ELSEVIER

Chemical Engineering Journal 136 (2008) 312–319

Chemical Engineering Journal

www.elsevier.com/locate/cej

Self-adaptive supervisory predictive functional control of a hybrid semi-batch reactor with constraints

Igor Škrjanc *

Laboratory of Process Automation and Informatisation, Laboratory of Modelling, Simulation and Control, Faculty of Electrical Engineering, University of Ljubljana, Tržaška 25, 1000 Ljubljana, Slovenia

Received 16 January 2007; received in revised form 26 March 2007; accepted 3 April 2007

Abstract

In this paper self-adaptive supervisory predictive functional control is studied for applications in a semi-batch reactor in which the optimal operation is to follow the reference trajectory without significant overshoot, and to minimize the overall batch time. The volume in the reactor varies, bending to increase with time, as does the heat-transfer surface inside the reactor. This causes variations in the batch-reactor dynamics which means serious problems with the reactor's core-temperature control. The semi-batch reactor is used in the pharmaceutical industry for the production of drugs, where quality control is extremely strict and it is necessary to follow the exact production recipe. The semi-batch reactor is an example of a hybrid process where there are some discrete on/off valves and a continuous mixing valve. The supervisory control is designed to cope with the constraints and the discrete actuators. A simulation study was carried out to investigate the possible use of the proposed self-adaptive control algorithm in a real application.

Keywords: Adaptive control; Predictive control; Semi-batch reactor

1. Introduction

In chemistry, pharmacy and biotechnology the batch reactors function as the most important part in process technology. The control of batch reactors is essentially a problem of temperature control which is difficult to overcome. The difficulties arise in part from the mixed continuous and discrete nature of the process behavior and the equipment, the various uses of these reactors, the drastic changes in set-point during the operation and the different modes of operation which requires an adaptive functioning. Large numbers of these batch reactors are semi-batch or fed-batch reactors in which the initial mixture of material is placed. The mixture is then heated to the desired temperature and additional reactant is gradually added in to the vessel during the procedure. The volume in the reactor varies, tending to increase with time, as does the heat-transfer surface of the reactor. The construction of the reactor induces the heat-transfer through the reactor's jacket to the reactor's core. From the dynamic point of view the reactor represents a time-varying process with unknown parameters. The optimal operation of the semi-batch reactor is to follow the reference trajectory, which is defined by the technological recipe, as precisely as possible and without overshoot. All the important variables should be within the prescribed intervals. A very important constraint is that of the reactor's jacket temperature, which should not exceed its upper limit because this can cause damage to the ingredients, which are very sensitive to the temperature. Another important goal of batch-reactor control is the minimization of the overall batch time.

In the literature a number of papers have been published that discuss the control of batch reactors. Initially, a various types of controllers were studied, together with the optimum batch trajectories. The state-of-the-art control schemes up to the year 1986 are given in [15]. During that time many different concepts of semi-batch reactor control were developed. The most promising of these were the concepts of adaptive control [3,18], optimal control [2,8,19] and especially model-predictive control schemes, which are the most frequently used [4,5,9,11–13,16,17]. Model predictive control was very successful in solving many industrial control problems [1,6,7]. One of the most frequently used predictive schemes in practice is the predictive functional control scheme [21,22], which has been

* Tel.: +386 1 4768 311; fax: +386 1 4264 631.
E-mail address: igor.skrjanc@fe.uni-lj.si.

1385-8947/$ – see front matter © 2007 Elsevier B.V. All rights reserved.
doi:10.1016/j.cej.2007.04.012

used in our study. The main advantage of this proposed algorithm is the analytical expression of the control law, which enables it to be used in real-time control and implemented on low-cost hardware. The main goal of our simulation study was to elaborate the possible use of the proposed self-adaptive supervisory control algorithm in a real application. The process control requirements are relatively difficult: fast reference-trajectory tracking, small overshoot of the controlled variable and a small number of switchings between cold and hot water at the inlet. Special difficulties arise due to the constraints of the mixing valve and due to the constraints that are the results of the chemical properties of the process and the mechanical structure of the batch reactor. Self-adaptive algorithms are a conceptually appealing scheme for the control of complex industrial processes where manual tuning of the controller parameters appear to be prolonged and cumbersome, when the parameters of the processes are time-varying, and when we are dealing with a number of similar plants that have to be controlled, i.e., the same algorithm can be used with special tuning of the controller parameter. The principal self-adaptive algorithms are either based on minimization of the quadratic index or, alternatively, they are derived by attempting to place the closed-loop poles at an arbitrary position, commonly denoted as sub-optimal as they are not designed to minimize any cost function [10,14,20]. In our case it is based on a recursive least-squares identification algorithm with exponential forgetting.

The paper is organized in the following way: in Section 2 the semi-batch reactor is described, in Section 3 the recursive least-squares algorithm is discussed, in Section 4 the predictive functional control algorithm and the supervisory level control are described, and in Section 5 the simulation results are presented.

2. The semi-batch reactor

The semi-batch reactor, in this case, is situated in a pharmaceutical company, used in the production of medicines. Dynamically, it is an example of a hybrid plant. The goal is to control the temperature of the ingredients stirred in the reactor's core so that they synthesize optimally into the final product. In order to achieve this, the temperature has to follow, as accurately as possible, the technologically prescribed reference trajectory given in the recipe.

A scheme of the semi-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 construction of the reactor enables measurements of the jacket temperature, T_j, and the reactor's core temperature, T. The temperature of the ingredients should not exceed the maximal temperature of 60 °C, because of the temperature sensitivity of the ingredients. This means that both temperatures, the water-jacket temperature and the reactor's core temperature, should not exceed the maximal temperature. This can be achieved with an explicitly controlled temperature inside the reactor, T, and by treating the limitation of the jacket temperature, T_j, which can be viewed as a state of the process, as the constraint control problem. The constraint of the jacket temperature will be denoted as $T_{j\max} = 60\,^{\circ}\mathrm{C}$.

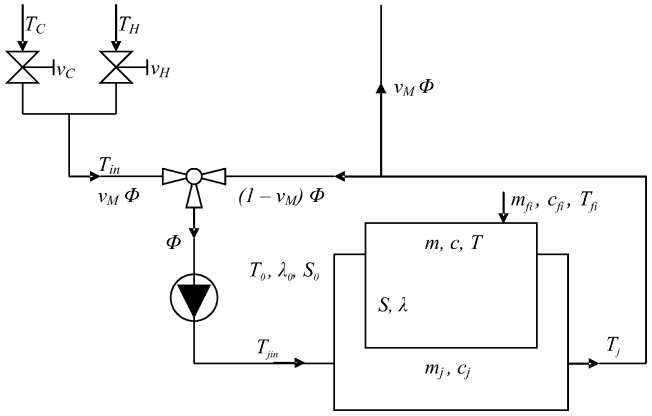

Fig. 1. The scheme of semi-batch reactor process.

The medium in the jacket is a mixture of fresh input water, which enters the reactor through on/off valves, and the reflux water. The temperature of the fresh input water depends on two inputs: the positions of the on/off valves v_H and v_C. However, there are two possible operating modes of the on/off valves. In the case when $v_C = 1$ and $v_H = 0$, the input water is cool ($T_{in} = T_C = 12\,^{\circ}\mathrm{C}$), whereas if $v_C = 0$ and $v_H = 1$, the input water is hot ($T_{in} = T_H = 75\,^{\circ}\mathrm{C}$). Both on/off valves are controlled by the signal v_{CH} which is defined as:

$$v_{CH} = \begin{cases} +1, & \text{if } v_C = 0 \text{ and } v_H = 1 \\ -1, & \text{if } v_C = 1 \text{ and } v_H = 0 \end{cases} \tag{1}$$

The ratio of fresh input water to reflux water is controlled by a third input, i.e., by the position of the mixing valve v_M, which is limited to the range $[v_{M\min}, v_{M\max}]$. The valve rate is constrained in the range $[\Delta v_{M\min}, \Delta v_{M\max}]$.

We are therefore dealing with a multivariable system with two discrete inputs (v_H and v_C), one continuous input, v_M, and two measurable outputs (T and T_j). The temperature of the mixed water or the input jacket temperature, which cannot be measured directly, although it can be estimated using the temperature of the input water, T_{in}, the water jacket temperature, T_j, and the position of the mixing valve v_M, which is denoted as T_{jin}. It is constrained in the range between T_C and T_H ($T_C \le T_{jin} \le T_H$). The time constants of the on/off valves are relatively small in comparison to the time constants of the process itself and can be neglected, but the dynamics of the mixing valve has to be considered in the model.

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 semi-batch reactor is considered as a stiff system.

The mathematical model of the semi-batch reactor is defined by the differential equations Eqs. (2), (3), (5), (6) and (7) and the algebraic equations Eqs. (4) and (8).

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

$$mc\frac{\mathrm{d}T}{\mathrm{d}t} = \lambda S(T_\mathrm{j} - (T + \Delta T\,\delta(t - t_i))) \tag{3}$$

$$\Delta T = \frac{m_{\mathrm{f}i}c_{\mathrm{f}i}(T_{\mathrm{f}i} - T)}{mc + m_{\mathrm{f}i}c_{\mathrm{f}i}} \tag{4}$$

where $m_\mathrm{j} = 200\,\mathrm{kg}$ stands for the mass of the water in the jacket, $c_\mathrm{j} = 4200\,\mathrm{J\,kg^{-1}\,K^{-1}}$the heat capacity of the water in the pipes, $\Phi = 1.6\,\mathrm{kg\,s^{-1}}$ the mass flow in the pipes of the reactor, $\lambda = 420\,\mathrm{W\,m^{-2}\,K^{-1}}$ the thermal conductivity between the reactor core and the jacket, $\lambda_0 = 84\,\mathrm{Wm^{-2}\,K^{-1}}$ and $S_0 = 4\,\mathrm{m^2}$ are the thermal conductivity between the jacket and the surroundings and the conduction surface. The temperature of the surroundings is equal to $T_0 = 17\,^\circ\mathrm{C}$. During the procedure additional ingredients are added to the reactor. This causes a change of the mass of ingredients inside the reactor, m, a change of the heat capacity, c, a change of the conduction surface, S, and a change of the reactor's core temperature T. These changes are much faster than the time constants of the reactor, and for this reason they are modeled as discontinuous jumps of variables. The discontinuous jumps, which occur at time instants t_i are in our case modeled using a Dirac impulse δ. The discontinuous phenomena of the system state, T, is modeled as follows from Eq. (3). The state jump, ΔT, is defined in Eq. (4), where $m_{\mathrm{f}i}$ stands for the mass of ingredient added to the reactor at the time instant t_i, $c_{\mathrm{f}i}$ defines the heat capacity of the ingredient that is added and $T_{\mathrm{f}i}$ stands for the temperature of the ingredient at the time of loading (t_i). The variation of the mass inside the reactor is given in Eq. (5). Eq. (6) denotes the change of the average heat capacity of the mixture inside the reactor, where

$$\Delta c_i = (c_{\mathrm{f}i} - c)\frac{m_{\mathrm{f}i}}{m + m_{\mathrm{f}i}}.$$

$$\frac{\mathrm{d}m}{\mathrm{d}t} = m_{\mathrm{f}i}\delta(t - t_i),\ m(0) \tag{5}$$

$$\frac{\mathrm{d}c}{\mathrm{d}t} = \Delta c_i\delta(t - t_i),\ c(0) \tag{6}$$

The time-varying profile of the conduction surface, S, is given in Eq. (7) as follows:

$$\frac{\mathrm{d}S}{\mathrm{d}t} = S_{\mathrm{f}i}\delta(t - t_i),\ S(0) \tag{7}$$

where $S_{\mathrm{f}i}$ stands for the change of the conduction surface at time t_i, due to the added ingredient. In our case it is roughly modeled as $S_{\mathrm{f}i} = Sm_{\mathrm{f}i}/m$.

The temperature in the reactor can be controlled indirectly by the input jacket temperature, T_jin, which is now called the indirect control variable and actually depends on the position of the mixing valve and on the temperature of the fresh water, as shown in Eq. (8) which follows

$$T_\mathrm{jin} = v_\mathrm{M}T_\mathrm{in} + (1 - v_\mathrm{M})T_\mathrm{j} \tag{8}$$

In our approach the control will be developed based on the indirect control variable, which after the supervisory level control will be transformed into the real control variables, i.e., the position of the mixing valve, v_M, and the position of the discrete valves, v_C and v_H.

3. Recursive least-squares identification

In our example the plant parameters are not known a priori; the semi-batch reactor is fed during the operation and causes the time-varying characteristics of the process ($m(t)$, $c(t)$ and $S(t)$). 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. The last right term in the differential equation from Eq. (2) exhibits the loss energy flow into the surroundings and represents an offset in this equation (affine equation). To obtain the model in incremental form, the offset has to be eliminated, which is realized by the filtration and differentiation of the measured signals.

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

$$G_\mathrm{f}(z) = \frac{\Delta(z)}{F(z)} \tag{9}$$

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 $T_\mathrm{s} = 20\,\mathrm{s}$. The behavior of the semi-batch reactor, which is presented in Eqs. (2) and (3) in continuous form is now transformed into the discrete-time domain as follows:

$$T_\mathrm{j}^\mathrm{f}(k) = \theta_{11}T_\mathrm{j}^\mathrm{f}(k-1) + \theta_{12}T^\mathrm{f}(k-1) + \theta_{13}T_\mathrm{jin}^\mathrm{f}(k-1) \tag{10}$$

$$T^\mathrm{f}(k) = \theta_{21}T_\mathrm{j}^\mathrm{f}(k-1) + \theta_{22}T^\mathrm{f}(k-1) \tag{11}$$

where superscript 'f' stands for the filtered signals.

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

$$\psi_{\mathrm{f}1}^\mathrm{T}(k) = [\,T_\mathrm{j}^\mathrm{f}(k-1) \quad T^\mathrm{f}(k-1) \quad T_\mathrm{jin}^\mathrm{f}(k-1)\,] \tag{12}$$

$$\psi_{\mathrm{f}2}^\mathrm{T}(k) = [\,T_\mathrm{j}^\mathrm{f}(k-1) \quad T^\mathrm{f}(k-1)\,] \tag{13}$$

$$y_{\mathrm{f}1}(k) = T_\mathrm{j}^\mathrm{f}(k) \tag{14}$$

$$y_{\mathrm{f}2}(k) = T^\mathrm{f}(k) \tag{15}$$

$$\theta_1^\mathrm{T} = [\,\theta_{11}(k) \quad \theta_{12}(k) \quad \theta_{13}(k)\,] \tag{16}$$

$$\theta_2^\mathrm{T} = [\,\theta_{21}(k) \quad \theta_{22}(k)\,] \tag{17}$$

the following incremental models of the semi-batch reactor are obtained:

$$y_{\mathrm{f}1}(k) = \psi_{\mathrm{f}1}^\mathrm{T}(k)\theta_1(k) \tag{18}$$

$$y_{\mathrm{f}2}(k) = \psi_{\mathrm{f}2}^\mathrm{T}(k)\theta_2(k) \tag{19}$$

The parameters θ_i, $i = 1, 2$ are estimated using the recursive least-square identification algorithm as follows:

$$\sigma_i(k) = P_i(k-1)\psi_{\mathrm{f}i}(k)(\gamma_i + \psi_{\mathrm{f}i}^\mathrm{T}(k)P_i(k-1)\psi_{\mathrm{f}i}(k))^{-1} \tag{20}$$

$$P_i(k) = (I_i - \sigma_i(k)\psi_{\mathrm{f}i}^\mathrm{T}(k))P_i(k-1)/\gamma_i \tag{21}$$

$$\theta_i(k)=\theta_i(k-1)+\sigma_i(k)(y_{fi}(k)-\psi_{fi}^{T}(k)\theta_i(k-1)),\quad i=1,2 \tag{22}$$

where $P_i(k)$, $i=1,2$ denotes the covariance matrix ($P_1(k)\in\mathbb{R}^{3\times3}$, $P_2(k)\in\mathbb{R}^{2\times2}$), $\theta_i(k)$, $i=1,2$ denotes the vector of the identified or estimated process parameter, 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 dynamics of the process is now given by the transfer functions $G_{mj}(z)$ and $G_m(z)$, which denote the behavior of the plant variables $T_j^f(k)$ and $T^f(k)$ according to the input jacket temperature $T_{jin}^f(k)$. Both transfer functions are obtained by transforming Eqs. (10) and (11) into the Z-domain, and explicitly expressing the given relations, which are then described as follows:

$$G_{mj}(z)=\frac{T_j^f(z)}{T_{jin}^f(z)}=\frac{b_{1j}z-b_{0j}}{z^2-a_1z-a_0} \tag{23}$$

$$G_m(z)=\frac{T^f(z)}{T_{jin}^f(z)}=\frac{b_0}{z^2-a_1z-a_0} \tag{24}$$

where $b_{0j}=\theta_{22}\theta_{13}$, $b_{1j}=\theta_{13}$, $b_0=\theta_{21}\theta_{13}$, $a_1=\theta_{22}+\theta_{11}$ and $a_0=\theta_{12}\theta_{21}-\theta_{11}\theta_{22}$.

Assuming the observability of the process plant, both transfer functions, $G_{mj}(z)$ and $G_m(z)$, are transformed to the observable canonical form. The obtained state-space matrices are A_{mj}, B_{mj}, C_{mj} and A_m, B_m, C_m, respectively, assuming that both input–output matrices are equal to zero and that $C_{mj}=[0\ldots0\,1]$ and $C_m=[0\ldots0\,1]$ due to the observable canonical form. The state-space equivalents of the transfer functions $G_{mj}(z)$ and $G_m(z)$ are given as follows:

$$x_{mj}(k+1)=A_{mj}x_{mj}(k)+B_{mj}T_{jin}^f,\quad T_j^f(k)=C_{mj}x_{mj}(k) \tag{25}$$

$$x_m(k+1)=A_mx_m(k)+B_mT_{jin}^f,\quad T^f(k)=C_mx_m(k) \tag{26}$$

where $x_{mj}(k)$ and $x_m(k)$ stand for the model states.

Using the recursive least-squares algorithm, we are faced with the problem of the covariance matrix $P_i(k)$, $i=1,2$, when there is not enough excitation. In that case the covariance matrix is exponentially increasing if the forgetting factor $\gamma_i<1$, $i=1,2$. This problem, which is called *bursting*, is solved by calculating the recursive algorithm only in the case of a satisfied excitation criterion:

$$\psi_{fi}^{T}(k)P_i(k-1)\psi_{fi}(k)>k_{DZ}(1-\gamma_i),\ i=1,2 \tag{27}$$

where k_{DZ} denotes the factor of the dead-zone, when the identification algorithm is frozen. The dead-zone parameter is defined heuristically.

4. The predictive functional control algorithm

In this section the well-known basic algorithm of predictive functional control is introduced [21,23]. 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 the 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 ($u(k)=u(k+1)=\cdots=u(k+H-1)$). This strategy is known as mean-level control. The H-step-ahead prediction of the plant output is estimated in Eq. (28):

$$y_m(k+H)=C_m(A_m^Hx_m(k)+(A_m^H-I)(A_m-I)^{-1}B_mu(k)) \tag{28}$$

where $I\in\mathbb{R}^{2\times2}$ is unity matrix.

The reference model is given by the following difference equation

$$\begin{aligned}x_r(k+1)&=a_rx_r(k)+b_rw(k)\\ y_r(k)&=c_rx_r(k)\end{aligned} \tag{29}$$

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

$$c_r(1-a_r)^{-1}b_r=1 \tag{30}$$

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

$$y_r(k+H)=a_r^Hy_r(k)+(1-a_r^H)w(k) \tag{31}$$

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, (31) is first rewritten as

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

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

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

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.,

$$\Delta_p=\Delta_m \tag{34}$$

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 $y_p(k)$

$$\Delta_p=y_r(k+H)-y_p(k) \tag{35}$$

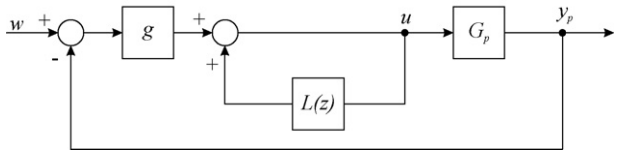

Fig. 2. The control scheme of PFC.

Substituting Eqs. (33) into (36) yields,

$$\begin{aligned}\Delta_{\mathrm{p}} &= y_{\mathrm{p}}(k+H) - y_{\mathrm{p}}(k)\\ &= w(k+H) - a_{\mathrm{r}}^{H}(w(k) - y_{\mathrm{p}}(k)) - y_{\mathrm{p}}(k)\end{aligned} \tag{36}$$

The model output increment vector Δ_{m} is defined by the following formula:

$$\Delta_{\mathrm{m}} = y_{\mathrm{m}}(k+H) - y_{\mathrm{m}}(k) \tag{37}$$

By substituting Eqs. (36) and (37) into (34) and making use of Eqs. (33) and (28) the following control law can be obtained,

$$u(k) = \eta^{-1}((1 - a_{\mathrm{r}}^{H})(w(k) - y_{\mathrm{p}}(k)) + y_{\mathrm{m}}(k) - C_{\mathrm{m}}A_{\mathrm{m}}^{H}x_{\mathrm{m}}(k)) \tag{38}$$

where

$$\eta = C_{\mathrm{m}}(A_{\mathrm{m}}^{H} - I)(A_{\mathrm{m}} - I)^{-1}B_{\mathrm{m}} \tag{39}$$

The closed-loop scheme with the basic control law defined in Eq. (38) is presented in Fig. 2 where

$$\begin{aligned}g &= \eta^{-1}(1 - a_{\mathrm{r}}^{H})\\ L(z) &= \eta^{-1}(1 - a_{\mathrm{r}}^{H})(zI - A_{\mathrm{m}})^{-1}B_{\mathrm{m}}\end{aligned} \tag{40}$$

Note that the control law (38) 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 [23]. The sensitivity to the parameter uncertainties is reduced by implicitly introduced integrative action into the control law and the asymptotic tracking of the reference variable is achieved. In [23] 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 equals the relative order of the controlled system, ρ ($H \geq \rho$), as proposed.

5. Supervisory predictive functional control for a semi-batch reactor

The control algorithm in the case of a semi-batch reactor should provide a fast reference tracking of the temperature in the reactor's core $T(k)$, taking into account the constraint of the jacket temperature, $T_{\mathrm{j}}(k)$, which should not exceed $T_{\mathrm{j_{max}}}$, and the constraints of the valves. It is also very important that the number of on/off valve switchings should be as small as possible. There are also the mechanical (physical) constraints of the mixing valve, for example, the minimal and the maximal values and the minimal and the maximal rate of the valve. The time constant of the mixing valve is taken into account by the proposed identification of the process dynamics.

The problem of the constraint jacket temperature, $T_{\mathrm{j}}(k)$, can be efficiently solved using supervisory level and analytical predictive functional control law. The supervisory level control means decision making according to the model-based jacket temperature monitoring. The decision making means switching between different predictive control laws. Next, the supervisory predictive functional control algorithm will be presented. In the first step, the unconstrained predictive control law $u_{\mathrm{m}}(k)$ will be calculated as given next:

$$u_{\mathrm{m}}(k) = \eta_{\mathrm{m}}^{-1}((1 - a_{\mathrm{r}}^{H})(w(k) - y_{\mathrm{p}}(k)) + y_{\mathrm{m}}(k) - C_{\mathrm{m}}A_{\mathrm{m}}^{H}x_{\mathrm{m}}(k)) \tag{41}$$

$$\eta_{\mathrm{m}} = C_{\mathrm{m}}(A_{\mathrm{m}}^{H} - I)(A_{\mathrm{m}} - I)^{-1}B_{\mathrm{m}} \tag{42}$$

where $y_{\mathrm{p}}(k)$ stands for the current core temperature, $x_{\mathrm{m}}(k)$ and y_{m} are the states and the output of the process model that defines the dynamics between the jacket input temperature, $T_{\mathrm{jin}}(k)$, and the output temperature, $T(k)$. In the second step, the constrained predictive control law $u_{\mathrm{mj}}(k)$ is calculated as follows:

$$\begin{aligned}u_{\mathrm{mj}}(k) &= \eta_{\mathrm{mj}}^{-1}((1 - a_{\mathrm{r}}^{H})(T_{\mathrm{j_{max}}} - y_{\mathrm{pj}}(k)) + y_{\mathrm{mj}}(k) - C_{\mathrm{mj}}A_{\mathrm{mj}}^{H}x_{\mathrm{mj}}(k))\\ \eta_{\mathrm{mj}} &= C_{\mathrm{mj}}(A_{\mathrm{mj}}^{H} - I)(A_{\mathrm{mj}} - I)^{-1}B_{\mathrm{mj}}\end{aligned} \tag{43}$$

where $y_{\mathrm{pj}}(k)$ stands for the current jacket temperature, $x_{\mathrm{mj}}(k)$ and $y_{\mathrm{mj}}(k)$ are the states and the output of the process model that defines the relation between the jacket input temperature, $T_{\mathrm{jin}}(k)$, and the jacket temperature $T_{\mathrm{j}}(k)$. This control law is called the constrained control law because we are calculating the control law that has $T_{\mathrm{j_{max}}}(k)$ as the reference value. In the third step, the prediction of the jacket temperature is calculated using the unconstrained control law $u_{\mathrm{m}}(k)$:

$$y_{\mathrm{mj}}(k+h) = C_{\mathrm{mj}}(A_{\mathrm{mj}}^{h}x_{\mathrm{mj}}(k) + (A_{\mathrm{mj}}^{h} - I)(A_{\mathrm{mj}} - I)^{-1}B_{\mathrm{mj}}u_{\mathrm{m}}(k)) \tag{44}$$

where $h \geq \rho_{\mathrm{in}}$ denotes the prediction horizon of the internal model, where ρ_{in} stands for relative order of the internal model.

Next, the most important part of the supervisory level is introduced as the decision logic that switches between the control law $u_{\mathrm{m}}(k)$ and the constrained control $u_{\mathrm{mj}}(k)$ in the following way:

$$\begin{aligned}&\text{if } y_{\mathrm{mj}}(k+h) - y_{\mathrm{mj}}(k) \leq T_{\mathrm{j_{max}}} - T_{\mathrm{j}}(k) \text{ then } T_{\mathrm{jin}}(k) = u_{\mathrm{m}}(k)\\ &\text{if } y_{\mathrm{mj}}(k+h) - y_{\mathrm{mj}}(k) > T_{\mathrm{j_{max}}} - T_{\mathrm{j}}(k) \text{ then } T_{\mathrm{jin}}(k) = u_{\mathrm{mj}}(k)\end{aligned} \tag{45}$$

where the jacket input temperature, $T_{\mathrm{jin}}(k)$, acts as the indirect control variable. This means that the position of the on/off valves and the position of the mixing valve, which both act as the direct control variables, have to be defined to fulfill the required jacket input temperature, $T_{\mathrm{jin}}(k)$, given in Eq. (45). The position of the

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

$$\text{if } e(k) < \delta_e \text{ then } v_{CH}(k) = -1 \text{ else } v_{CH}(k) = 1 \quad (46)$$

where δ_e defines the switching threshold ($\delta_e = -1\,^\circ\text{C}$) and the position of the mixing valve $v_M(k)$ is calculated from Eq. (8) as follows:

$$v_M(k) = \frac{T_{jin}(k) - T_j(k)}{T_{in}(k) - T_j(k)} \quad (47)$$

where $T_{in}(k)$ is defined by the position of the on/off valves. The position and the rate of the mixing valve are limited according to the physical limitation of the valve (the position [0,1] and the valve rate $[-0.01, 0.01]$).

6. Simulation results

The self-adaptive supervisory predictive functional control algorithm was tested on a semi-batch reactor by means of a simulation. The study was meant to show the potential of the proposed approach for further real applications using semi-batch reactors in the pharmaceutical industry. The obtained results are very promising, especially because of the very elegant way of tuning the controller, the possibility to handle the signal constraints together with high control performance and adaptation.

In the simulation the following initialization of the identification algorithm parameters was made: the signals were sampled with the sampling time $T_s = 20\,\text{s}$, the initial covariance matrices are equal to $P_1(0) = 100I_3$ and $P_2(0) = 100I_2$. The vectors of the 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 $a_r = 0.925$.

In the simulated experiment the initial mass in the reactor's core equals $m(0) = 600\,\text{kg}$, the conduction surface $S(0) = 2\,\text{m}^2$, the heat capacity $c(0) = 4200\,\text{J kg}^{-1}\,\text{K}^{-1}$ and the mass in the jacket equals $m_j = 200\,\text{kg}$. The reactor is fed with an additional ingredient ($m_{f1} = 100\,\text{kg}$, $c_{f1} = 4200\,\text{J kg}^{-1}\,\text{K}^{-1}$, $T_{f1} = 17\,^\circ\text{C}$) at the time $t_1 = 8000\,\text{s}$, and with the second additional ingredient ($m_{f2} = 150\,\text{kg}$, $c_{f2} = 4200\,\text{J kg}^{-1}\,\text{K}^{-1}$, $T_{f2} = 17\,^\circ\text{C}$) at the time $t_2 = 30{,}000\,\text{s}$. These parameters are only used to simulate the process and are not used in the controller design procedure. All the information about the process parameters θ is obtained by recursive identification.

The prescribed temperature profile is the following: the ingredient of the reactor should first be heated to 42 ° C (in this phase the first additive is added), at the time 12,500 s the temperature is changed to 54 ° C (in this phase the second additive is added), at time 25,000 s the temperature is cooled down to 38 ° C and after that at time 37,500 s the ingredient is cooled down to the outer temperature, which equals 17 °C.

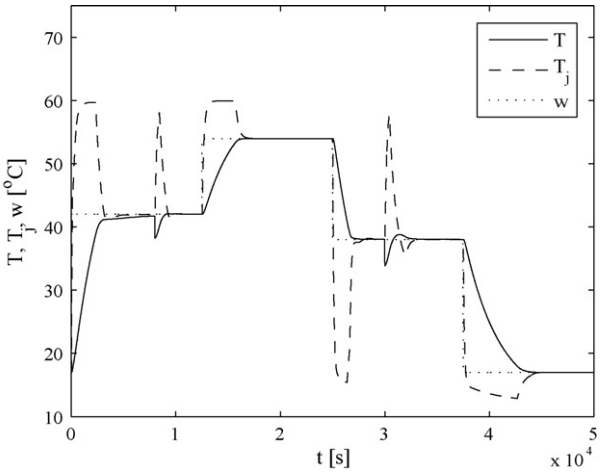

Fig. 3. The control of the semi-batch reactor ($T(k)$, $T_j(k)$, $w(k)$).

In Fig. 3 the output signal, $T(k)$, the jacket temperature, $T_j(k)$, and the reference signal, $w(k)$, are shown. The position of the mixing valve and the positions of the on/off valves are shown in Fig. 4. The algorithm succeeds in controling the temperature $T(k)$ in the tolerance intervals that are required, also when the additional ingredients are fed in the reactor. In the stationary state the discrete valve for hot water is open ($v_{CH} = 1$) together with the mixing valve v_M slightly open, because of the energy loss in the surroundings. The switching of the discrete valves is minimal, as required. In Figs. 5 and 6 the time courses of the identified process parameters θ_{11}, θ_{12}, θ_{13}, θ_{21} and θ_{22} are shown. The process parameters, θ_{ij}, are adapted when the reference is changed or in the case of a disturbance (the addition of ingredients influences the change in the process parameter θ_{22}, as seen in Fig. 6). In these situations the excitation of the system is large enough to fulfill Eq. (27) and trigger the recursive identification.

The simulation study was done to elaborate the possible use of the proposed self-adaptive supervisory control algorithm in the real application. Using the simulation study the implemen-

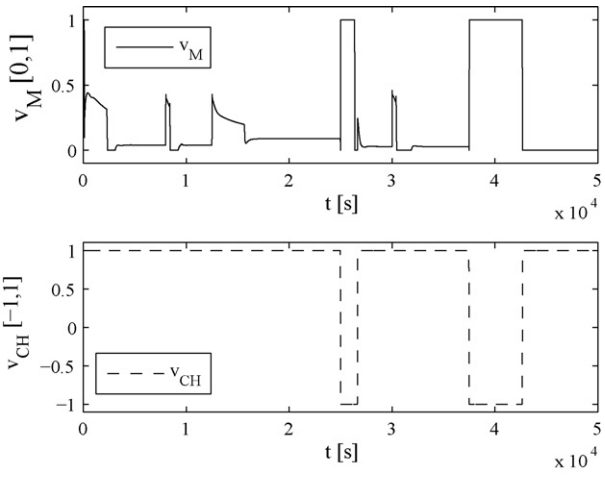

Fig. 4. The control of the semi-batch reactor (position of the mixing valve v_M and the position of the on/off valves v_{CH}).

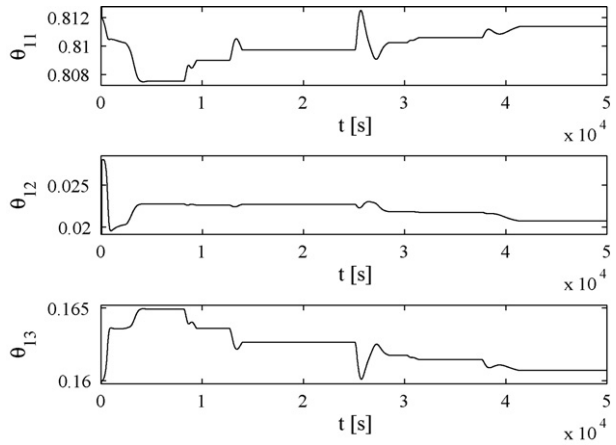

Fig. 5. The identified process parameters θ_{11}, θ_{12} and θ_{13}.

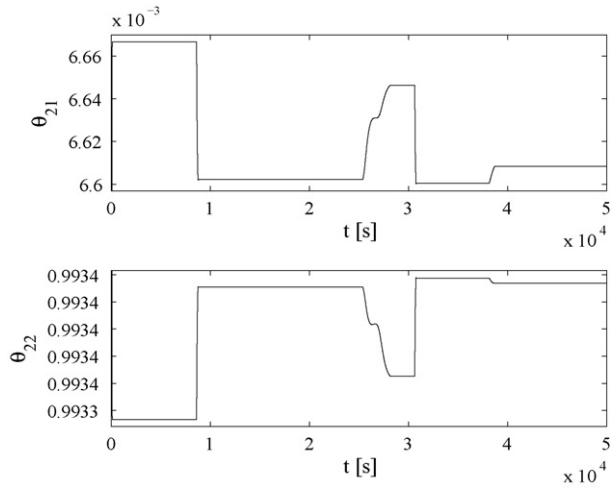

Fig. 6. The identified process parameters θ_{21} and θ_{22}.

tation of a self-adaptive predictive functional control algorithm was justified. It has been shown that the obtained results meet the desired criteria: fast and suitable reference-trajectory tracking, which results in a shorter time for the whole batch; a small overshoot of the controlled variable which results in higher-quality production; and a small number of switchings between cold and hot water in the inlet, which is important for the longevity of the actuators.

7. Conclusion

In this paper a self-adaptive supervisory predictive functional control algorithm was tested to control the temperature in a reactor's core. The semi-batch reactor is used in the pharmaceutical industry for the production of medicines. The semi-batch reactor is an example of a hybrid process where some discrete on/off valves and a continuous mixing valve are used. The continuous control with supervision is used to control the hybrid type of process. A simulation study was carried out to elaborate the possible use of the proposed self-adaptive supervisory control algorithm in the real application. Using the simulation study the implementation of a self-adaptive predictive functional control algorithm was justified. It has been shown that the obtained results meet the desired criteria: rapid and suitable reference-trajectory tracking, which results in a shorter time for the whole batch; a small overshoot of the controlled variable, which results in higher-quality production; and a small number of switchings between cold and hot water in the inlet, which is important for the longevity of the actuators.

Acknowledgement

The work was done in the frame of the industrial project between University of Ljubljana, Faculty of Electrical Engineering, Ljubljana and pharmaceutical company Lek d.d., Sandoz, a Division of the Novartis AG group.

References

[1] B.W. Bequette, Nonlinear control of chemical processes: a review, Ind. Eng. Chem. Res 30 (1991) 1391–1413.
[2] J.-S. Chang, W.Y. Hseih, Optimization and control of semibatch reactors, Ind. Eng. Chem. Res. 33 (1995) 545–556.
[3] L. Chen, G. Bastin, V. Van Breusegam, A case study of adaptive nonlinear regulation of fed-batch reactors, Automatica 31 (1995) 55–65.
[4] C. Mohtadi, D.W. Clarke, Generalized predictive control, LQ, or pole-placement: a unified approach, in: Proceedings of 25th Conference on Decision and Control, 1986, pp. 1536–1541.
[5] D.W. Clarke, C. Mohtadi, P.S. Tuffs, Generalized predictive control—Parts 1 and 2, Automatica 24 (1987) 137–160.
[6] D.W. Clarke, C. Mohtadi, Properties of generalized predictive control, Automatica 25 (6) (1989) 859–875.
[7] C.R. Cutler, B.L. Ramaker, Dynamic Matrix Control—A Computer Control Algorithm, ACC, San Francisco, 1980.
[8] J.E. Cuthrell, L.T. Biegler, Simultaneous optimization and solution methodes for batch reactor control, Comput. Chem. Eng. 13 (1989) 49–62.
[9] D. Clarke, Advances in Model-Based Predictive Control, Science Publication, 1994.
[10] R.M.C. De Keyser, P.G.A. Van de Valde, F.A.G. Dumortier, A comparative study of self-adaptive long-range predictive control methods, Automatica 24 (2) (1988) 149–163.
[11] R.A.J. De Vries, H.B. Verbruggen, Multivariable unified predictive control, in: Advances in Model-Based Predictive Control, Oxford University Press, 1994.
[12] B.A. Foss, T.A. Johansen, A.V. Sorensen, Nonlinear predictive control using local models-applied to a batch fermentation process, Control Eng. Pract. 3 (1995) 389–396.
[13] M.A. Henson, D.E. Seborg, Input–output linerization of general processes, AIChE J. 36 (1990) 1753.
[14] M.A. Henson, Nonlinear model predictive control: current status and future directions, Comput. Chem. Eng. 23 (1998) 187–202.
[15] M.R. Juba, J.W. Hamer, Progress and challanges in batch process control, Chem. Process Control—CPC II (1986) 139–183.
[16] N. Lakshmanan, Y. Arkun, Estimation and control of batch processes using multiple models, Int. J. Control 72 (7/8) (1999) 659–675.
[17] C. Loeblin, J.D. Perkins, B. Srinivasan, D. Bonvin, Economic performance analysis in the design of on line batch optimization system, J. Process Control 9 (1999) 61–78.
[18] Z. Louleh, M. Cabassud, M.V. Le Lann, A new strategy for temperature control of batch reactors: experimental application, Chem. Eng. J. 75 (1999) 11–20.
[19] R. Luus, O.N. Okongwu, Towards practical optimal control of batch reactors, Chem. Eng. J. 75 (1999) 1–9.

[20] J.D. Morningred, B.E. Paden, D.A. Mellichamp, An adaptive nonlinear predictive controller, Chem. Eng. Sci. 47 (1992) 755–762.
[21] J. Richalet, Industrial application of model based predictive control, Automatica 29 (5) (1993) 1251–1274.
[22] I. Škrjanc, D. Matko, Predictive functional control based on fuzzy model for heat-exchanger pilot plant, IEEE Trans. Fuzzy Syst. 8 (6) (2000) 705–712.
[23] I. Škrjanc, D. Matko, Fuzzy predictive functional control in the state space domain, J. Intell. Robot. Syst. 31 (2001) 283–297.