Chemical Engineering Journal 87 (2002) 351–356

Chemical Engineering Journal

www.elsevier.com/locate/cej

Reaction heat estimation in continuous chemical reactors using high gain observers

Ricardo Aguilar [a,b,*], Rafael Martínez-Guerra [b], Alexander Poznyak [b]

[a] Departamento de Energía, Universidad Autónoma Metropolitana-Azcapotzalco, CINVESTAV-IPN, Apartado Postal 75-338, CP 07300, Mexico, D.F., Mexico

[b] Departamento de Control Automático, Universidad Autónoma Metropolitana-Azcapotzalco, CINVESTAV-IPN, Apartado Postal 75-338, CP 07300, Mexico, D.F., Mexico

Received 9 August 2000; accepted 28 September 2001

Abstract

The problem of the on-line estimation of the reaction heat in a continuous stirred tank reactor (CSTR) from temperature measurements is addressed in this paper. The proposed uncertainty observer is based on differential algebraic techniques, such that the algebraic observability condition of the uncertainty from temperature measurements is easily verified and the observer structure is very simple, which lead to feasible implementation. The observer proposed is robust against noisy measurements and sustained disturbances. The good performance of the observer is shown by means of numerical simulations.

Keywords: Uncertainty observer; Noisy measurements; Sustained disturbances; Robustness

1. Introduction

The continuous stirred tank reactors (CSTRs) are widely used in the chemical industry, e.g. in polymerization, petrochemical, pharmaceutical, biochemical, etc. Therefore, their importance in the industry is great, nowadays the demands in security, efficiency, environmental restrictions and so on makes the process engineers to apply more sophisticated techniques in modeling, monitoring and controlling strategies for obtaining high performance in the processes.

Generally speaking, the evaluation of reaction heats is a difficult task in chemical processes, due the complexity of the related physico-chemical phenomena. This led us to construct uncertain mathematical models of this process, such that the problem of on-line estimation of reaction heats must be tackled. Currently, estimation theory is one of the most active research area necessary to obtain on-line estimates of unknown terms related to mathematical models for process identification and control purposes. Schuler and Schmidt [1] used an uncertainty estimator based on calorimetric balances to infer the reaction heats in chemical reactors. Alvarez-Ramirez et al. [2] used this estimation methodology coupled with a linearizing controller to regulate temperature in FCC units like Aguilar et al. [3] who employed this control scheme too for the substrate regulation in a continuous bioreactor, but for dynamic estimation of uncertain terms, these class of strategies become unstable when the measurements are noisy, because the derivative related to the accumulation terms cannot be calculated adequately, which can lead to poor closed-loop performance or instabilities in the process.

Georgakis and coworkers [4] proposed a Kalman filtering technique to estimate kinetics terms in a polymerization reactor with good results, and following this research line, Aguilar et al. [5] using filtering techniques, designed a nonlinear controller based on observer for the regulation of temperature in a CSTR with complex behavior. In this kind of estimation methodologies based on observer Kalman structures, the convergence analysis of the observer is difficult because the observer gain is based on an approximation of the covariance matrix related with the estimation error. Besides, it has the problem of the initial condition proposed for the observer equation and the *peaking* phenomena can become closed-loop leading to the unstable behavior of the system.

2. Mathematical background

In the beginning of the century, Ritt [6] introduced the differential algebra with the main idea related to bring

* Corresponding author. Present address: Departamento de Energía, Universidad Autónoma Metropolitana-Azcapotzalco, CINVESTAV-IPN, Apartado Postal 75-338, CP 07300, Mexico, D.F., Mexico.

E-mail addresses: raguilar@correo.azc.uam.mx (R. Aguilar), rguerra@ctrl.cinvestav.mx (R. Martínez-Guerra), apoznyak@ctrl.cinvestav.mx (A. Poznyak).

1385-8947/02/$ – see front matter © 2002 Elsevier Science B.V. All rights reserved.
PII: S1385-8947(01)00232-7

the theory of systems of differential equations, which are algebraic in the unknowns and their derivatives some of the completeness enjoyed by the theory of systems of algebraic equations. This mathematical approach has recently been shown to be the most effective tool for understanding basic questions such as input–output inversions and realizations [7–9]. Now, before showing the proposed estimation methodology, the following definitions must be considered [10,11]:

Definition 1. A differential field extension L/K is given by two differential field, L and K, such that:

1. $K \subseteq L$.
2. The derivation of K is the restriction to K of the derivation of L.

Definition 2. Let u be a differential scalar indeterminate and let k be a differential field, with derivation denoted by d( )/dt.

Definition 3. A dynamics is a finitely generated differentially algebraic extension $\mathfrak{J}/k\langle u\rangle$. This means that any element of $\mathfrak{J}$ satisfies a differential algebraic equation with coefficients which are rational functions over k in the components of u and a finite number of their time derivatives.

Definition 4. Let $\{u, y\}$ be a subset of $\mathfrak{J}$ in a dynamics $\mathfrak{J}/k\langle u\rangle$. An element in $\mathfrak{J}$ is said to be observable with respect to $\{u, y\}$ if it is algebraic over $k\langle u, y\rangle$. Therefore a state x is said to be observable if and only if it is observable with respect to $\{u, y\}$.

Definition 5. A dynamics $\mathfrak{J}/k\langle u\rangle$ with output y is said to be observable if and only if any state is so.

3. Problem statement

Consider the following nonlinear dynamic system related with a mathematical model of a CSTR [12]:

Mass balance:

$$\dot{X}_0 = \theta(X_{0e} - X_0) - KX_0^2 \tag{1}$$

Energy balance:

$$\dot{X}_1 = \theta(X_{1e} - X_1) + X_2 + \gamma(u - X_1) \tag{2}$$

Uncertainty dynamics (reaction heat):

$$\dot{X}_2 = f(X_1, X_2) \tag{3}$$

System output:

$$Y = X_1 \tag{4}$$

where X_0 is the reactive concentration, K the kinetic constant, X_1 the reactor temperature, X_2 the uncertain term related with the heat generation by chemical reaction, Y the system output, u the system input (temperature of the cooling jacket) and θ and γ are the inverse of the residence time and the heat transfer global coefficient, respectively.

We consider the subsystem given by Eqs. (2)–(4). From this, the following differential algebraic equations can be obtained:

$$X_1 - Y = 0 \tag{5}$$

$$\dot{Y} + (\theta + \gamma)Y - \theta X_{1e} - \gamma u - X_2 = 0 \tag{6}$$

Now, a new concept called uncertainty algebraically observable is introduced:

Definition 6. An element X_u in $\mathfrak{J}$ is said to be uncertainty algebraically observable if X_u satisfies a differential algebraic equation with coefficients over $k\langle u, y\rangle$.

From Definitions 5 and 6, along with the differential algebraic equations (5) and (6), the pair uncertainty–temperature i.e. $\{X_1, X_2\}$ is universally observable in the Diop–Fliess sense [11].

The corresponding input–output representation of the system (2) and (3) is given by:

$$\ddot{Y} + (\theta + \gamma)\dot{Y} = \gamma\dot{u} + f(X_1, X_2) \tag{7}$$

which can be represented in a generalized observability canonical form using the following change of variables:

$$\eta_i = \frac{\mathrm{d}^{i-1}Y}{\mathrm{d}t^{i-1}} \tag{8}$$

to obtain

$$\dot{\eta}_1 = \eta_2, \qquad \dot{\eta}_2 = \Phi(\eta_1, \eta_2, \dot{u}), \qquad Y = \eta_1 \tag{9}$$

Now, as it can be seen from the nature of the system given by Eq. (9), a standard structure of a Luenberger type observer based with a copy of the system plus measurement error correction is not realizable since the term Φ is unknown. Therefore, the following observer is proposed in order to filter an estimate of η_1 and η_2, respectively:

$$\dot{\hat{\eta}}_1 = \hat{\eta}_2 - l\tau^{-1}(\eta_1 - \hat{\eta}_1) \tag{10}$$

$$\dot{\hat{\eta}}_2 = -l^2\tau^{-1}(\eta_1 - \hat{\eta}_1) \tag{11}$$

finally from Eq. (6), the reaction heat is evaluated by the following equation:

$$\hat{X}_2 = \hat{\eta}_2 - \theta(X_{1e} - \hat{\eta}_1) - \gamma(u - \hat{\eta}_1) \tag{12}$$

the idea to estimate η_1 and filtering it is that this variable is directly the reactor temperature (system output) and in accordance with Eq. (12), if the temperature measurements are noisy, the noise would be transmitted to the estimation of the reaction heat which can lead to poor performance. In this work, it is assumed that the reactor temperature $X_1 \geq 0$ is bounded for all $t > 0$. Consequently, the concentrations inside the reactor are bounded input to bounded output

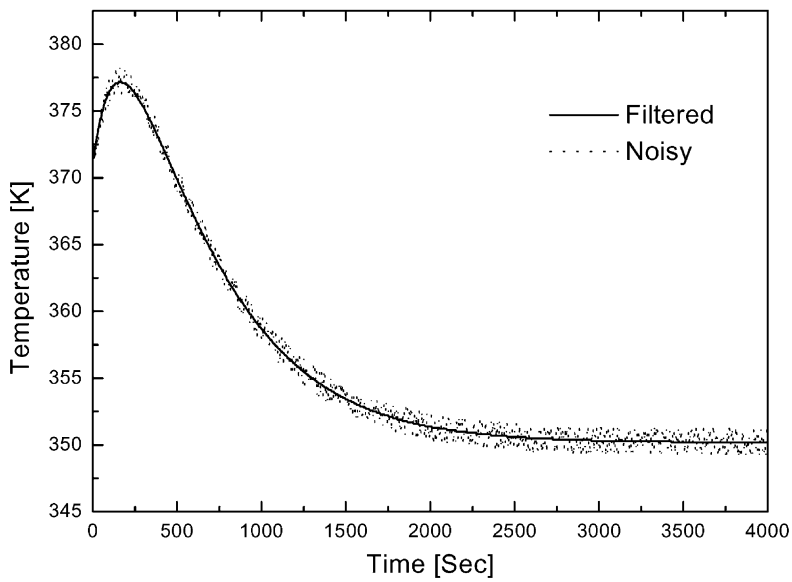

Fig. 1. Filtering process of the reactor temperature measurements ($l = 0.01$).

state. It is also assumed that the uncertain term remains bounded. The restraint of the heat of reaction (uncertain term) is common for a wide class of chemical reactions and is a consequence of the characteristics of the mathematical modeling commonly employed; chemical reactions are usually Lipschitz with respect to temperature. It is not hard to see that global Lipschitz of $\Delta H_f R(y_f, T_r)$ property is found if the functionality $R(y_f, T_r)$ with respect to temperature is of Arrhenius type.

The estimation errors are defined as:

$$e_1 = \eta_1 - \hat{\eta}_1 \tag{13}$$

$$e_2 = \frac{\eta_2 - \hat{\eta}_2}{l} \tag{14}$$

Considering Eqs. (13) and (14), the dynamic of the estimation error is defined as

$$\dot{E} = lAE + \Omega(\eta_1, \eta_2) \tag{15}$$

where:

$$E = \begin{bmatrix} e_1 \\ e_2 \end{bmatrix}, \qquad A = \begin{bmatrix} \tau^{-1} & 1 \\ \tau^{-1} & 0 \end{bmatrix}, \qquad \Omega = \begin{bmatrix} 0 \\ \dfrac{\Phi}{l} \end{bmatrix}$$

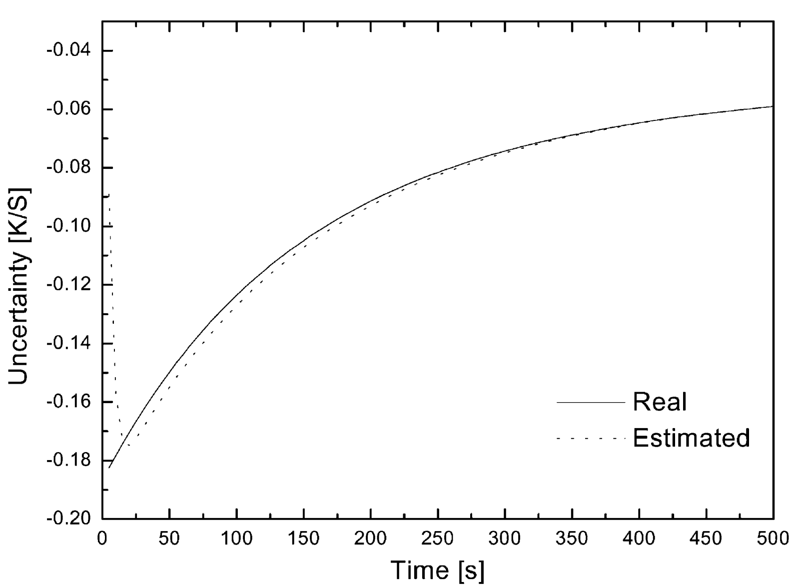

Fig. 2. On-line estimation of the reaction heat ($l = 0.01$).

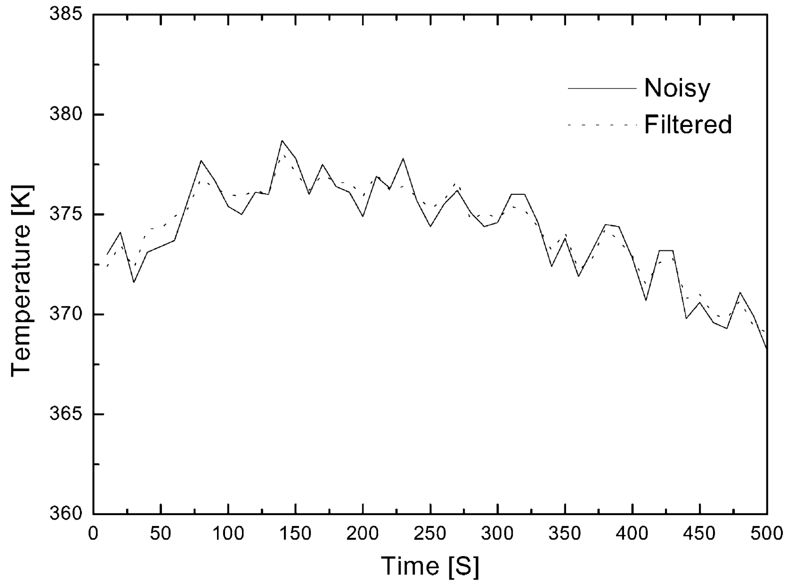

Fig. 3. Filtering process of the reactor temperature measurements considering sustained disturbances ($l = 0.01$).

Considering the following assumptions:

1. Ω is bounded, i.e. $||\Omega|| \leq \Gamma$.
2. There exist two positive constants $j > 0$ and $\lambda > 0$, such that:

$$||\exp(lAt)E|| \leq j\exp(-l\lambda t)||E||$$

Now, solving Eq. (15), the next expression is obtained:

$$E = \exp(lAt)E_0 + \int_0^t \exp\{lA(t-s)\}\Omega\, \mathrm{d}s \tag{16}$$

Considering the assumptions 1 and 2 and taking norms for both sides of the Eq. (16), the following equation is generated:

$$||E|| \leq j\exp(-l\lambda t)\left[||E_0|| - \frac{j\Gamma}{l^2\lambda}\right] + \frac{j\Gamma}{l^2\lambda} \tag{17}$$

in the limit, when $t \to \infty$:

$$||E|| \leq \frac{j\Gamma}{l^2\lambda} \tag{18}$$

The above inequality implies that the estimation error can be as small as is desired if the observer gain l is chosen large enough.

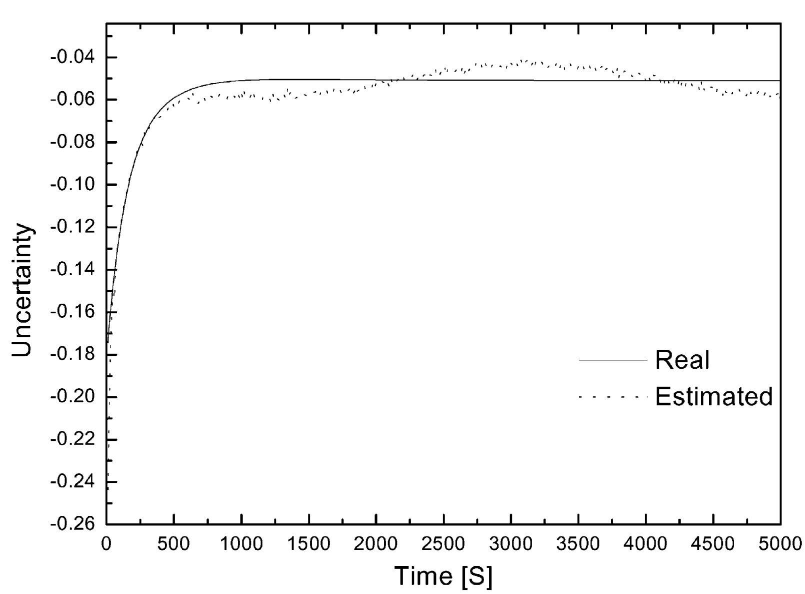

Fig. 4. On-line estimation of the reaction heat, considering sustained disturbances ($l = 0.01$).

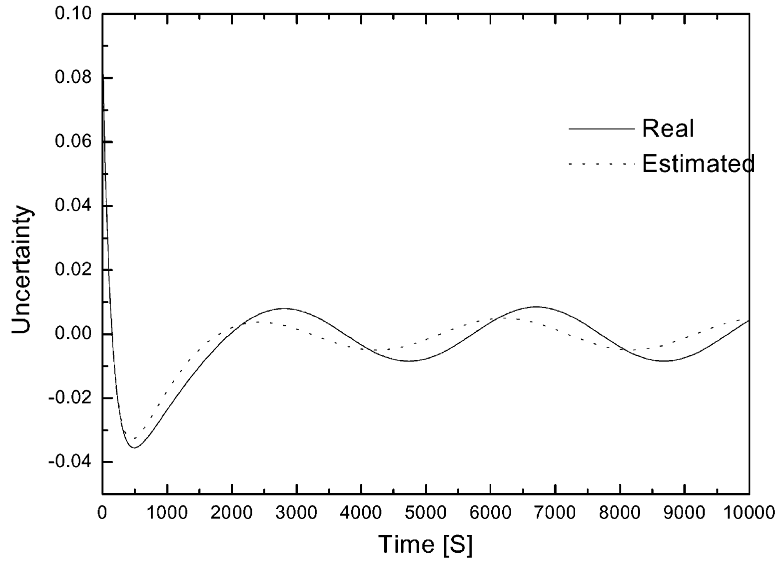

Fig. 5. Uncertainty estimation in the transformed space ($l = 0.01$).

Note that if the system output is corrupted by additive noise i.e. $Y = \eta_1 + \delta$ and the noise is considered bounded such that $||\delta|| \leq \Delta$, a similar methodology used to analyze the estimation error E can be applied in order to prove that the steady-state estimation error becomes $j(\Gamma + \Delta)/l^2\lambda$ which proves robustness against noisy measurements.

4. Numerical experiments

In this section, numerical simulations were carried out in order to show the performance of the proposed observer. The reaction heat generated in a CSTR is estimated via temperature measurements, which are corrupted with a white noise of ± 2 K around the current temperature value. The observer filters adequately the noisy temperature measurements as can be observed in the Fig. 1, which are used in the estimation of the reaction heat although it corresponds to the differential algebraic structure. The observer is able to infer the reaction heat with a good performance as shown in Fig. 2.

Additionally to the noisy temperature measurements, a sustained disturbance in the reactor temperature inlet $X_{1e} = X_{1eo} + 4\sin(\Pi t)$ is now introduced to the system and the observer proposed is able to estimate the corresponding terms, as can be seen in Fig. 3 corresponding to noisy reactor temperature measurement and the related temperature filtered. Fig. 4 shows the performance of the observer to infer the reaction heat in the chemical reactor and finally Fig. 5 shows the performance of the observer in the new coordinates, which is adequate too, in spite of

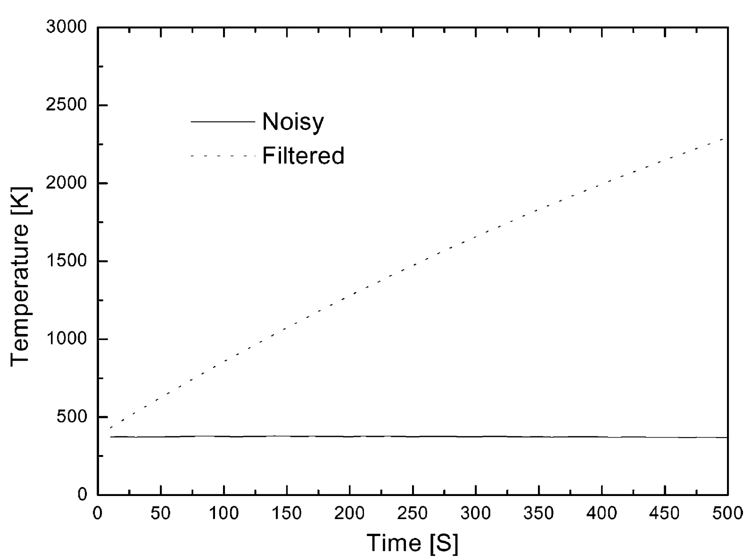

Fig. 6. Filtering process of the reactor temperature measurements ($l = 0.001$).

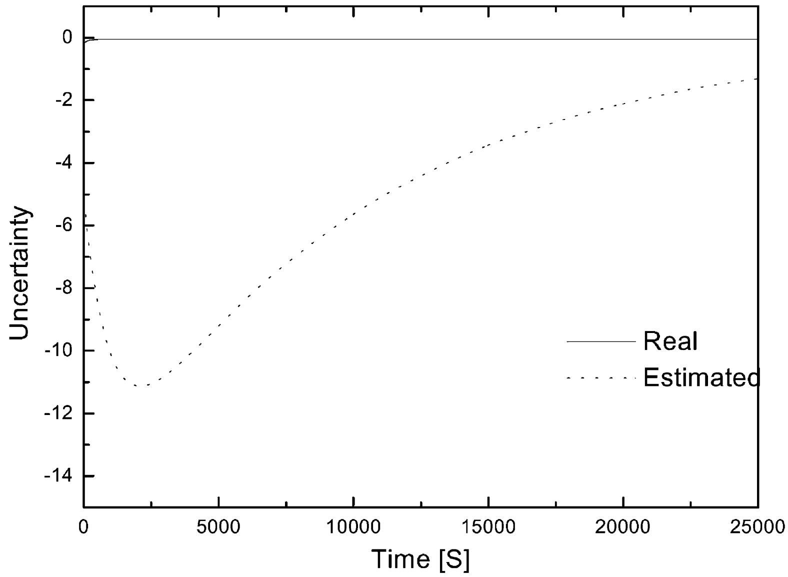

Fig. 7. On-line estimation of the reaction heat ($l = 0.001$).

different initial conditions for the system and the observer. For Figs. 1–5 the value of the observer parameter gain l is $l = 0.01$ and the parameter $\tau = 1.0$.

Figs. 6 and 7 are related with the effect of the observer parameter gain l. The value $l = 0.001$ is chosen to show the effect of a small gain, as can be seen the observer do not converge to the values of the corresponding terms, temperature and heat of reaction, respectively, which is in accordance with the theoretical convergence properties developed in Section 3.

5. Concluding remarks

A high gain observer to infer reaction heats in a CSTR via temperature measurements is designed using differential algebraic tools. The concept of uncertainty algebraic observability condition was introduced to estimate the uncertain term from the output selected and is easily obtained from this approach, besides the implementation of the observer is very simple with the transformation proposed. The performance of the observer developed is satisfactory in spite of noisy temperature measurements and sustained disturbances under the high gain condition.

Acknowledgements

This work is supported under project FIES-98-111-II of Instituto Mexicano del Petróleo and CONACYT under Grant 31982-A.

References

[1] H. Schuler, C. Schmidt, Calorimetric-state estimator for chemical reactors diagnosis and control: review of methods and applications, Chem. Eng. Sci. 47 (1992) 899–915.
[2] J. Alvarez-Ramirez, R. Aguilar, F. López-Isunza, Robust regulation of temperature in reactor-regenerator fluid catalytic cracking units, Ind. Eng. Chem. Res. 35 (1996) 1652–1659.
[3] R. Aguilar, J. Alvarez, J. González, M.A. Barrón, A strategy to regulate continuous fermentation process with unknown reaction rates, J. Chem. Technol. Biotechnol. 37 (4) (1996) 357–361.
[4] G.E. Elicabe, E. Ozdeger, C. Georgakis, On line estimation of reaction rate in a polymerization process, Ind. Eng. Chem. Res. 34 (1995) 1219.
[5] R. Aguilar, J. González, J. Alvarez, M. Angel Barrón, Temperature regulation of a class of continuous chemical reactor based on a nonlinear Luenberger-like observer, J. Chem. Technol. Biotechnol. 70 (3) (1997) 209–216.
[6] J.F. Ritt, Differential Equations from the Algebraic Standpoint, American Mathematical Society, New York, 1932.
[7] M. Fliess, M. Hasler, Questioning the classical state-space description via circuit example, Mathematical Theory of Networks and Systems, Birkhauser, Boston, MA, 1990.
[8] M. Hasler, J. Neirynck, Nonlinear Circuits, Artech House, Boston, MA, 1986.
[9] M.I. Freedman, J.C. Willems, Smooth representation of systems with differentiated inputs, IEEE Trans. Aut. Contr. 23 (1978) 16—21.
[10] M. Fliess, Generalized controller canonical forms for linear and nonlinear dynamics, IEEE Trans. Aut. Contr. 35 (9) (1990) 994–1001.
[11] R. Martínez-Guerra, J. de León-Morales, Nonlinear estimators: a differential algebraic approach, Appl. Math. Lett. 9 (4) (1996) 21-25.
[12] C.A. Smith, A. Corripio, Principles and Practice of Automatic Process Control, Wiley, New York, 1980.