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Integral observers for uncertainty estimation in continuous chemical reactors: algebraic-differential approach

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Abstract

In this paper, the on-line estimation of reaction heat in continuous stirred tank reactors, from noisy temperature measurements is addressed. An alternative representation of the original system is proposed in order to transform the output system disturbance on a system disturbance; this allows using a high gain-type observer without noise amplification problems. The uncertainty observer developed consists of integral (I)-type action and it is related with differential-algebraic concepts, where the observability condition for the uncertainty estimation from temperature measurements can be corroborated easily and the observer structure is simple enough to leads a feasible implementation. The structure of the proposed observer is robust against noisy measurements and model uncertainties. The performance of the observer is illustrated with numerical experiments.

Keywords: Noisy measurements; Integral observer; Robustness; Model uncertainties; Uncertainty estimation

1. Introduction

Currently, due to the necessity of on-line estimates of unknown terms related to mathematical models for process identification and control purposes, estimation theory is one of the most active research fields. In order to obtain effective operation management, on-line monitoring and control of chemical processes, the estimation of unknown variables is a task that spontaneously arises. A particular example, which is widely used in the chemical industry, is the continuous stirred tank reactor (CSTR). This kind of reactors is involved, for example in pharmaceutical, polymerization, petrochemical, biochemical industries and so on. As is well known the nonlinearities present in chemical reactor modeling are related with kinetic and chemical heat generation. The evaluation of temperature changes due to heat generation by chemical reaction is a difficult task, because of the complexity of the physical and chemical phenomena related, this is a serious drawback from modeling, monitoring and controller synthesis point of view.

The estimators or observers for states and uncertainties can play a key role during the early detection of hazardous and unsafe operating conditions, besides of the issues mentioned earlier. Following this spirit, several researches have been focused in the proposition of estimation methodologies for states and uncertainties present in chemical processes. For example, uncertainty estimation based on calorimetric balances to infer heats of reaction in chemical reactors was proposed by Schuler and Schmidt [1] and it has been very successful in steady state operation, but if the system measurements are noisy could lead to instabilities during transient operation.

Another approach is related to the construction of asymptotic observers for nonlinear processes using geometric-differential methods [2]. The main idea is to find a state transformation to represent the system as a linear equation plus a nonlinear term, which is function of the system output. However, finding a nonlinear transformation that places a system of order n into observer form requires the integration of n coupled partial differential equations. Furthermore, this approach needs accurate knowledge of the nonlinear dynamics of the system.

The approach to design observers in nonlinear systems, developed by Thau [3], does not include a systematic technique for the synthesis of the observer; it gives sufficient conditions for asymptotic stability around the origin of the error differential equation.

The extended Kalman filters have been widely used in the process industry, because of their easy implementation and capabilities to deal with errors in the modeling and

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Nomenclature

e_i	estimation errors
k_i	observer gains (1/s)
K	kinetic constant (l/(kmol s))
u	system input (temperature of the cooling jacket) (K)
X_1	reactive concentration (kmol/l)
X_2	reactor temperature (K)
X_3	reaction heat (uncertain term) (K/s)
$X_{i,\text{in}}$	inlet conditions
Y	system measured output (reactor temperature) (K)

Greek letters

δ	temperature noise (K)
γ	heat transfer global coefficient (kcal/(m^2 K s))
θ	inverse of the residence time (1/s)
ζ_i	variables in the transformed space

Superscripts

$\cdot$	time derivative
$\hat{}$	estimate variables

the measurements in its structure. Nonetheless, this design is based on linearized approaches of the nonlinear system, where robustness and convergence properties are difficult to prove [4,5].

Another kind of methodology is related to the differential-algebra, which is a mathematical approach that has been recently shown to be a very effective tool for understanding basic questions such as input–output inversions and observer realizations [6–9]. Algebraic-differential methodologies have been employed to construct asymptotic and even exponential observers [10,11] however, up to date, these designs only include full order observers for state estimation and do not include uncertainty estimation.

In this paper an uncertainty integral-type observer based on algebraic-differential techniques is designed for a class of CSTRs, in order to infer, on-line, the reaction heat from noisy temperature measurements. The main advantages are that the observability condition of the pair uncertainty-temperature is easily done and the implementation of the uncertainty observer in the transformed space is very simple. Additionally, the observer contains, inside its structure, an alternative form of the integral contributions of the measurement error, which provides robustness against disturbances to the system and noisy measurements with a high gain condition, given that the disturbances and the noise are *decoupled* from the observer gains, which allows to increase the stabilizing part of the structure of the observer, thanks to new system representation. The proposed methodology could be employed in the synthesis of controllers based model (I/O linearizing control laws), fault detection and on-line monitoring.

2. Problem statement

The following nonlinear dynamic plant, which represents the mathematical model of a CSTR where a second order reaction takes place [12], is considered as case of study:

Heat balance:

$$\dot{X}_2 = \theta(X_{2,\text{in}} - X_2) + X_3 + \gamma(u - X_2) \tag{1}$$

Mass balance:

$$\dot{X}_1 = \theta(X_{1,\text{in}} - X_1) - KX_1^2 \tag{2}$$

Uncertainty dynamics:

$$\dot{X}_3 = f(X_1, X_2) \tag{3}$$

System output:

$$Y = X_2 + \delta \tag{4}$$

In order to give a background previous to the estimation methodology proposed, the following definitions are considered [6,11]:

D1. A differential field extension L/M is given by two differential fields, L and M, such that:

(i) $M \subseteq L$
(ii) The derivation of M is the restriction to K of the derivation of L.

D2. A dynamics is a finitely generated differentially algebraic extension $\mathfrak{I}/M\langle u\rangle$. This means that any element of $\mathfrak{I}$ satisfies a differential-algebraic equation with coefficients, which are rational functions over M in the components of u and a finite number of their time derivatives.

D3. Let a subset $\{u, y\}$ of $\mathfrak{I}$ in a dynamics $\mathfrak{I}/M\langle u\rangle$. An element in $\mathfrak{I}$ is said to be observable with respect to $\{u, y\}$ if it is algebraic over $M\langle u, y\rangle$. Therefore, a state x is said observable if, and only if, it is observable with respect to $\{u, y\}$.

The following concept is introduced in order to define an algebraically observable uncertainty condition:

D4. An element X_u in $\mathfrak{I}$ is said to be an algebraically observable uncertainty if X_u satisfies a differential-algebraic equation with coefficients over $M\langle u, y\rangle$.

Now, consider Eqs. (1) and (4), which according to **D2** define an algebraic-differential dynamic system. From this subsystem, the following differential-algebraic equations can be obtained:

$$X_2 - Y = 0 \tag{5}$$

$$\dot{Y} + (\theta + \gamma)Y - \theta X_{2,\text{in}} - \gamma u - X_3 = 0 \tag{6}$$

From **D3** and **D4**, the pair X_2, X_3 is universally observable in the Diop-Fliess sense, under the assumption that the additive noise does not affect the observability condition.

3. Integral observer design

Now, the corresponding input–output representation of Eqs. (1) and (3) is given by Eq. (7).

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

Eq. (7) can be represented in a generalized observability canonical form (Eq. (9)), using the following change of variables:

$$\zeta_i = \frac{d^{i-1}Y}{dt^{i-1}} \quad (8)$$

$$\begin{aligned} \dot{\zeta}_1 &= \zeta_2 \\ \dot{\zeta}_2 &= \Phi(\zeta_1, \zeta_2, \dot{u}) \\ Y &= \zeta_1 + \delta \end{aligned} \quad (9)$$

This representation is more adequate for our purposes such that the system given by Eqs. (1) and (3) is high nonlinear in comparison with system (9).

Now, it is necessary to design an observer to infer ζ_2 (the uncertainty term in the transformed space). However, as it can be seen from the nature of the system given by Eq. (9), a standard structure of a Luenberger type observer based on a copy of the system plus measurement error correction is not realizable since the term Φ is unknown. Besides, as is well known, the proportional observers tend to amplify the measurement noise, which can lead to degradation of the observer performance. In order to save these drawbacks, the following representation of the system (9) is done:

$$\begin{aligned} \dot{\zeta}_1 &= \zeta_2 \\ \dot{\zeta}_2 &= \Phi(\zeta_1, \zeta_2, \dot{u}) \\ \dot{\zeta}_3 &= \zeta_1 + \delta \\ Y_0 &= \zeta_3 \end{aligned} \quad (10)$$

The main issue of this new representation of the system is to eliminate the additive noise from the new output system Y_o, transform it on system disturbance.

Proposition 1. *The following dynamic system* (Eqs. (11)–(13)) *is an asymptotic-type observer of system (10).*

$$\dot{\hat{\zeta}}_1 = \hat{\zeta}_2 + k_1(Y_0 - \hat{Y}_0) \quad (11)$$

$$\dot{\hat{\zeta}}_2 = k_2(Y_0 - \hat{Y}_0) \quad (12)$$

$$\dot{\hat{\zeta}}_3 = \hat{\zeta}_1 + k_3(Y_0 - \hat{Y}_0) \quad (13)$$

Now, to back into the original space of states, from Eq. (6), the reaction heat is evaluated by Eq. (14).

$$\hat{X}_3 = \hat{\zeta}_2 - \theta(X_{2,\mathrm{in}} - \hat{\zeta}_1) - \gamma(u - \hat{\zeta}_1) \quad (14)$$

According to the variable change given by Eq. (8), the variable ζ_1 is the thermodynamic reactor temperature. From Eq. (14), if temperature measurements were noisy, the noise would be transmitted to the estimation of the heat of reaction, which would lead to poor performance in the estimation procedure. Therefore, it was necessary to filter the temperature measurements; this is the main reason of the structure of the proposed observer given by Eqs. (11)–(13). Furthermore, note that the observer Eqs. (11)–(13) contains an integral-type contribution; this is considered in its structure in order to increase the robustness against inaccurate modeling of measurements, process noisy and disturbance rejection. The disturbance rejection is a property of the integral action as was pointed out by Linder and Shafai [13]. When this property is used with a single output system, integral action allows the integral observers to reject any type of rank one perturbations, as long as the form of the perturbation is known and the effect of it is slower than the time constant of the integral action. Hence, on the one hand, the increase of the integral gain allows the rejection of faster perturbations and on the other hand, it has negative side effects on decreasing the observer's stability margin [14].

It is important to note that Eq. (14), used to infer the heat of reaction, is equivalent to the calorimetric balance technique, where the difference lies in the approximation of the derivative term related to energy accumulation, dT/dt. As it was mentioned earlier, in the calorimetric balance methodology the derivative of reactor temperature is approximated by finite difference techniques, which become unstable for noisy measurements. Nonetheless, using the algebraic-differential approach the derivative term (ζ_2 in the transformed space) is estimate using an uncertainty observer that is robust against noisy temperature measurements and model uncertainties.

3.1. *Convergence observer comments (sketch of proof of Proposition 1)*

Now, let us define the following estimation errors (Eqs. (15)–(17)):

$$e_1 = \zeta_1 - \hat{\zeta}_1 \quad (15)$$

$$e_2 = \zeta_2 - \hat{\zeta}_2 \quad (16)$$

$$e_3 = \zeta_3 - \hat{\zeta}_3 \quad (17)$$

Now, it is possible to evaluate the dynamics of the estimation error as is given by Eq. (18).

$$\dot{E} = AE + \Omega(\zeta_1, \zeta_2, \dot{u}, \delta) \quad (18)$$

where,

$$E = \begin{bmatrix} e_1 \\ e_2 \\ e_3 \end{bmatrix}$$

$$A = \begin{bmatrix} 0 & 1 & -k_1 \\ 0 & 0 & -k_2 \\ 1 & 0 & -k_3 \end{bmatrix}$$

$$\Omega = \begin{bmatrix} 0 \\ \Phi \\ \delta \end{bmatrix}$$

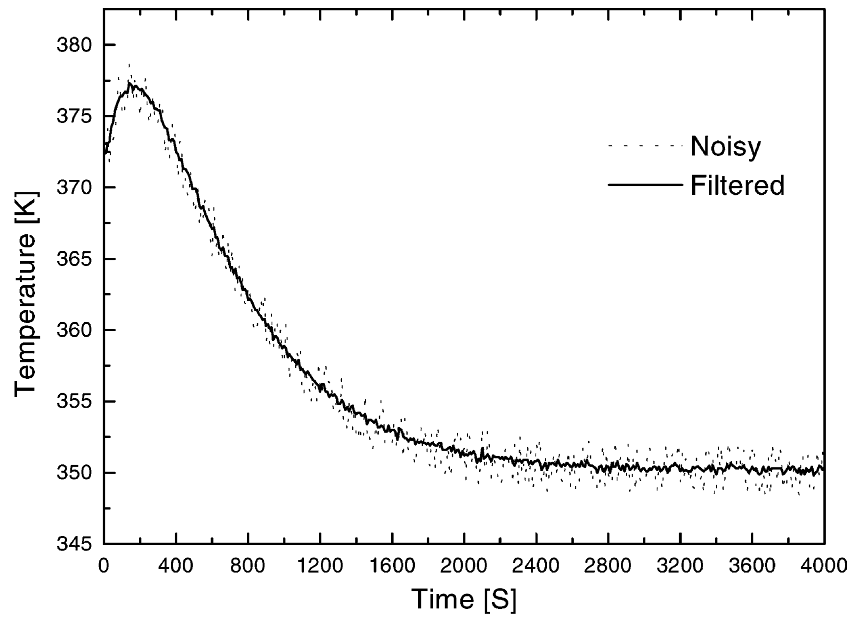

Fig. 1. Reactor temperature estimation with integral-type observer ($k_1 = 1 \times 10^{-2}\,s^{-1}$).

under the following assumption:

A1. Ω is bounded, i.e. $||\Omega|| \leq \Gamma$ for some $\Gamma > 0$.

It can choose the observer gains *ki* such that the matrix ***A*** is Hurwitz stable. Therefore, the system (11)–(13) is an asymptotic-type observer for the system (10).

3.2. Remarks

The uncertainty observer designed has several important characteristics:

1. To transform the space given by Eq. (8) back into the original space state, only algebraic relationships are used.
2. Considering the alternative system representation, when a *large enough* observer gains, k_i are chosen, the stabilizing term of the dynamic estimation error prevails over the disturbance term. Then, the integral-type action provides robustness under unmodelled dynamics and additive noisy measurements.
3. The earlier remark can be done, given that the disturbances and the measurement noisy are decoupled of the observer gains, thanks to the system representation given by Eq. (9).

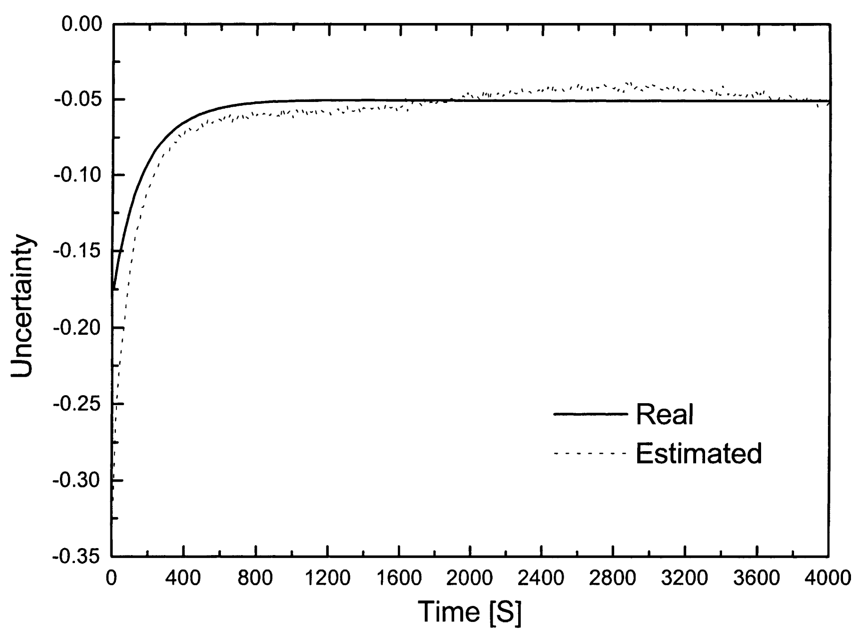

Fig. 2. Reaction heat estimation (K/min), with integral-type observer ($k_2 = 2 \times 10^{-2}\,s^{-1}$).

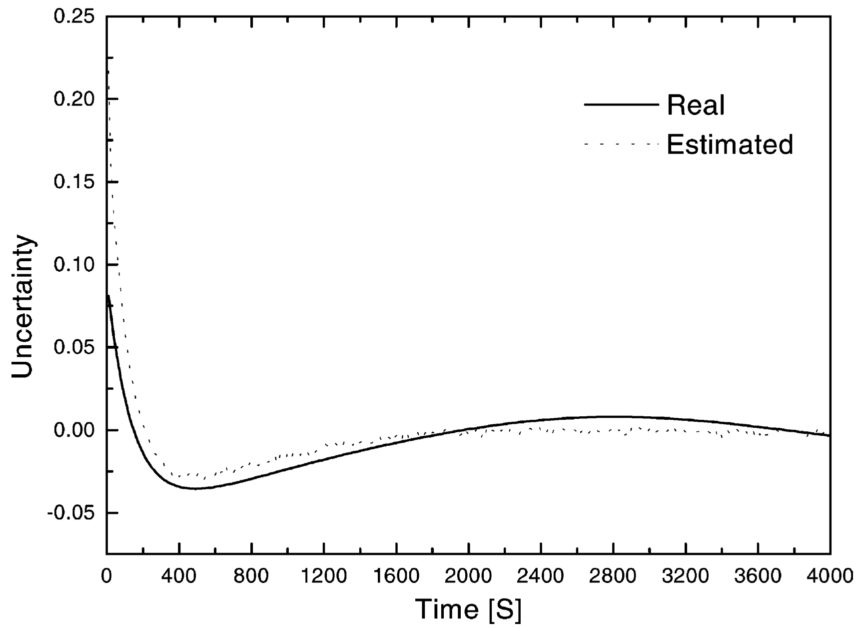

Fig. 3. Uncertainty (ζ_2, (K/min)) estimation in the transformed space, with integral-type observer ($k_2 = 2 \times 10^{-2}\,s^{-1}$).

4. The restraint of the reaction heat (uncertain term) is common for a wide class of chemical reactions and is consequence of 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 $\Delta H_f\, R(X_1,X_2)$ property is found if the functionality $R(X_1,X_2)$ with respect to temperature is of Arrhenius type.
5. The proposed observer can be employed in calorimetric analysis, in order to evaluate reaction heats of complex reacting systems; besides of on-line process monitoring, controllers based on observers and fault detection issues.
6. Practical implementation of the proposed observer would be feasible in commercial hardware, because it only needs temperature measurements and basic system structure knowledge.

4. Numerical simulation

In order to show the improved features of the observer proposed, numerical simulations were performed. The heat

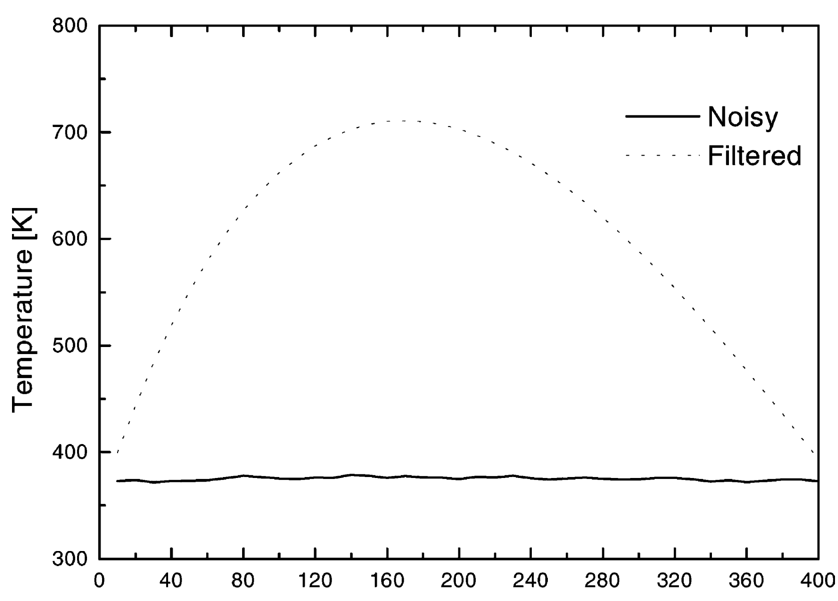

Fig. 4. Reactor temperature estimation with integral-type observer ($k_1 = 1 \times 10^{-3}\,s^{-1}$).

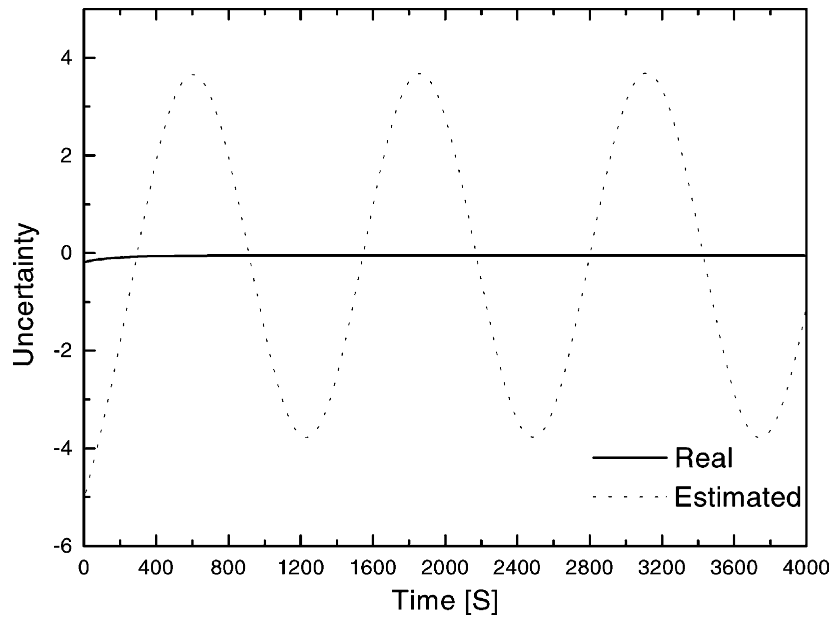

Fig. 5. Reaction heat (K/min) estimation with integral-type observer ($k_2 = 2 \times 10^{-3}\,\mathrm{s}^{-1}$).

of reaction generated in a CSTR is estimated via temperature measurements. These measurements are corrupted by a white noise of $\delta = \pm 2\,\mathrm{K}$ around the actual temperature value. Additionally, there is a sustained disturbance in the reactor temperature inlet $X_{2,\mathrm{in}} = X_{20,\mathrm{in}} + 4\sin(\pi t)$. For Figs. 1–3 the value of the observer gain is $k_1 = 1 \times 10^{-2}\,\mathrm{s}^{-1}$, $k_2 = 2 \times 10^{-2}\,\mathrm{s}^{-1}$, $k_3 = 0.5 \times 10^{-2}\,\mathrm{s}^{-1}$, which are choose of the order of the sampling time. The proposed observer estimates adequately the noisy temperature measurements, as it can be noticed in Fig. 1. This filtered temperature is used in the estimation of the reaction heat in accordance with the differential-algebraic structure. The observer is able to infer the uncertain term (reaction heat, (K/s)) with good precision, as it can be seen in Fig. 2.

Despite of different initial conditions for the system and the observer, the performance of the observer in transformed coordinates, is adequate too as is shown in Fig. 3.

Figs. 4 and 5 show the effect of the observer parameter gain k_i. The values $k_1 = 1 \times 10^{-3}\,\mathrm{s}^{-1}$, $k_2 = 2 \times 10^{-3}\,\mathrm{s}^{-1}$, $k_3 = 0.5 \times 10^{-3}\,\mathrm{s}^{-1}$, which are considered less than

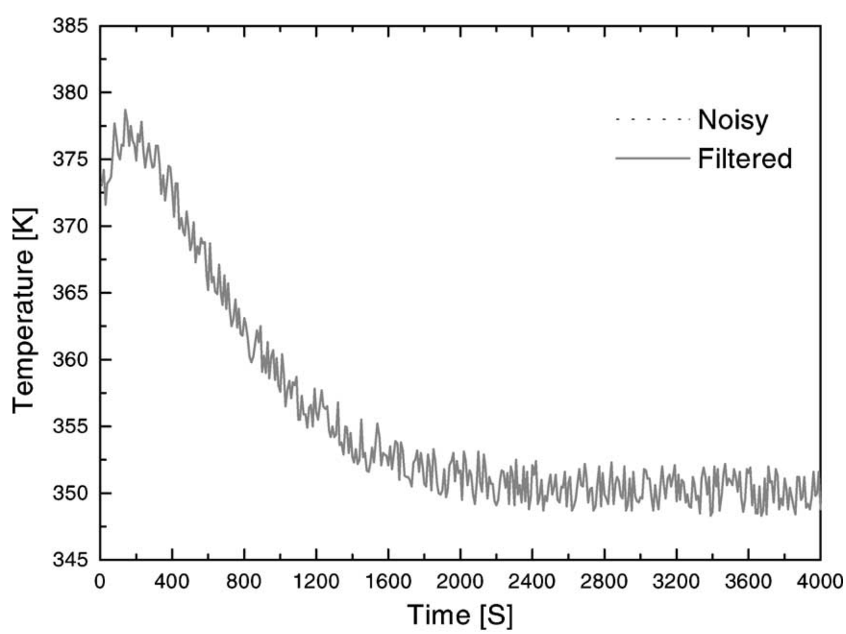

Fig. 6. Reactor temperature estimation with proportional observer ($k_2 = 1 \times 10^{-2}\,\mathrm{s}^{-1}$).

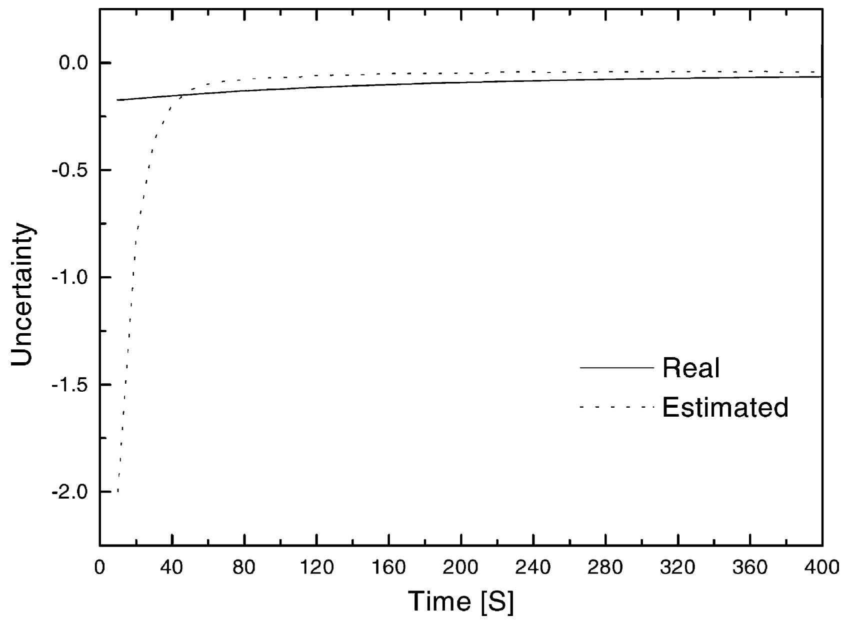

Fig. 7. Reaction heat (K/min) estimation with proportional observer ($k_2 = 2 \times 10^{-2}\,s^{-1}$) during start-up.

temperature sampling time, they are selected to show the effect of a small gain. As it can be seen, the observer cannot converge to the values of the corresponding terms, temperature and reaction heat, respectively, which is in agreement with the theoretic converge properties developed in Section 3; because the proposed observer must be is an integral *high* gain observer.

In order to compare the performance of the proposed methodology, a classical proportional observer was implemented. Fig. 6 is related with the performance of standard proportional observer with the following gain values $k_1 = 1 \times 10^{-2}\,s^{-1}$ and $k_2 = 2 \times 10^{-2}\,s^{-1}$, with it the effects of the noise propagation is shown. As can be seen, the observer tends to reproduce the noise output signal; consequently the filtered temperature and the noise temperature measured are overlapped, as is characteristic of proportional observers. Figs. 7 and 8 show the performance of the standard uncertainty proportional observer during the start-up and steady state operation, respectively. The uncertainty estimated presents peaking phenomena in the start-up of the estimation procedure and besides the additive noise and the disturbance are transmitted to the uncertainty estimated at steady state.

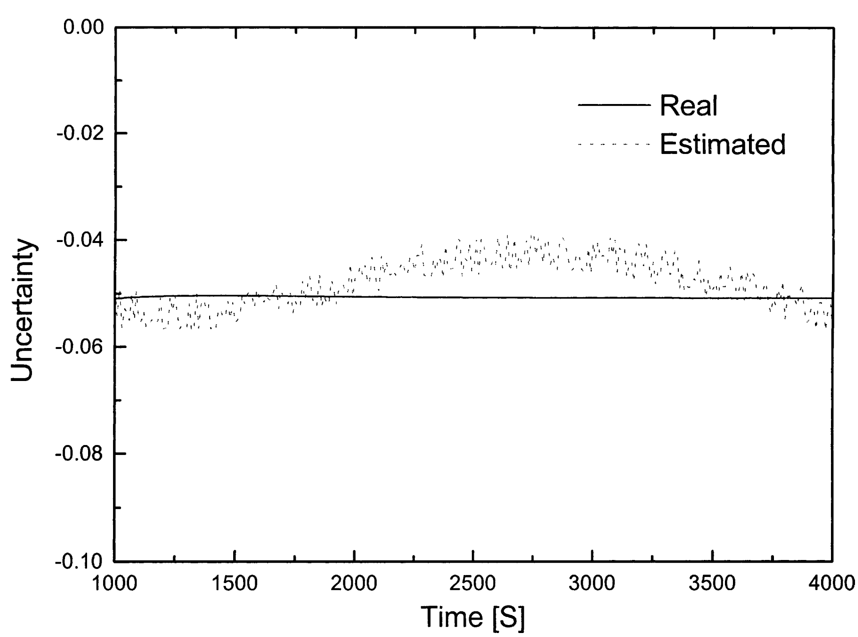

Fig. 8. Reaction heat (K/min) estimation with proportional observer ($k_2 = 2 \times 10^{-2}\,s^{-1}$), steady state.

5. Conclusions

A high gain integral-type observer to infer the reaction heat in CSTRs via temperature measurements was designed using differential-algebraic tools. The concept of uncertainty algebraic observability condition was employed to estimate the uncertain term from the output selected, such that the observability condition is easily obtained from this approach. Moreover, the implementation of the observer is very simple following the proposed transformation of the system. Despite of noisy temperature measurements and sustained disturbances, the performance of the observer developed is very satisfactory when the high gain condition is imposed, thanks to the new system representation. It is important to notice that the same observer presents bad performance when using small gains, relative to the sampling time, because the stabilizing part of the observer cannot compensate the system disturbances.

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