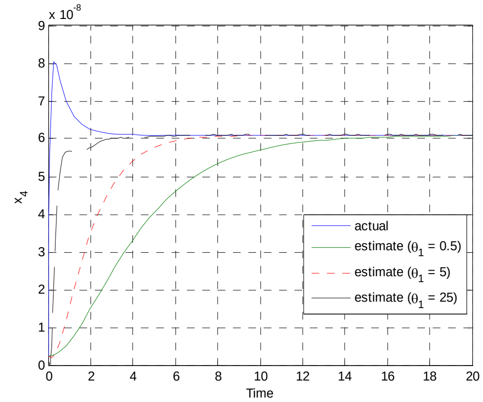

Figure 5. Real and estimated dimensionless growing polymer concentration

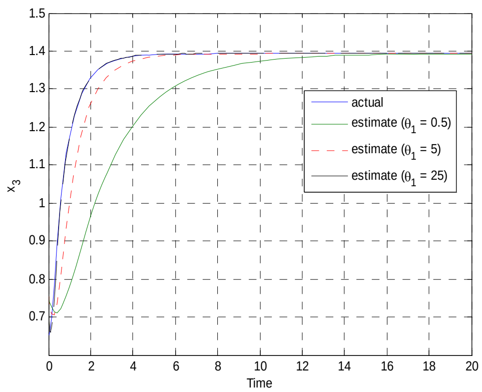

Figure 4. Real and estimated dimensionless reactor temperature

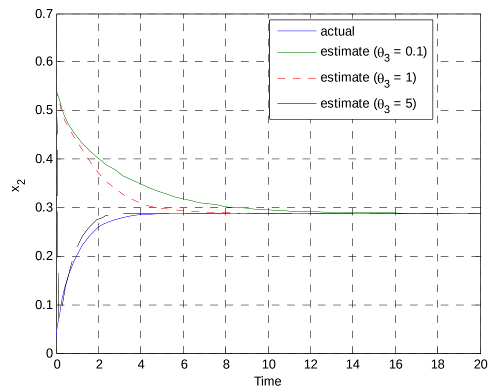

Figure 6. Real and estimated dimensionless monomer concentration

In order to test the behavior of the proposed nonlinear observer in the presence of measurement noise, several estimations were performed. For this purpose, white Gaussian noises with variances of $\pm 5\%$ are simultaneously added to the outputs x_3, x_5 and x_6. Figures 8-13 show the estimation results obtained in this case. It clearly appears that the observer conserve its performances and robustness in presence of noises. In these figures, the influence of θ on the robustness with respect to measurement noise is shown. Here it is seen that the bigger values of θ, increases the sensitivity of the estimated state to the measurement noise.

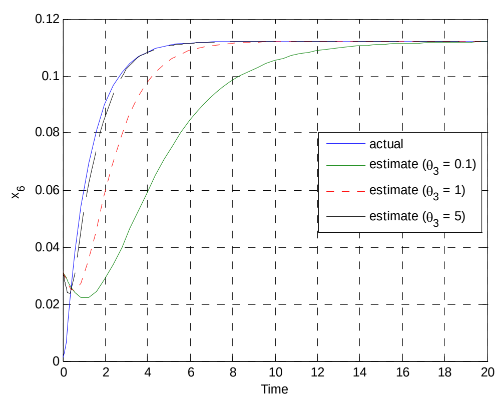

Figure 7. Real and estimated dimensionless of concentration of monomer units present as polymer

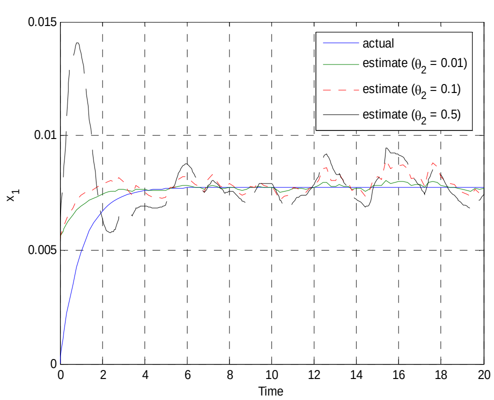

Figure 8. Real and estimated dimensionless initiator concentration in presence of measure noises

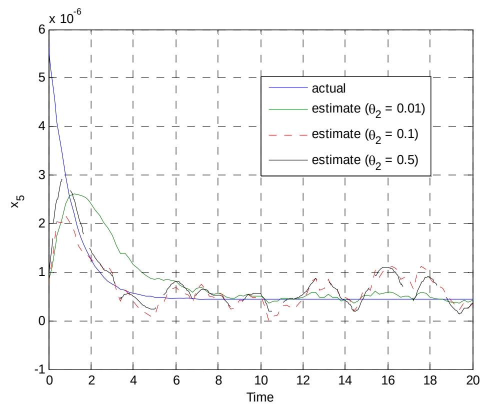

Figure 9. Real and estimated dimensionless dead polymer concentration in presence of measure noises

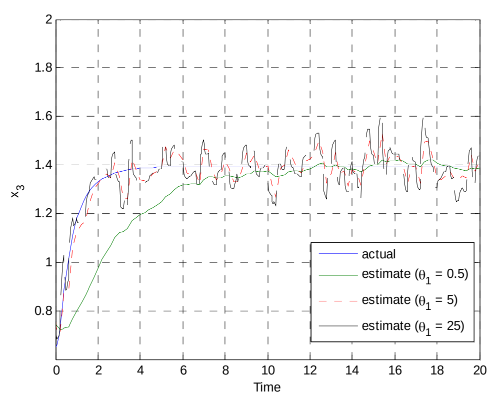

Figure 10: Real and estimated dimensionless reactor temperature in presence of measure noises

To test the observer performance in other disadvantageous conditions, additional simulations were carried out based on model uncertainty. For this purpose, it was considered a mismatch between the real activation energy and its value in the model. In this work, a difference up to 2% between the real parameter and its value in the model was considered.

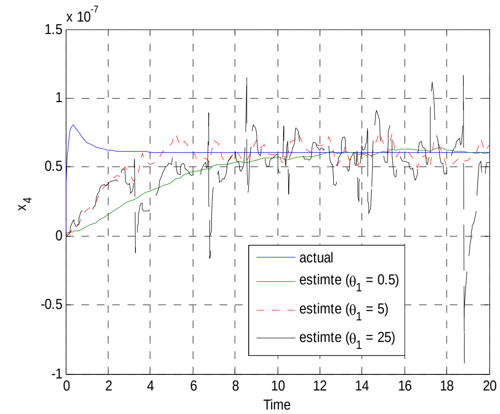

Figure 11. Real and estimated dimensionless growing polymer concentration in presence of measure noises

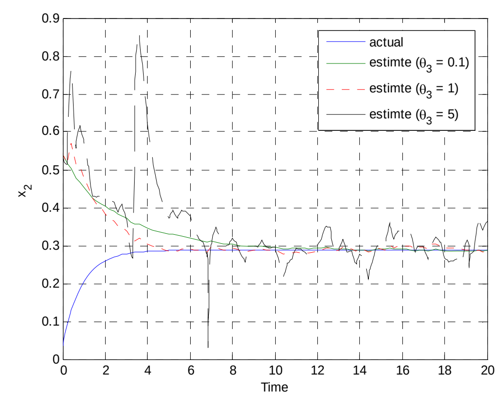

Figure 12. Real and estimated dimensionless monomer concentration in presence of measure noises

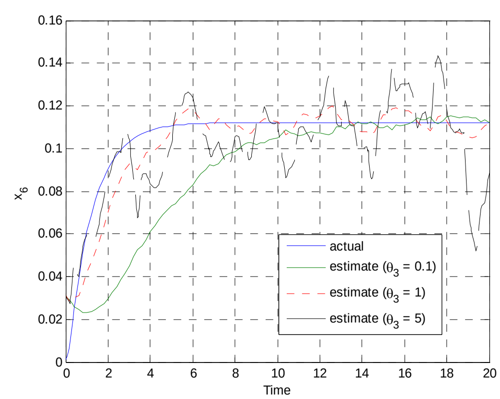

Figure 13: Real and estimated dimensionless of concentration of monomer units present as polymer in presence of measure noises.

Figures 14-19 shows the influence of θ on the robustness with respect to modeling errors. It is seen that for small values of θ there is a large error between the observed states and the real ones, due to the modeling error.

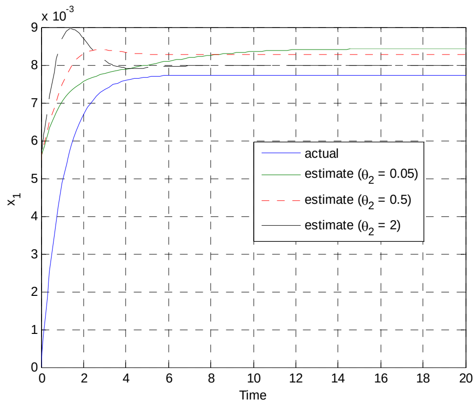

Figure 14. Real and estimated dimensionless initiator concentration in presence of modeling error

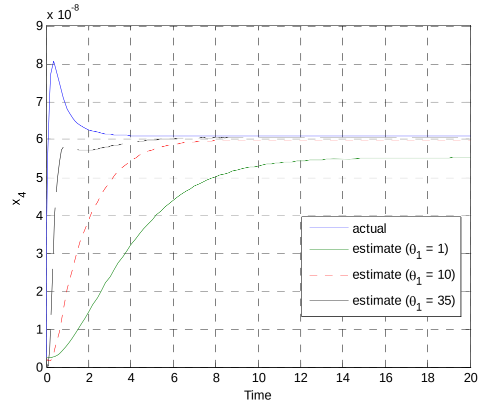

Figure 17. Real and estimated dimensionless growing polymer concentration in presence of modeling error

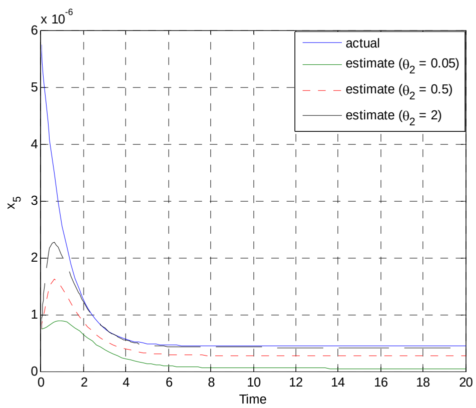

Figure 15. Real and estimated dimensionless dead polymer concentration in presence of modeling error

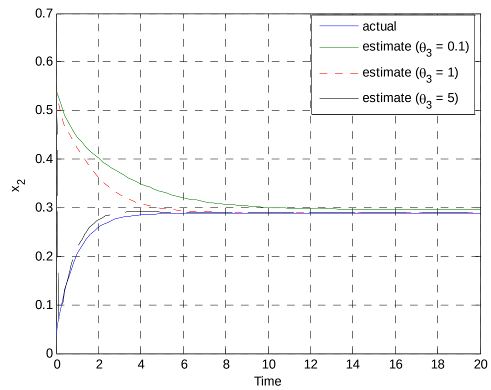

Figure 18. Real and estimated dimensionless monomer concentration in presence of modeling error

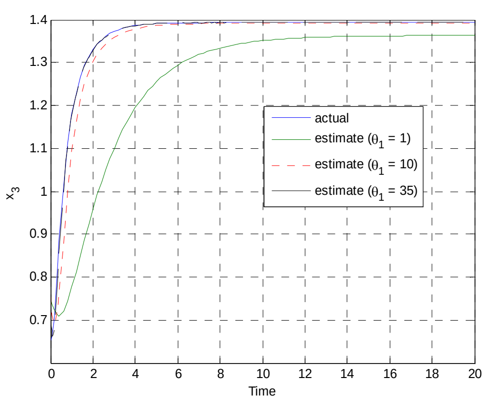

Figure 16: Real and estimated dimensionless reactor temperature in presence of modeling error

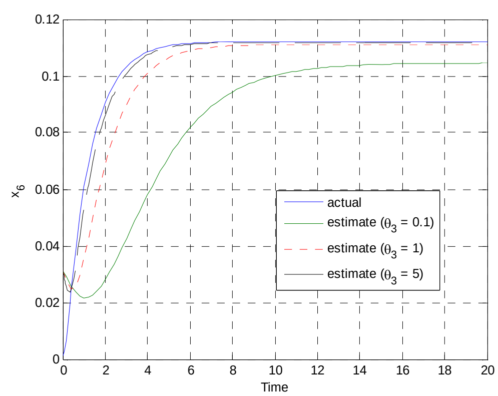

Figure 19: Real and estimated dimensionless of concentration of monomer units present as polymer in presence of modeling error

5. CONCLUSION

A nonlinear interconnected high gain observer for estimating states variables in MIMO free radical polymerization system has been introduced. Convergence of the estimated states to the true ones is obtained. The observer implementation is simple and it requires small computational effort. Moreover, the nonlinear observer exhibits a satisfactory performance when used with noisy measurements and dynamics uncertainty. The observer gain can be easily tuned in order to find an optimum compromise between fast convergence and robustness. Finally, computer simulations were developed to illustrate the performance of the nonlinear observer. Simulation results showed the good performance that can be achieved with the proposed method.

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NOTATION

C_I : Initiator concentration.

C_{I_0} : Initiator feed concentration.

C_m : Monomer concentration.

C_{m_0} : Monomer feed concentration.

C_{gp} : Growing polymer concentration.

T : Reactor temperature.

T_0 : Reactor feed temperature.

T_j : Cooling jacket temperature.

k_I : Rate constant for termination.

k_p : Rate constant for propagation.

k_t : Rate constant for termination.

F_I : Initiator flowrate.

F_m : Monomer flowrate.

F_s : Solvent flowrate.

F : Total flowrate through reactor.

V : Reactor volume.

ΔH : Heat of reaction.

ρ : Density of the reaction mixture.

C_p : Heat capacity of the reaction mixture.

U : Overall heat transfer coefficient.

A : Heat transfer area.

f^* : Initiator efficiency.

λ_0 : Concentration of dead polymer.

λ_1 : Concentration of monomer units present as polymer.