

SELF-ADAPTIVE PREDICTIVE FUNCTIONAL CONTROL OF TEMPERATURE IN AN EXOTHERMIC BATCH REACTOR

Gorazd Karer¹, Igor Škrjanc¹, Borut Zupančič¹

¹University of Ljubljana, Faculty of Electrical Engineering
1000 Ljubljana, Tržaška 25, Slovenia

gorazd.karer@fe.uni-lj.si (Gorazd Karer)

Abstract

In this paper we study a self-adaptive predictive functional control algorithm as an approach to control of temperature in an exothermic batch reactor. The batch reactor is situated 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. Furthermore, 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 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 switching of the on/off valves to minimum and therefore relieve the wear-out of the actuators as well as reduce the energy consumption needed for control.

Keywords: Self-adaptive control, Predictive functional control, Batch reactor, Exothermic chemical reaction, Hybrid systems.

Presenting Author's Biography

Gorazd Karer received a B.Sc. in electrical engineering from the University of Ljubljana in 2004. He is currently a Ph.D. student at the Faculty of Electrical Engineering, University of Ljubljana. His research interests are in hybrid systems and model predictive 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 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 [1]. 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 event can cause a loss of the batch and even presents a risk for the plant and operators. For most reaction systems of industrial interest detailed kinetic models are not known [2]. In rapidly changing chemical business, there is often not enough time or financial benefit in carrying out detailed kinetic studies of the reactions.

What is more, sometimes the same reactor has to be able to deal with different batches and thus different reaction dynamics. This calls for special control strategies. The most promising seem to be the concepts of adaptive control [3], optimal control [4, 5, 6], and especially model predictive control schemes [7, 8, 9]. The principle 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 [10], 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. Section 3 summarizes the exothermic chemical reaction dynamics. Next, the recursive least-squares identification is explained in Section 4. In Section 5, the predictive functional control algorithm is presented. Finally, the simulation results and conclusions are discussed in Section 6 and Section 7.

2 Batch Reactor

The batch reactor in the experiment is a simulation example of a real batch reactor, which is situated 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.

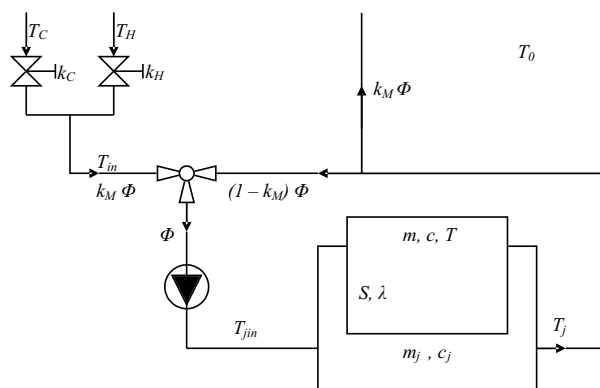


Fig. 1 Scheme of the batch reactor.

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, namely, 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 position of the on/off valves k_H and k_C . However, there are two possible operating modes of the on/off valves. In case $k_C = 1$ and $k_H = 0$, the input water is cool ($T_{in} = T_C = 12^\circ\text{C}$), whereas if $k_C = 0$ and $k_H = 1$, the input water is hot ($T_{in} = T_H = 150^\circ\text{C}$). 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.

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

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 $[0,1]$.

2.1 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.

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

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

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

Here, $m_j = 200$ kg stands for the mass of the water in the jacket, $c_j = 4200$ J kg⁻¹ K⁻¹ is the heat capacity of the water in the pipes, $\Phi = 1.6$ kg s⁻¹ is the mass flow in the pipes of the reactor, $\lambda = 420$ W m⁻² K⁻¹ stands for the thermal conductivity between the reactor core and the jacket, $\lambda_0 = 84$ W m⁻² K⁻¹ is the thermal conductivity between the jacket and the surroundings. $S = 2$ m² and $S_0 = 4$ m² denote the conduction surfaces between the reactor core and the jacket and between the jacket and the surrounding, respectively. The temperature of the surroundings is equal to $T_0 = 17^\circ\text{C}$.

The variables m and c stand for the mass and the heat capacity of the ingredients in the core of the reactor (see Eqs. (15) and (17) in section 3).

Q_r in Eq. (3) denotes the heat released due to exothermic nature of the reaction among the ingredients in the core of the batch reactor (see Eq. (18) in section 3).

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 [11, 2, 12]. A well-mixed liquid-phase reaction system is treated, in which two reactions are modelled.



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

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

$$\frac{dM_A}{dt} = -R_1 - R_2 \quad (7)$$

$$\frac{dM_B}{dt} = -R_1 \quad (8)$$

$$\frac{dM_C}{dt} = +R_1 - R_2 \quad (9)$$

$$\frac{dM_D}{dt} = +R_2 \quad (10)$$

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

$$R_1 = k_1 M_A M_B \text{ kmol}^{-1} \text{ s}^{-1} \quad (11)$$

$$R_2 = k_2 M_A M_C \text{ kmol}^{-1} \text{ s}^{-1} \quad (12)$$

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

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

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

The remaining physical variables are calculated as follows.

$$m = w_A M_A + w_B M_B + w_C M_C + w_D M_D \quad (15)$$

$$M = M_A + M_B + M_C + M_D \quad (16)$$

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

$$Q_r = -\Delta H_1 R_1 - \Delta H_2 R_2 \quad (18)$$

The parameters of the reaction are given below:

molar weight of the components

$$\begin{aligned} w_A &= 30 \text{ kg kmol}^{-1}, \\ w_B &= 100 \text{ kg kmol}^{-1}, \\ w_C &= 130 \text{ kg kmol}^{-1}, \\ w_D &= 1600 \text{ kg kmol}^{-1}; \end{aligned}$$

molar heat capacity of the components

$$\begin{aligned} c_A &= 75.31 \text{ kJ kmol}^{-1} \text{ }^\circ\text{C}^{-1}, \\ c_B &= 167.36 \text{ kJ kmol}^{-1} \text{ }^\circ\text{C}^{-1}, \\ c_C &= 217.57 \text{ kJ kmol}^{-1} \text{ }^\circ\text{C}^{-1}, \\ c_D &= 334.73 \text{ kJ kmol}^{-1} \text{ }^\circ\text{C}^{-1}; \end{aligned}$$

reaction rate constants

$$\begin{aligned} k_1^1 &= 20.9057, \\ k_1^2 &= 10000 \text{ }^\circ\text{C}, \\ k_2^1 &= 38.9057, \\ k_2^2 &= 17000 \text{ }^\circ\text{C}; \end{aligned}$$

heat of reaction

$$\begin{aligned} \Delta H_1 &= -41840 \text{ kJ kmol}^{-1}, \\ \Delta H_2 &= -25105 \text{ kJ kmol}^{-1}. \end{aligned}$$

4 Recursive least-squares identification

In our example the plant parameters are not known a priori. What is more, the chemical reaction causes the time-varying characteristics of the process. This is the reason why the parameters of the plant are estimated online. In our case we used the standard recursive estimator with exponential forgetting. To obtain the model in incremental form, the offset has to be eliminated, which is realized by filtration and differentiation of the measured signals.

The filtration and differentiation of the measured variables is realized by the filter transfer function defined as

$$G_f(z) = \frac{\Delta(z)}{F(z)}, \quad (19)$$

where $F(z) = (1 - fz^{-1})^p$, the parameter f is defined experimentally (in our example $f = 0.95$, $p = 3$), $\Delta(z) = 1 - z^{-1}$ is the differential operator and the sampling time equals $T_s = 20$ s. The behavior of the semi-batch reactor which is in continuous form presented in Eq. 2 and Eq. 3 is now transformed into the discrete-time domain as follows.

$$T_j^f(k) = \theta_{11}T_j^f(k-1) + \theta_{12}T^f(k-1) + \theta_{13}T_{jin}^f(k-1) \quad (20)$$

$$T^f(k) = \theta_{21}T_j^f(k-1) + \theta_{22}T^f(k-1) \quad (21)$$

Here, superscript f stands for the filtered signals.

Defining the regression vector $\psi_{f1}^T(k) \in \mathbb{R}^{1 \times 3}$, $\psi_{f2}^T(k) \in \mathbb{R}^{1 \times 2}$, the output variables y_{f1} and y_{f2} , and the vectors of identified parameters θ_1^T and θ_2^T as follows;

$$\psi_{f1}^T(k) = [T_j^f(k-1) \ T^f(k-1) \ T_{jin}^{*f}(k-1)], \quad (22)$$

$$\psi_{f2}^T(k) = [T_j^f(k-1) \ T^f(k-1)], \quad (23)$$

$$y_{f1}(k) = T_j^f(k), \quad (24)$$

$$y_{f2}(k) = T^f(k), \quad (25)$$

$$\theta_1^T = [\theta_{11}(k) \ \theta_{12}(k) \ \theta_{13}(k)], \quad (26)$$

$$\theta_2^T = [\theta_{21}(k) \ \theta_{22}(k)], \quad (27)$$

the following incremental model of the semi-batch reactor in is obtained.

$$y_{f1}(k) = \psi_{f1}^T(k)\theta_1(k) \quad (28)$$

$$y_{f2}(k) = \psi_{f2}^T(k)\theta_2(k) \quad (29)$$

The parameters of the model are estimated using the recursive least-square identification algorithm.

$$\sigma_i(k) =$$

$$P_i(k-1)\psi_{fi}(k) (\gamma_i + \psi_{fi}^T(k)P_i(k-1)\psi_{fi}(k))^{-1} \quad (30)$$

$$P_i(k) = (I_i - \sigma_i(k)\psi_{fi}^T(k))P_i(k-1)/\gamma_i \quad (31)$$

$$\theta_i(k) = \theta_i(k-1) + \sigma_i(k) (y_{fi}(k) - \psi_{fi}^T(k)\theta_i(k-1)), \quad i = 1, 2 \quad (32)$$

Here, $P_i(k)$, $i = 1, 2$ denotes the covariance matrix ($P_1(k) \in \mathbb{R}^{3 \times 3}$, $P_2(k) \in \mathbb{R}^{2 \times 2}$), $\theta_i(k)$, $i = 1, 2$ denotes the vector of identified or estimated process parameter, γ_i , $i = 1, 2$ denotes the forgetting factor and $I_1 \in \mathbb{R}^{3 \times 3}$ and $I_2 \in \mathbb{R}^{2 \times 2}$ 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 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 Eq. 28 into Z-domain and explicitly expressing the given relations, which are then described as follows.

$$G_{mj}(z) = \frac{T_j^f(z)}{T_{jin}^{*f}(z)} = \frac{b_{1j}z - b_{0j}}{z^2 - a_1z - a_0} \quad (33)$$

$$G_m(z) = \frac{T^f(z)}{T_{jin}^{*f}(z)} = \frac{b_0}{z^2 - a_1z - a_0} \quad (34)$$

Here, $b_{0j} = \theta_{22}\theta_{13}$, $b_{1j} = \theta_{13}$, $b_0 = \theta_{21}\theta_{13}$, $a_1 = \theta_{22} + \theta_{11}$, $a_0 = \theta_{12}\theta_{21} - \theta_{11}\theta_{22}$ and $\theta_{23} = 0$. The parameter θ_{23} equals zero ($\theta_{23} = 0$) because there is no relation between variables $T^f(k)$ and $T_{jin}^{*f}(k)$.

Assuming the observability of the process plant, both transfer functions, $G_{mj}(z)$ and $G_m(z)$, can be transformed to the observable canonical form.

Using the recursive least-squares algorithm we are always faced with the problem of the singularity of the covariance matrix $P_i(k)$, $i = 1, 2$. The covariance matrix is exponentially increasing in the case of $\gamma_i < 1$, $i = 1, 2$. The problem is solved by calculating the recursive algorithm only in the case of a satisfied dead-zone criterion.

$$\psi_{fi}^T(k)P_i(k-1)\psi_{fi}(k) > k_{DZ}(1-\gamma_i), \quad i = 1, 2 \quad (35)$$

Here, k_{DZ} denotes the factor of the dead-zone, which is defined heuristically.

5 Predictive functional control algorithm

In this section the well-known basic algorithm of predictive functional control is introduced [10], [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 a coincidence horizon and it is denoted by H . The prediction is calculated assuming of constant future manipulated variables

($u(k) = u(k+1) = \dots = u(k+H-1)$). This strategy is known as mean-level control. The H-step-ahead prediction of the plant output is estimated in Eq. (36).

$$y_m(k+H) = C_m(A_m^H x_m(k) + (A_m^H - I)(A_m - I)^{-1} B_m u(k)) \quad (36)$$

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

The reference model is given by the following difference equation.

$$\begin{aligned} x_r(k+1) &= a_r x_r(k) + b_r w(k) \\ y_r(k) &= c_r x_r(k) \end{aligned} \quad (37)$$

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

$$c_r (1 - a_r)^{-1} b_r = 1, \quad (38)$$

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

$$y_r(k+H) = a_r^H y_r(k) + (1 - a_r^H) w(k), \quad (39)$$

where a constant and bounded reference signal ($w(k+i) = w(k)$, $i = 1, \dots, H$) 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, (39) is first rewritten as

$$w(k+H) - y_r(k+H) = a_r^H (w(k) - y_r(k)). \quad (40)$$

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

$$y_p(k+H) = w(k+H) - a_r^H (w(k) - y_p(k)). \quad (41)$$

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.,

$$\Delta_p = \Delta_m. \quad (42)$$

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 $y_p(k)$.

$$\Delta_p = y_r(k+H) - y_p(k) \quad (43)$$

Substituting Equation (41) into (44) yields

$$\begin{aligned} \Delta_p &= y_p(k+H) - y_p(k) = \\ &= w(k+H) - a_r^H (w(k) - y_p(k)) - y_p(k). \end{aligned} \quad (44)$$

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

$$\Delta_m = y_m(k+H) - y_m(k) \quad (45)$$

By substituting Equations (44) and (45) into (42) and making use of Equations (41) and (36) the following control law can be obtained:

$$u(k) = \eta^{-1} ((1 - a_r^H)(w(k) - y_p(k)) + y_m(k) - C_m A_m^H x_m(k)), \quad (46)$$

where,

$$\eta = C_m (A_m^H - I) (A_m - I)^{-1} B_m. \quad (47)$$

Note that the control law (46) 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 is by introducing the integrative action into the control law reduced 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 or equals 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 supervisory level by introducing the decision logic which is as follows.

$$\begin{aligned} \text{if } T_{ref}(k) - T(k) < \delta_e \text{ then } k_{CH}(k) &= -1 \\ \text{else } k_{CH}(k) &= 1 \end{aligned} \quad (48)$$

Here, δ_e defines the switching threshold ($\delta_e = -1^0 C$). This approach is a rather straightforward way of dealing with the hybrid nature of the batch reactor.

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

$$k_M(k) = \frac{T_{jin}^*(k) - T_j(k)}{T_{in}(k) - T_j(k)} \quad (49)$$

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

6 Results

The control algorithm has been verified on the batch reactor simulation example. Simulation work in [11] concerning the reaction described in section 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 that drops from 95 °C to 25 °C so as to cool the ingredients down after the reaction has settled.

The initial charge of the ingredients A and B was $M_A = M_B = 2$ kmol. 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 $T_s = 20s$, the initial covariance matrices are equal to $P_1(0) = 100I_3$ and $P_2(0) = 100I_2$. The vectors of estimated process parameters were initialized as $\theta_{11} = \theta_{22} = 1$ and the other parameters were equal to zero. The forgetting factors of the identification algorithms were set to $\gamma_1 = \gamma_2 = 0.995$, and the factor of the dead-zone was set to $k_{DZ} = 0.01$. The initialization of the generalized predictive control algorithm was the following: $H = 10$ and $a_r = 0.925$. Noise at the batch reactor outputs has also been presumed in the simulation.

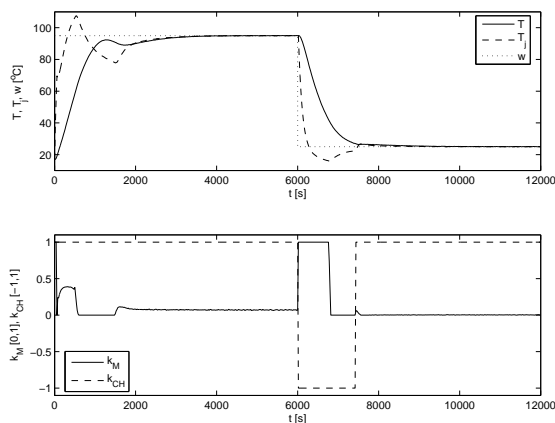


Fig. 2 Temperature trajectories and valve input signals

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 .

Fig. 3 depicts the chemical reaction dynamics, i.e. the concentrations of the ingredients M_A , M_B , M_C , M_D and the heat generation trajectory.

Fig. 4 and Fig. 5 show the identified process parameters θ .

7 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.

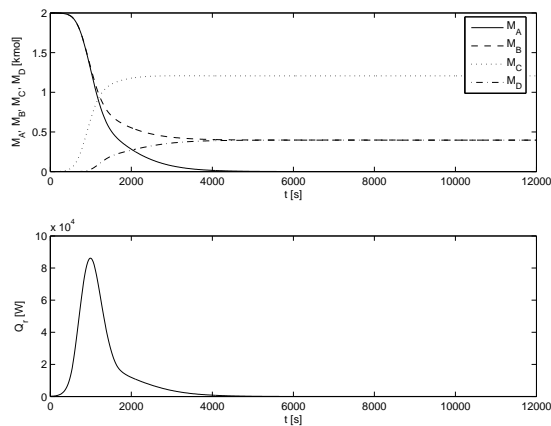


Fig. 3 Concentration trajectories and heat generation

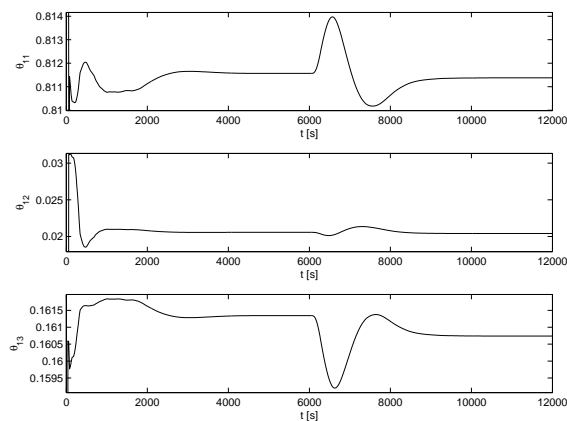


Fig. 4 The identified parameters

The results suggest that such 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 switching of the on/off valves to minimum and therefore relieve the wear-out of the actuators as well as reduce the energy consumption needed for control.

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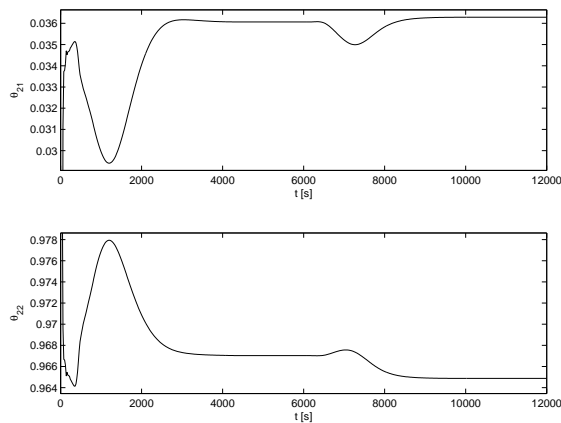


Fig. 5 The identified parameters

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