Self-adaptive predictive functional control of the temperature in an exothermic batch reactor

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Abstract

In this paper we study a self-adaptive predictive functional control algorithm as an approach to the control of the temperature in an exothermic batch reactor. The batch reactor is located in a pharmaceutical company in Slovenia and is used in the production of medicines. Due to mixed discrete and continuous inputs the reactor is considered as a hybrid system. The model of the reactor used for the simulation experiment is explained in the paper. Next, we assumed an exothermic chemical reaction that is carried out in the reactor core. The dynamics of the chemical reaction that comply with the Arrhenius relation have been well documented in the literature and are also summarized in the paper. In addition, the online recursive least-squares identification of the process parameters and the self-adaptive predictive functional control algorithm are thoroughly explained. We tested the proposed approach on the batch-reactor simulation example that included the exothermic chemical reaction kinetic model. The results suggest that such an implementation meets the control demands, despite the strongly exothermic nature of the chemical reaction. The reference is suitably tracked, which results in a shorter overall batch-time. In addition, there is no overshoot of the controlled variable T, which yields a higher-quality production. Finally, by introducing a suitable discrete switching logic in order to deal with the hybrid nature of the batch reactor, we were able to reduce the switching of the on/off valves to a minimum and therefore relieve the wear-out of the actuators as well as reduce the energy consumption needed for control.

1. Introduction

Batch reactors that are cooled and heated through a water jacket are common in chemical, pharmaceutical, biotechnological and similar industries. Therefore, many papers discussing the temperature control of such systems have been published. Dynamic systems that involve continuous and discrete states are called *hybrid systems*. Most industrial processes contain both continuous and discrete components, for instance, discrete valves, on/off switches, logical overrides, etc. The continuous dynamics are often inseparably interlaced with the discrete dynamics; therefore, a special approach to modelling and control is required. At first this topic was not treated systematically [14]. In recent years, however, hybrid systems have received a great deal of attention from the computer science and control community. Due to the mixed discrete and continuous inputs, batch reactors can also be regarded as hybrid systems.

Many times in industrial practice the dynamics of the batch reactor are not known in advance. Furthermore, often an exothermic (or endothermic) chemical reaction is carried out in a batch reactor, which can result in a thermal runaway. Such an event can cause the loss of the batch and can even represent a risk to the plant and the operators. For most reaction systems of industrial interest detailed kinetic models are not known [6]. In the rapidly changing chemical business, there is often not enough time or financial benefit in carrying out detailed kinetic studies of the reactions.

Some industrial batch reactors have to be able to deal with different batches and ingredients, and, therefore, different reaction dynamics are involved. This calls for special control strategies, since a classic approach, where a time-invariant process is presumed, is not suitable. The concepts of adaptive control [4], optimal control [7,3,11], and especially model predictive control schemes [8–10] seem to be the most appropriate. The principle

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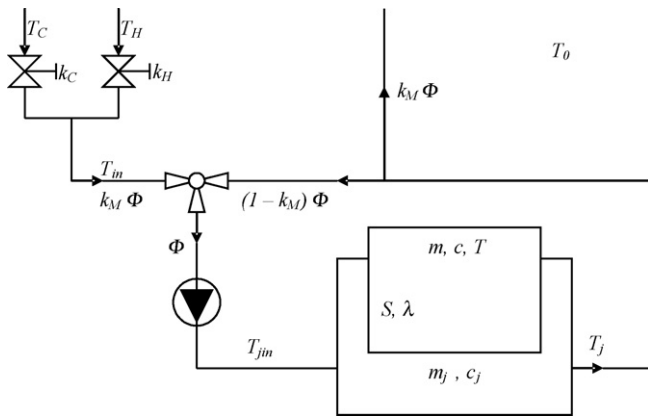 *E-mail address:* gorazd.karer@fe.uni-lj.si (G. Karer).

Fig. 1. Scheme of the batch reactor.

of model predictive control is based on forecasting the future behavior of a system at each sampling instant using the process model.

One of the most frequently used approaches in practice is predictive functional control [12], which is also treated in this paper. The main advantage of the approach is the analytical explicit expression of the control law, which does not require high computational capabilities and can therefore be implemented in real-time using low-cost hardware on most systems.

The paper is organized as follows. In Section 2, the batch reactor and its mathematical model are presented, and the exothermic chemical reaction dynamics are summarized. In Section 3, the recursive least-squares identification is explained and the predictive functional control algorithm is presented. Finally, the simulation results and conclusions are discussed in Sections 4 and 5.

2. The plant

2.1. Batch reactor

The experimental batch reactor is a simulation example of a real batch reactor, which is located in a pharmaceutical company and is used in the production of medicines. The goal is to control the temperature of the ingredients stirred in the reactor core so that they synthesize into the final product. In order to achieve this, the temperature has to follow the reference trajectory prescribed in the recipe as accurately as possible.

A scheme of the batch reactor is shown in Fig. 1. The reactor's core (temperature T) is heated or cooled through the reactor's water jacket (temperature T_j). The heating medium in the water jacket is a mixture of fresh input water, which enters the reactor through on/off valves, and reflux water. The water is pumped into the water jacket with a constant flow ϕ. The dynamics of the system depend on the physical properties of the batch reactor, i.e. the mass m and the specific heat capacity c of the ingredients in the reactor's core and in the reactor's water jacket (here, index j denotes the water jacket). λ is the thermal conductivity, S is the contact area and T_0 is the temperature of the surroundings.

The temperature of the fresh input water T_{in} depends on two inputs: the positions of the on/off valves k_H and k_C. How-

ever, there are two possible operating modes for the on/off valves. In case $k_C = 1$ and $k_H = 0$, the input water is cool ($T_{in} = T_C = 12\,^\circ C$), whereas if $k_C = 0$ and $k_H = 1$, the input water is hot ($T_{in} = T_H = 150\,^\circ C$). Both on/off valves are controlled by the signal k_{CH} that is defined in the following equation. Due to the mixed discrete and continuous inputs, the batch reactor is regarded as a hybrid system.

$$k_{CH} = \begin{cases} +1, & \text{if } k_C = 0 \text{ and } k_H = 1 \\ -1, & \text{if } k_C = 1 \text{ and } k_H = 0 \end{cases} \tag{1}$$

The ratio of fresh input water to reflux water is controlled by the third input, i.e., by the position of the mixing valve k_M. The value range of the mixing valve is in [0,1].

2.2. Mathematical model of the batch reactor

We are dealing with a hybrid multivariable system with three discrete inputs (k_M, k_H and k_C) and two measurable outputs (T and T_j).

The temperature of the mixed water or the input-jacket temperature, which is denoted as T_{jin}^*, cannot be measured directly. However, it is possible to estimate it using the temperature of the input water T_{in}, the water-jacket temperature T_j, and the position of the mixing valve k_M (see Eq. (4)). T_{jin}^* is constrained in the range between T_C and T_H ($T_C \leq T_{jin}^* \leq T_H$).

Due to the nature of the system, the time constant of the temperature in the water jacket is obviously much shorter than the time constant of the temperature in the reactor's core. Therefore, the batch reactor is considered as a stiff system.

The mathematical model of the batch reactor is defined by the following two differential equations and one algebraic equation.

$$m_j c_j \frac{dT_j}{dt} = k_M \Phi c_j T_{in} + (1 - k_M) \Phi c_j T_j - \Phi c_j T_j$$
$$- \lambda S(T_j - T) - \lambda_0 S_0(T_j - T_0) \tag{2}$$

$$mc \frac{dT}{dt} = \lambda S(T_j - T) + Q_r \tag{3}$$

$$T_{jin}^* = k_M T_{in} + (1 - k_M) T_j \tag{4}$$

The parameters of the model are presented in Table 1.

2.3. Exothermic chemical reaction model

The exothermic reaction considered in this experiment is based on a dynamic model benchmark originally developed for the Warren Springs Laboratory [2,6,5]. A well-mixed liquid-phase reaction system is treated, in which two reactions are modelled.

$$A + B \rightarrow C \tag{5}$$

$$A + C \rightarrow D \tag{6}$$

The concentration (number of moles) of the components A, B, C and D changes according to the rates of production of the

Table 1
Parameters of the batch reactor

Parameter	Value	Meaning
m_j	200 kg	Mass of the water in the jacket
c_j	4200 J kg^{-1} K^{-1}	Heat capacity of the water in the pipes
Φ	1.6 kg s^{-1}	Mass flow in the pipes of the reactor
λ	420 W m^{-2} K^{-1}	Thermal conductivity between the reactor core and the jacket
λ_0	84 W m^{-2} K^{-1}	Thermal conductivity between the jacket and the surroundings
S	2 m^2	Conduction surface between the reactor core and the jacket
S_0	4 m^2	Conduction surface between the jacket and the surroundings
T_0	17 °C	Temperature of the surroundings
m	See Eq. (15)	Mass of the ingredients in the core of the reactor
c	See Eq. (17)	Heat capacity of the ingredients in the core of the reactor
Q_r	See Eq. (18)	Heat released due to the exothermic nature of the reaction among the ingredients in the core of the batch reactor

Table 2
Parameters of the reaction

Parameter	Value	Meaning
w_A	30 kg kmol^{-1}	Molar weight of component A
w_B	100 kg kmol^{-1}	Molar weight of component B
w_C	130 kg kmol^{-1}	Molar weight of component C
w_D	1600 kg kmol^{-1}	Molar weight of component D
c_A	75.31 kJ kmol^{-1}°C^{-1}	Molar heat capacity of component A
c_B	167.36 kJ kmol^{-1}°C^{-1}	Molar heat capacity of component B
c_C	217.57 kJ kmol^{-1}°C^{-1}	Molar heat capacity of component C
c_D	334.73 kJ kmol^{-1}°C^{-1}	Molar heat capacity of component D
k_1^1	20.9057	Reaction rate constant
k_1^2	10, 000 °C	Reaction rate constant
k_2^1	38.9057	Reaction rate constant
k_2^2	17, 000 °C	Reaction rate constant
ΔH_1	−41, 840 kJ kmol^{-1}	Heat of reaction
ΔH_2	−25, 105 kJ kmol^{-1}	Heat of reaction

components C (R_1) and D (R_2), as given in the equations below.

$$\frac{dM_A}{dt} = -R_1 - R_2 \tag{7}$$

$$\frac{dM_B}{dt} = -R_1 \tag{8}$$

$$\frac{dM_C}{dt} = +R_1 - R_2 \tag{9}$$

$$\frac{dM_D}{dt} = +R_2 \tag{10}$$

The rates of production R_1 and R_2 depend on the reactant concentrations and the rate constants k_1 and k_2.

$$R_1 = k_1 M_A M_B \ \text{kmol}^{-1}\,\text{s}^{-1} \tag{11}$$

$$R_2 = k_2 M_A M_C \ \text{kmol}^{-1}\,\text{s}^{-1} \tag{12}$$

The rate constants k_1 and k_2 are dependent on the reaction temperature through the Arrhenius relation.

$$k_1 = \exp(k_1^1 - k_1^2/(T + 273, 15\,°C)) \tag{13}$$

$$k_2 = \exp(k_2^1 - k_2^2/(T + 273, 15\,°C)) \tag{14}$$

The remaining physical variables are calculated as follows:

$$m = w_A M_A + w_B M_B + w_C M_C + w_D M_D \tag{15}$$

$$M = M_A + M_B + M_C + M_D \tag{16}$$

$$c = \frac{c_A M_A + c_B M_B + c_C M_C + c_D M_D}{M} \tag{17}$$

$$Q_r = -\Delta H_1 R_1 - \Delta H_2 R_2 \tag{18}$$

The parameters of the reaction are given in Table 2.

3. Control algorithm

3.1. Estimation of model parameters

The online determination of the process parameters is a key element in adaptive control. The selection of the model's structure and the determination of its parameters depend on the a-priori knowledge of the process we want to control.

In the case of the batch reactor, some fundamental dynamic properties are known in advance, therefore, the structure of the presumed model of the batch reactor in incremental form can be derived and transformed into a discrete-time domain from Eqs. (2)–(4).

We assume that the plant parameters and the time-varying properties of the chemical reaction that takes place in the reactor have to be estimated online, i.e., during the normal operation of the reactor.

As shown in Eqs. (19) and (20), we are dealing with two independently estimated models. To obtain the model in incremental form, the offset has to be eliminated, which is realized by filtration and differentiation of the measured signals. Superscript f denotes the filtered signals.

$$y_{f1}(k) = \psi_{f1}^T(k)\theta_1(k) \tag{19}$$

$$y_{f2}(k) = \psi_{f2}^T(k)\theta_2(k) \tag{20}$$

Here, $y_{f1}(k) = T_j^f(k)$ is the filtered output of the first model and $y_{f2}(k) = T^f(k)$ stands for the filtered output of the second model, denoting the temperature of the water jacket and the temperature of the core, respectively. In the regressors, the temperature of the water jacket, the temperature of the core, and the input jacket temperature are considered: $\psi_{f1}^T(k) = [T_j^f(k-1) \ T^f(k-1) \ T_{jin}^{*f}(k-1)]$, $\psi_{f2}^T(k) = [T_j^f(k-1) \ T^f(k-1)]$. The parameter vectors $\theta_1^T = [\theta_{11}(k) \ \theta_{12}(k) \ \theta_{13}(k)]$ and $\theta_2^T = [\theta_{21}(k) \ \theta_{22}(k)]$ consist of three and two parameters that have to be estimated, respectively.

The filtration and differentiation of the measured variables is realized by the filter transfer function defined in Eq. (21).

$$H_f(z) = \frac{\Delta(z)}{F(z)} \tag{21}$$

Here, $\Delta(z) = 1 - z^{-1}$ is the differential operator. The filter denominator $F(z) = (1 - fz^{-1})^p$ is defined experimentally: in our case $f = 0.95$, $p = 3$. The sampling time used in the experiment is $T_s = 20$ s. Both models in Eqs. (19) and (20) are linear in the parameters, which makes it possible to calculate a least-squares estimate analytically. One of the main advantages of an adaptive controller is the ability to track variations in the process dynamics. In order to achieve this, it has to discount the old data and calculate the estimates with an emphasis on new data. We used a recursive least-squares identification algorithm with exponential forgetting [1], which is based on a least-squares loss function that discounts old data exponentially with time. The parameters of the model are estimated as shown in the equations below.

$$\hat{\theta}_i(k) = \hat{\theta}_i(k-1) + K_i(k)(y_{fi}(k) - \psi_{fi}^T(k)\hat{\theta}_i(k-1)) \tag{22}$$

$$K_i(k) = P_i(k-1)\psi_{fi}(k)(\gamma_i + \psi_{fi}^T(k)P_i(k-1)\psi_{fi}(k))^{-1} \tag{23}$$

$$P_i(k) = (I_i - K_i(k)\psi_{fi}^T(k))P_i(k-1)/\gamma_i \tag{24}$$

Here, $P_i(k)$, $i = 1, 2$ denotes the covariance matrix ($P_1(k) \in \mathbb{R}^{3\times3}$, $P_2(k) \in \mathbb{R}^{2\times2}$), $\hat{\theta}_i(k)$, $i = 1, 2$ denotes the vector of the identified or estimated process parameters, γ_i, $i = 1, 2$ denotes the forgetting factor and $I_1 \in \mathbb{R}^{3\times3}$ and $I_2 \in \mathbb{R}^{2\times2}$ are unity matrices. This means that two recursive identification algorithms are running in parallel to estimate the process parameters $\theta_1(k)$ and $\theta_2(k)$.

The forgetting factor γ_i, $i = 1, 2$ is defined in Eq. (25), where T_{γ_i} stands for the time constant for the exponential forgetting. In our case: $\gamma_1 = \gamma_2 = 0.995$.

$$\gamma_i = e^{-(T_s/T_{\gamma_i})} \tag{25}$$

The dynamical behavior of the plant variables $T_j^f(k)$ and $T^f(k)$ according to the input-jacket temperature $T_{jin}^f(k)$ is given by the transfer functions $G_{mj}(z)$ and $G_m(z)$, which are obtained by transforming Eqs. (19) and (20) into the Z-domain and explicitly expressing the given relations, which are then described as follows:

$$G_{mj}(z) = \frac{T_j^f(z)}{T_{jin}^{*f}(z)} = \frac{b_{1j}z - b_{0j}}{z^2 - a_1 z - a_0} \tag{26}$$

$$G_m(z) = \frac{T^f(z)}{T_{jin}^{*f}(z)} = \frac{b_0}{z^2 - a_1 z - a_0} \tag{27}$$

Here, $b_{0j} = \theta_{22}\theta_{13}$, $b_{1j} = \theta_{13}$, $b_0 = \theta_{21}\theta_{13}$, $a_1 = \theta_{22} + \theta_{11}$ and $a_0 = \theta_{12}\theta_{21} - \theta_{11}\theta_{22}$. Assuming the observability of the process plant, the transfer functions formulation, $G_{mj}(z)$ and $G_m(z)$ in Eqs. (26) and (27), can be merged into the state-space domain and written in the observable canonical form.

Exponential forgetting works properly all the time only if the process is appropriately excited. On the other hand, in practice there are many processes that cannot be excited during steady-state in normal operation. In such cases, the estimates $\hat{\theta}_i(k)$ and the covariance matrix $P_i(k)$ become unstable, which means that the estimates would change abruptly as soon as ψ_{fi} becomes different from 0. The phenomenon is known as estimator windup and has to be taken care of. An easy way to avoid it is to update the estimates and the covariance only when there is excitation. We therefore introduced a dead-zone criterion in the recursive algorithm (see Eq. (28)), which is calculated only if the criterion is satisfied, i.e., only when the process is properly excited.

$$\psi_{fi}^T(k)P_i(k-1)\psi_{fi}(k) > k_{DZ}(1 - \gamma_i), \quad i = 1, 2 \tag{28}$$

Here, k_{DZ} denotes the factor of the dead-zone, which is defined heuristically. In our case, $k_{DZ} = 0.01$.

3.2. Predictive functional control algorithm

In this section the well-known basic algorithm of predictive functional control is introduced [12,13]. In this instance, the prediction of the plant output is given by its model in the state-space domain.

The behavior of the closed-loop system is defined by a reference trajectory, which is given in the form of a reference model. The control goal, in general, is to determine the future control action so that the predicted output trajectory coincides with the reference trajectory. The coincidence point is called the coincidence horizon and it is denoted by H. The prediction is calculated assuming constant future manipulated variables ($u(k) = u(k + 1) = \ldots = u(k + H - 1)$). This strategy is known as mean-level control. The H-step-ahead prediction of the plant output is estimated in Eq. (29).

$$y_m(k + H) = C_m(A_m^H x_m(k) + (A_m^H - I)(A_m - I)^{-1}B_m u(k)) \tag{29}$$

Here, $I \in \mathbb{R}^{2\times2}$ is a unity matrix.

The reference model is given by the following difference equation:

$$\begin{aligned} x_r(k + 1) &= a_r x_r(k) + b_r w(k) \\ y_r(k) &= c_r x_r(k) \end{aligned} \tag{30}$$

Here, w stands for the reference signal. The reference model parameters should be chosen to fulfil the following equation:

$$c_r(1 - a_r)^{-1}b_r = 1, \tag{31}$$

which results in a unity gain and where $c_r = 1$ and b_r has to be equal to $1 - a_r$. This enables reference trajectory tracking without the control error (the asymptotic reference tracking).

The prediction of the reference trajectory is then written in the following form

$$y_r(k + H) = a_r^H y_r(k) + (1 - a_r^H)w(k), \tag{32}$$

where a constant and bounded reference signal ($w(k + i) = w(k), i = 1, \ldots, H$) is assumed. The main goal of the proposed

algorithm is to find a control law that enables the controlled signal $y_p(k)$ to track the reference trajectory.

To develop the control law, (32) is first rewritten as

$$w(k + H) - y_r(k + H) = a_r^H(w(k) - y_r(k)). \tag{33}$$

Taking into account the main idea of the proposed control law, the reference trajectory tracking ($y_r(k + i) = y_p(k + i)$, $i = 0, 1, \ldots, H$), is given by

$$y_p(k + H) = w(k + H) - a_r^H(w(k) - y_p(k)). \tag{34}$$

The idea of PFC is introduced by the equivalence of the objective increment vector Δ_p and the model output increment vector Δ_m, i.e.,

$$\Delta_p = \Delta_m. \tag{35}$$

The former is defined as the difference between the predicted reference signal vector $y_r(k + H)$ and the actual output vector of the plant $y_p(k)$.

$$\Delta_p = y_r(k + H) - y_p(k) \tag{36}$$

Substituting Eq. (34) into (37) yields

$$\Delta_p = y_p(k + H) - y_p(k)$$
$$= w(k + H) - a_r^H(w(k) - y_p(k)) - y_p(k). \tag{37}$$

The model output increment vector Δ_m is defined by the following formula.

$$\Delta_m = y_m(k + H) - y_m(k) \tag{38}$$

By substituting Eqs. (37) and (38) into (35) and making use of Eqs. (34) and (29) the following control law can be obtained:

$$u(k) = \eta^{-1}((1 - a_r^H)(w(k) - y_p(k)) + y_m(k) - C_m A_m^H x_m(k)), \tag{39}$$

where,

$$\eta = C_m(A_m^H - I)(A_m - I)^{-1}B_m. \tag{40}$$

Note that the control law (39) is realizable if $\eta \neq 0$. This condition is true if the plant is stable, controllable and observable. This means that the PFC control law in its common form can be implemented only for open-loop stable systems. It can also be proven that the control law is integrative and the stability conditions can also be given [13]. The sensitivity to the parameter uncertainties reduced is by introducing the integrative action into the control law and also the asymptotic tracking of the reference variable is achieved. In [13] it is shown that a stable control law can always be obtained for open-loop stable systems, when the coincidence horizon H is greater than or is equal to the relative order of the controlled system ρ ($H \geq \rho$) as proposed. The control algorithm in the case of the batch reactor should provide a fast reference $T_{ref}(k)$ tracking of the temperature in the reactor's core $T(k)$. It is also very important that the number of on/off valve switchings should be as small as possible. The position of

the on/off valves ($k_{CH}(k)$) is defined on the supervisory level by introducing the decision logic, which is as follows:

$$\begin{aligned} \textbf{if} \quad & T_{ref}(k) - T(k) < \delta_e \quad \textbf{then} \quad k_{CH}(k) = -1 \\ & \textbf{else} \quad k_{CH}(k) = 1 \end{aligned} \tag{41}$$

Here, δ_e defines the switching threshold ($\delta_e = -1\,°C$). This approach is a rather straightforward way of dealing with the hybrid nature of the batch reactor.

The position of the mixing valve $k_M(k)$, which acts as the direct control variable, is calculated in the next step from Eq. (4).

$$k_M(k) = \frac{T_{jin}^*(k) - T_j(k)}{T_{in}(k) - T_j(k)} \tag{42}$$

Here, $T_{in}(k)$ is defined by the position of the on/off valves.

4. Results

The control algorithm was verified on the batch-reactor simulation example. The simulation work in [2] concerning the reaction described in Section 2.3 suggests that an equimolar initial charge of the ingredients A and B yields the best results. In addition, the optimal reaction temperature is 95 °C.

Therefore, we have established the reference trajectory T_{ref} as a step function. The initial value of the reference trajectory is 95 °C, so that the ingredients react at the optimal temperature, as specified in [2]. After the reaction has settled, the reference drops to 25 °C so as to cool the ingredients down before engaging a new batch.

The initial charge of the ingredients A and B was $M_A = M_B = 2$ kmol, as suggested in [2]. The initial temperature was $T = T_j = T_0 = 17\,°C$.

In the simulation the following initialization of the identification algorithm parameters was made:

- The signals were sampled with the sampling time $T_s = 20$ s, which was chosen by considering the relevant time-constants of the plant.
- The initial covariance matrices were equal to $P_1(0) = 100 I_3$ and $P_2(0) = 100 I_2$. Here I_j denotes an identity matrix of size j. The initial values have to be positive definite and sufficiently large. By using the Kalman-filter interpretation of the least-squares parameter-estimation method, it may be seen that this way of starting the recursion corresponds to the situation in which the parameters have an initial distribution with covariance $P_1(0)$ and $P_2(0)$ [1].
- The vectors of the estimated process parameters were initialized as $\theta_{11} = \theta_{22} = 1$. The other parameters were equal to 0. Again, by using the Kalman-filter interpretation of the least-squares parameter-estimation method, it may be seen that this way of starting the recursion corresponds to the situation in which the parameters have an initial distribution with the previously specified mean value.
- The forgetting factors of the identification algorithms were set to $\gamma_1 = \gamma_2 = 0.995$. The method for dealing with time-varying parameters involves using a recursive least-squares
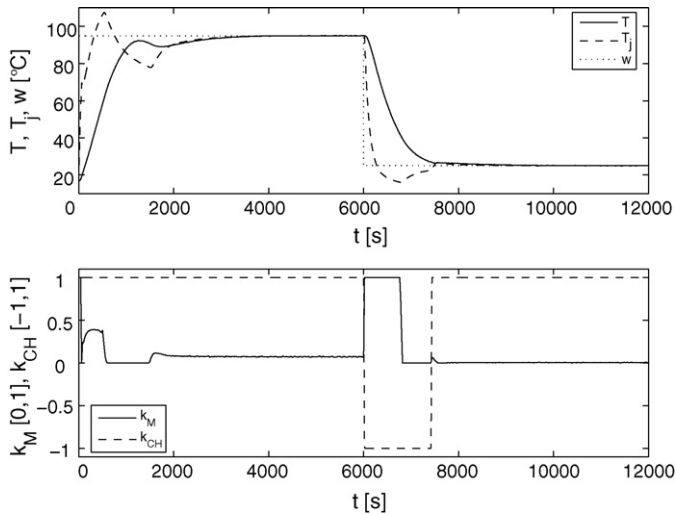
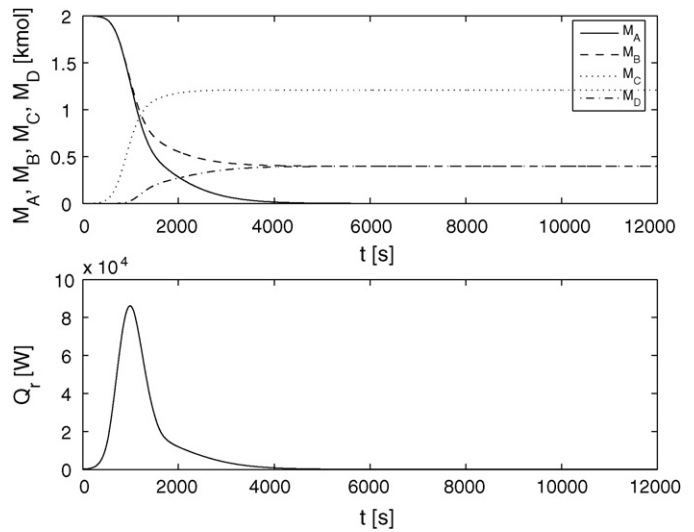Fig. 2. Temperature trajectories and valve input signals.

Fig. 3. Concentration trajectories and heat generation.

algorithm with exponential forgetting [1]. The forgetting factor has to be set between $0 < \gamma \le 1$, so as to introduce a time-varying weighting of the data used for parameter estimation. The most recent data is given a unit weight, whereas k-steps-old data is weighted by γ^k.

- The factor of the dead-zone was set to $k_{DZ} = 0.01$. The introduction of the dead-zone switches off the estimator when the input signal is not appropriate by updating the estimates only when the error is large enough.

The initialization of the generalized predictive control algorithm was as follows:

- The coincidence horizon was set to $H = 10$. This means that the predicted output will coincide with the output of the reference model after 10 time steps.
- The reference-model parameter was set to $a_r = 0.925$. This parameter defines the time-constant of the reference model and should be set according to the time-constants of the real plant. Changing this parameter results in a faster or slower control response.

The noise at the batch-reactor outputs was also presumed in the simulation.

Fig. 2 shows the control signals, i.e., the reference trajectory T_{ref}, the temperature in the reactor core T and the temperature in the reactor water jacket T_j. We can see that the reference trajectory was followed well by the temperature in the reactor core T. What is more, the adaptive algorithm allows the control actions to compensate for the strong exothermic reaction that takes place in the reactor core and to prevent a thermal runaway as well as to enable a response without an overshoot, which would not be possible when using a time-invariant process model.

Fig. 3 depicts the chemical reaction dynamics, i.e., the concentrations of the components M_A, M_B, M_C, M_D. We can see a decrease in the concentration of the components A and B and an increase in the concentration of the components C and D during the reactions. We can establish the rate of the reaction from the
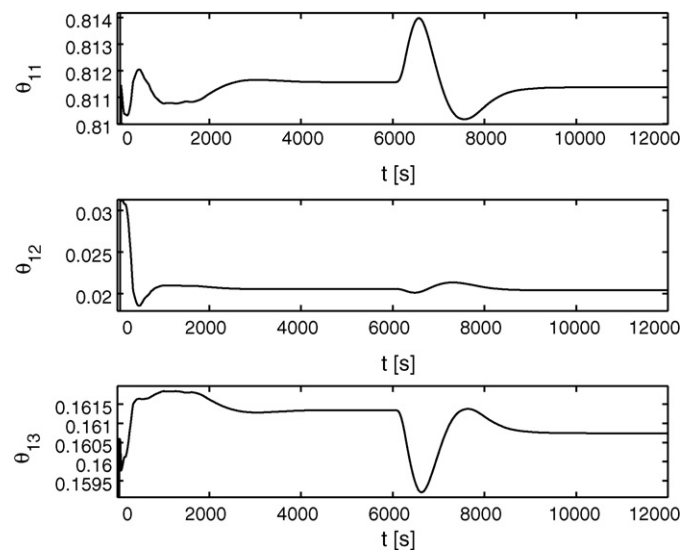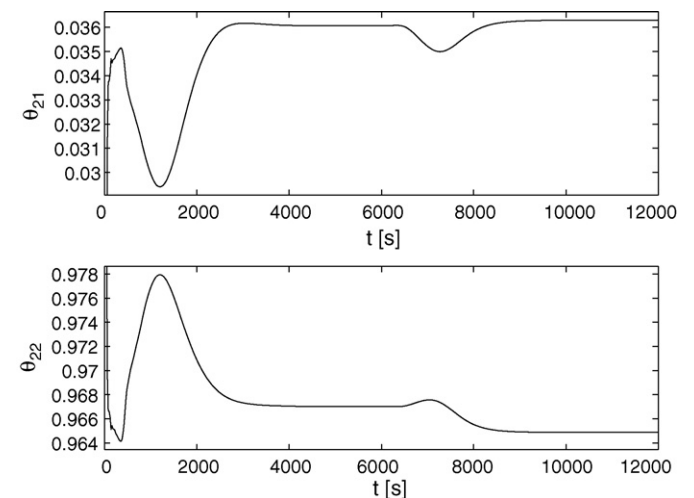

Fig. 4. The identified parameters.

Fig. 5. The identified parameters.

inclination of the relevant concentration trajectories. The heating power generated by both exothermic reactions is also shown in Fig. 3.

Figs. 4 and 5 show the identified process parameters θ. The figures are zoomed-in in order to show the changes of the parameters more clearly. However, we cannot see the initial values of the process parameters.

5. Conclusion

In this study we justified the usability of the self-adaptive predictive functional control algorithm. We tested the algorithm on a batch-reactor simulation example that included a well-known exothermic chemical reaction kinetic model.

The results suggest that such an implementation meets the control demands, despite the strongly exothermic nature of the chemical reaction. The reference is suitably tracked, which results in a shorter overall batch-time. In addition, there is no overshoot of the controlled variable T, which results in higher-quality production.

Batch reactors, such as the one used in the experiment, have a highly nonlinear and hybrid nature. What is more, such a process cannot be treated as a simple time-invariant process, especially when a strong exothermic reaction with unknown kinetics is involved. In this paper we showed how to avoid some of the difficulties in the control design for such processes.

Firstly, we introduced an auxiliary state $T^*_{j\text{in}}$, which cannot be measured directly. In this way we were able to linearize the system by treating $T^*_{j\text{in}}$ as a process input.

The linearized system allowed us to apply the self-adaptive predictive functional control algorithm that can only be used with linear systems. In such a manner we were able to cope with the time-varying parameters of the process, which is essential because of the exothermic reaction with unknown kinetics that takes place in the reactor core.

Finally, by introducing a suitable discrete switching logic in order to deal with the hybrid nature of the batch reactor, we were able to reduce the switching of the on/off valves to a minimum and therefore relieve the wear-out of the actuators as well as reduce the energy consumption needed for the control.

We believe that this paper presents a new approach to dealing with control synthesis problems that arise from the complex non-linear, time varying and hybrid dynamics of exothermic batch reactors.

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