Adaptive Supervisory Predictive Control of a Hybrid Fed-Batch Reactor with Slow Actuator

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

In this paper, adaptive supervisory predictive functional control is discussed for applications in a fed-batch reactor with slow continuous mixing valve, which acts as an actuator. The optimal operation regime of the reactor is to follow the reference trajectory without significant overshoot and to minimize the overall batch time. By adding the ingredients during the batch procedure, the volume in the reactor varies, tending to increase with time, as does the heat-transfer surface inside the reactor. This change causes variations in the batch-reactor dynamics, which can produce serious problems with the reactor's core-temperature control. Another problem that arises is the disturbance in the temperature inside the reactor, when additional ingredients added are at the outside temperature. In the pharmaceutical industry, a huge number of fed-batch reactors similar to ours are used for the production of drugs. The quality control is extremely strict, and it is necessary to follow the exact production recipe. The adaptive algorithm based on recursive identification is used to deal with varying dynamics of the systems; the predictive functional control algorithm is used because of its simple implementation, which can be realized also in programmable logic controllers; and the supervisory control level is designed to cope with the physical constraints and the discrete on/off valves that are used as actuators. The possible use of the proposed adaptive control algorithm in a real application was studied by taking into account a very slow actuator.

1. Introduction

The fed-batch reactors are the most important part in process technology in chemistry, pharmacy, and biotechnology. Essentially, the control of fed-batch reactors is mostly reduced to the problem of temperature control, which is difficult to overcome. The problem becomes more difficult because of the mixed, continuous, and discrete nature of the process behavior and the equipment. The other difficulties arise because of the various uses of fed-batch reactors; the nonlinearities of the reactors, which have a huge influence on the behavior because of the drastic changes in set point during the operation; and the different modes of operation, which require an adaptive functioning and physically constrained actuators. Special difficulties arise because of the constraints of the mixing valve and those that are the results of the chemical properties of the process and the mechanical structure of the batch reactor. Feeding the reactor means that the ingredients are gradually added in to the vessel during the procedure. The additional ingredient increases the volume inside the reactor, as does the heat-transfer surface between the reactor's jacket and the reactor's core. From the dynamic point of view, the reactor represents a time-varying process. The operation of the fed-batch reactor is defined by the technological recipe. The recipe in our case defines the temperature during the whole procedure and the addition of the ingredients. The reference temperature should be followed as precisely as possible and without overshoot in spite of added ingredients with different temperatures and taking into account the constraint 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. The overall goal of the batch-reactor optimization is to increase the production by minimizing the overall batch time and taking into account all important control requirements. The process control requirements are relatively demanding: fast reference-trajectory tracking, small overshoot of the controlled variable, and a small number of switchings of the on/off valves for cold and hot water at the inlet.

In the literature, a number of papers have been published that discuss the control of batch reactors. Initially, various types of controllers were studied, together with the optimum batch trajectories. The state-of-the-art of the classical control schemes is given in ref 11. Industrial batch reactors are equipped with jackets/coils, such that the actual manipulated variable is the flow rate of the cooling/heating fluid. Under this situation, the temperature controller can be implemented in a cascade configuration where the proposed controller becomes the master controller that provides the jacket temperature reference to a slave controller.[24] In this way, the slave controller manipulates the flow rate of the cooling/heating fluid to achieve the performance asked by the (proposed in this paper) master controller. During that time, many different concepts of fed-batch reactor control were developed. The nonlinear time-scaling techniques for robust controller design of isothermal chemical and biochemical reactors are given in ref 18. The most promising of these were the concepts of adaptive control,[5,15] optimal control,[4,8,16] recurrent neural network models,[25] methodologies based on Lyapunov theory,[2] on-line dynamic optimization,[1] and especially model-predictive control schemes, which are the most frequently used.[9,12,14] Model predictive control was very successful in solving many industrial control problems.[3,6,7] The recent survey of batch reactor control strategies is given in ref 20. One of the most frequently used predictive schemes in practice is the predictive functional control scheme,[19] which has been applied to a fed-batch reactor in our simulation study.

A very important feature of the 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,

* To whom correspondence should be addressed. Fax: +386 1 4264 631. Tel.: +386 1 4768 311. E-mail: igor.skrjanc@fc.uni-lj.si.

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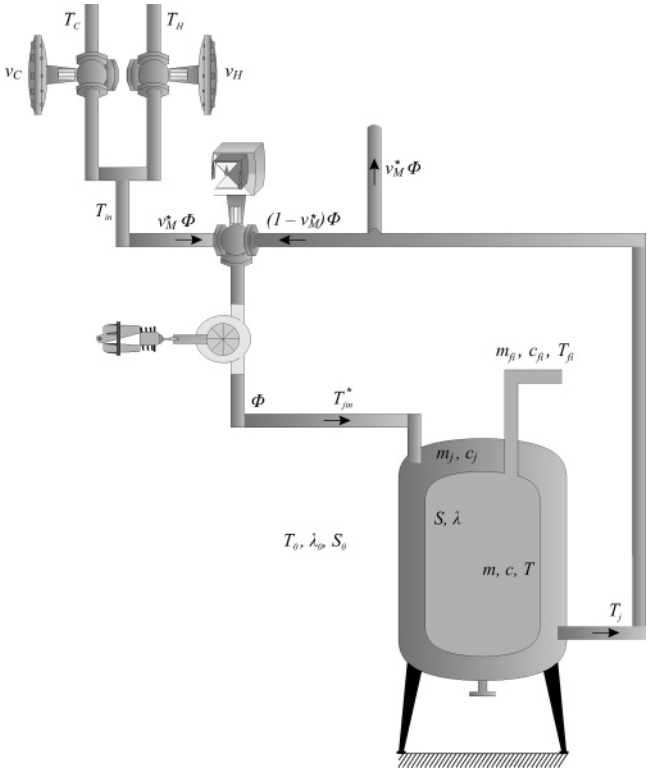

Figure 1. Scheme of fed-batch reactor process.

such as programmable logic controllers. The self-tuning and adaptive algorithms are a conceptually appealing scheme for the control of complex industrial processes where manual tuning of the controller parameters appears 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 predictive functional controller can be efficiently used, particularly in the case of constrained control problems, such as the constraints of internal variables and the physical constraints of the actuators. In this paper, special attention will be given to the problem of slow actuators.

The paper is organized in the following way: in Section 2, the fed-batch reactor is described, the process model that is used to design the control is presented, and the recursive least-squares algorithm is discussed; in Section 3, the predictive functional control law for a fed-batch reactor is presented; the supervisory level control is described in Section 4; and in Section 5, the simulation results are presented.

2. Fed-Batch Reactor

In our case, we are dealing with a pharmaceutical fed-batch reactor, used in the production of medicines. It is an example of a hybrid plant, because we have some discrete valves, a continuous mixing valve, and a continuous process. 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 fed-batch reactor is shown in Figure 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 55 °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 $T_{j\max} = 55$ °C.

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 ($T_{in} = T_C = 12$ °C), whereas if $v_C = 0$ and $v_H = 1$, the input water is hot ($T_{in} = T_H = 65$ °C). Both on/off valves are controlled by the signal v_{CH}, which is defined as

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

and the temperature of the input water is then defined as follows:

$$T_{in} = \begin{cases} T_H, & \text{if } v_{CH} = 1 \\ T_C, & \text{if } v_{CH} = -1 \end{cases} \quad (2)$$

The ratio of fresh input water to reflux water is controlled by a third input, i.e., by the position of the continuous mixing valve v_M, which is limited to the range $[v_{Mmin}, v_{Mmax}]$. The valve rate is constrained in the range $[\dot{v}_{Mmin}, \dot{v}_{Mmax}]$. This means that the opening time (from 0 to 1) of the valve equals $1/\dot{v}_{Mmax}$ and the closing time equals $1/\dot{v}_{Mmin}$. In our case, the opening and closing times are equal to 500 s. The slow dynamics of the valve, which cannot be neglected, incorporate additional delay into the process dynamics. The input to the valve is denoted as v_M, and the real-current position of the valve is denoted as v_M^*. The actual position of the mixing valve is presented with the following equation

$$v_M^*(t) = \int \dot{v}_M(t)\, dt \quad (3)$$

$$\dot{v}_M(t) = \begin{cases} \dot{v}_{Mmax}, & \text{if } \dot{v}_M(t) \geq \dot{v}_{Mmax} \\ \dot{v}_M(t), & \text{if } \dot{v}_{Mmin} < \dot{v}_M(t) < \dot{v}_{Mmax} \\ \dot{v}_{Mmin}, & \text{if } \dot{v}_M(t) \leq \dot{v}_{Mmin} \end{cases} \quad (4)$$

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 is denoted as T_{jin}^* and cannot be measured directly. It is constrained in the range between T_C and T_H ($T_C \leq T_{jin} \leq T_H$). The time constants (the opening and closing times of the valves) 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.

The mathematical model of the fed-batch reactor is defined by the differential equations 5, 6, and 8−10 and the algebraic equations 7 and 11.

$$m_j c_j \frac{dT_j}{dt} = v_M^* \Phi c_j T_{in} + (1 - v_M^*)\Phi c_j T_j - \Phi c_j T_j - \lambda S(T_j - T) - \lambda_0 S_0 (T_j - T_0) \quad (5)$$

$$mc\frac{dT}{dt} = \lambda S[T_j - (T + \Delta T\delta(t - t_i))] \quad (6)$$

$$\Delta T = \frac{m_{fi}c_{fi}(T_{fi} - T)}{mc + m_{fi}c_{fi}} \quad (7)$$

where $m_j = 200$ 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} and $S_0 = 4$ m^2 are the thermal conductivity between the jacket and the surroundings and the conduction surface, respectively. The temperature of the surroundings is equal to $T_0 = 17$ °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. The mixing of ingredients is modeled as an ideal one, given in eq 7. This is justified by the fact that the time constants of feeding and mixing together are negligible comparing to the time constants of the reactor. Assumption of ideal mixing implies the modeling of the feeding process 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 6. The state jump, ΔT, is defined in eq 7, where m_{fi} stands for the mass of ingredient added to the reactor at the time instant t_i, c_{fi} defines the heat capacity of the ingredient that is added, and T_{fi} 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 8. Equation 9 denotes the change of the average heat capacity of the mixture inside the reactor, where $\Delta c_i = (c_{fi} - c)m_{fi}/(m + m_{fi})$.

$$\frac{dm}{dt} = m_{fi}\delta(t - t_i), \quad m(0) \quad (8)$$

$$\frac{dc}{dt} = \Delta c_i\delta(t - t_i), \quad c(0) \quad (9)$$

The time-varying profile of the conduction surface, S, is given in eq 10 as follows,

$$\frac{dS}{dt} = S_{fi}\delta(t - t_i), \quad S(0) \quad (10)$$

where S_{fi} stands for the change of the conduction surface at time t_i, because of the added ingredient. In our case, it is roughly modeled as $S_{fi} = S(m_{fi}/m)$.

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 current position of the mixing valve, v^*_M (which cannot be measured), and on the temperature of the fresh water, T_{in}, and the jacket temperature, T_j, as follows

$$T^*_{jin} = v^*_M T_{in} + (1 - v^*_M)T_j \quad (11)$$

The input jacket temperature T^*_{jin} cannot be measured directly (no temperature sensor at that position), although it can be estimated using eq 11, where the desired position of the mixing valve, v_M, is used instead of the current mixing valve position, v^*_M. The estimated input jacket temperature is denoted as T_{jin} (without the asterisk) and is given in eq 12.

$$T_{jin} = v_M T_{in} + (1 - v_M)T_j \quad (12)$$

The control will be developed based on the indirect control variable T_{jin}, 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 positions of the discrete valves, v_C and v_H.

2.1. Process Model Used for Control Design. Next, the development of the discrete-time model, which is used for control design purposes, is presented. To obtain the model in the discrete-time incremental form, the filtration and discrete differentiation of the measured signals has to be performed. The last right term in the differential equation from eq 5, namely, exhibits the loss energy flow into the surroundings and represents an offset in this equation (affine equation). The filtration and differentiation of the measured variables is realized by the filter transfer function defined as

$$G_f(z) = \frac{\Delta(z)}{F(z)} \quad (13)$$

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 fed-batch reactor, which is presented in eqs 5 and 6 in continuous form, is now transformed into the discrete-time domain as follows,

$$T^f_j(k) = \boldsymbol{\theta}_{11}T^f_j(k-1) + \boldsymbol{\theta}_{12}T^f(k-1) + \boldsymbol{\theta}_{13}T^f_{jin}(k-1) \quad (14)$$

$$T^f(k) = \boldsymbol{\theta}_{21}T^f_j(k-1) + \boldsymbol{\theta}_{22}T^f(k-1) \quad (15)$$

where superscript f stands for the filtered signals.

The Z-transform of the jacket temperature is obtained from eq 15, and it is written as

$$T^f_j(z) = \frac{1}{\boldsymbol{\theta}_{21}}(z - \boldsymbol{\theta}_{22})T^f(z) \quad (16)$$

Incorporating eq 16 into eq 14 written in Z-domain results in the transfer function $G_m(z)$ between the core temperature, T, and the input jacket temperature, T_{jin}, as follows

$$G_m(z) = \frac{T^f(z)}{T^f_{jin}(z)} = \frac{\boldsymbol{\theta}_{21}\boldsymbol{\theta}_{13}}{z^2 - (\boldsymbol{\theta}_{11} + \boldsymbol{\theta}_{22})z + \boldsymbol{\theta}_{11}\boldsymbol{\theta}_{22} - \boldsymbol{\theta}_{12}\boldsymbol{\theta}_{21}} \quad (17)$$

The dynamics of the heat transfer between the input jacket temperature T^f_{jin} and the jacket temperature T^f_j is given by the transfer functions $G_{mj}(z)$ as follows

$$G_{mj}(z) = \frac{T^f_j(z)}{T^f_{jin}(z)} = \frac{\boldsymbol{\theta}_{13}z - \boldsymbol{\theta}_{22}}{z^2 - (\boldsymbol{\theta}_{11} + \boldsymbol{\theta}_{22})z + \boldsymbol{\theta}_{11}\boldsymbol{\theta}_{22} - \boldsymbol{\theta}_{12}\boldsymbol{\theta}_{21}} \quad (18)$$

In both transfer functions, the input jacket temperature, T^f_{jin}, acts as the input and will be used as the indirect control variable, because it cannot be defined directly, and the transfer functions $G_m(z)$ and $G_{mj}(z)$ will be used to design the control law. Before that, the parameters of the transfer function have to be estimated. The scheme of the process model that is used as an internal model in the predictive functional design is given in Figure 2, where $x_{mj}(k)$ and $x_m(k)$ stand for the model states, $T^m_{jin}(k)$ stands for the internal model input jacket temperature, $T^m_j(k)$ is the internal model jacket temperature, and $T^m(k)$ denotes the internal model reactor core temperature. The dynamics of the continuous

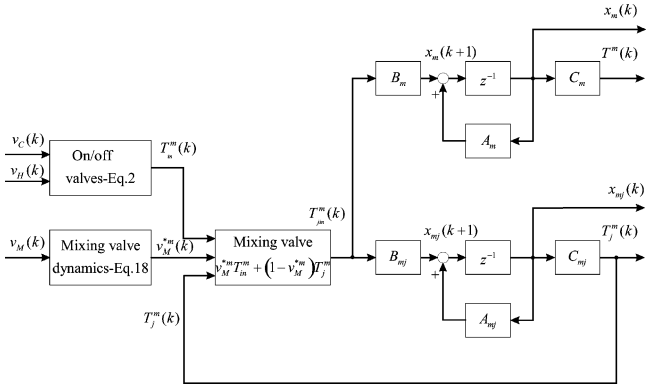

Figure 2. Internal process model in discrete-time space.

mixing valve is given as follows

$$\upsilon_{\mathrm{M}}^{*\mathrm{m}}(k) = \upsilon_{\mathrm{M}}^{*\mathrm{m}}(k-1) + \Delta\upsilon_{\mathrm{M}}^{\mathrm{m}}(k)$$

$$\Delta\upsilon_{\mathrm{M}}^{\mathrm{m}}(k) = \begin{cases} \dot{\upsilon}_{\mathrm{Mmax}}T_{\mathrm{s}}, & \text{if } \upsilon_{\mathrm{M}}^{\mathrm{m}}(k) - \upsilon_{\mathrm{M}}^{*\mathrm{m}}(k-1) \geq \dot{\upsilon}_{\mathrm{Mmax}}T_{\mathrm{s}} \\ \upsilon_{\mathrm{M}}^{\mathrm{m}}(k) - \upsilon_{\mathrm{M}}^{*\mathrm{m}}(k-1), & \text{if } \dot{\upsilon}_{\mathrm{Mmin}}T_{\mathrm{s}} < \upsilon_{\mathrm{M}}^{\mathrm{m}}(k) - \upsilon_{\mathrm{M}}^{*\mathrm{m}}(k-1) < \dot{\upsilon}_{\mathrm{Mmax}}T_{\mathrm{s}} \\ \dot{\upsilon}_{\mathrm{Mmin}}T_{\mathrm{s}}, & \text{if } \upsilon_{\mathrm{M}}^{\mathrm{m}}(k) - \upsilon_{\mathrm{M}}^{*\mathrm{m}}(k-1) \leq \dot{\upsilon}_{\mathrm{Mmin}}T_{\mathrm{s}} \end{cases} \tag{19}$$

The estimation of the model parameters is realized by the use of the recursive least-squares identification, which is given next.

2.2. Recursive Least-Squares Identification. The predictive control design is based on the process model given by the transfer functions $G_{\mathrm{m}}(z)$ and $G_{\mathrm{mj}}(z)$. The parameters of the transfer functions are time varying and are not known in advance. The fed-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. To estimate the model parameters, the standard recursive estimator with exponential forgetting is used.

When using the recursive identification in the adaptive control system, we are faced with the problem of identifiability of the process parameters when the process is running in the closed loop. This means that, in the case of the closed loop, the output of the process influences the input to the process. In that case, the process parameters can be identified only when the following criteria is fulfilled,

$$\max\{m_{\mathrm{a}} + \mu, m_{\mathrm{b}} + \nu\} \geq m_{\mathrm{a}} + m_{\mathrm{b}} \tag{20}$$

where m_{a} and m_{b} stand for the orders of the process transfer function numerator and denominator, respectively, and μ and ν are the orders of the controller transfer function numerator and denominator, respectively.[21] In the case of predictive functional control, the control law is based on the internal model of the process. This means that, in the case of structurally proper modeling, the problem of identifiability is solved.

Defining the regression vector $\boldsymbol{\psi}_{\mathrm{f1}}^{\mathrm{T}}(k) \in \mathrm{R}^{1\times 3}$, $\boldsymbol{\psi}_{\mathrm{f2}}^{\mathrm{T}}(k) \in \mathrm{R}^{1\times 2}$, the output variables y_{f1} and y_{f2}, and the vectors of the identified parameters $\boldsymbol{\theta}_1^{\mathrm{T}}$ and $\boldsymbol{\theta}_2^{\mathrm{T}}$ as follows,

$$\boldsymbol{\psi}_{\mathrm{f1}}^{\mathrm{T}}(k) = [T_{\mathrm{j}}^{\mathrm{f}}(k-1)T^{\mathrm{f}}(k-1)T_{\mathrm{jin}}^{\mathrm{f}}(k-1)] \tag{21}$$

$$\boldsymbol{\psi}_{\mathrm{f2}}^{\mathrm{T}}(k) = [T_{\mathrm{j}}^{\mathrm{f}}(k-1)T^{\mathrm{f}}(k-1)] \tag{22}$$

$$y_{\mathrm{f1}}(k) = T_{\mathrm{j}}^{\mathrm{f}}(k) \tag{23}$$

$$y_{\mathrm{f2}}(k) = T^{\mathrm{f}}(k) \tag{24}$$

$$\boldsymbol{\theta}_1^{\mathrm{T}} = [\boldsymbol{\theta}_{11}(k) \;\; \boldsymbol{\theta}_{12}(k) \;\; \boldsymbol{\theta}_{13}(k)] \tag{25}$$

$$\boldsymbol{\theta}_2^{\mathrm{T}} = [\boldsymbol{\theta}_{21}(k) \;\; \boldsymbol{\theta}_{22}(k)] \tag{26}$$

The following incremental models of the fed-batch reactor are obtained:

$$y_{\mathrm{f1}}(k) = \boldsymbol{\psi}_{\mathrm{f1}}^{\mathrm{T}}(k)\boldsymbol{\theta}_1(k) \tag{27}$$

$$y_{\mathrm{f2}}(k) = \boldsymbol{\psi}_{\mathrm{f2}}^{\mathrm{T}}(k)\boldsymbol{\theta}_2(k) \tag{28}$$

It should be emphasized that the regression vector $\boldsymbol{\psi}_{f1}^{T}(k)$ is fed with the estimated variable T_{jin}, which incorporates the dynamics of the actuator. The actuator dynamics is, therefore, implicitly incorporated into the process model.

The parameters $\boldsymbol{\theta}_i$, $i = 1, 2$, are estimated using the recursive least-squares identification algorithm as follows,

$$\sigma_i(k) = \mathbf{P}_i(k-1)\boldsymbol{\psi}_{fi}(k)(\gamma_i + \boldsymbol{\psi}_{fi}^{T}(k)\mathbf{P}_i(k-1)\boldsymbol{\psi}_{fi}(k))^{-1} \quad (29)$$

$$\mathbf{P}_i(k) = (\mathbf{I}_i - \sigma_i(k)\boldsymbol{\psi}_{fi}^{T}(k))\mathbf{P}_i(k-1)/\gamma_i \quad (30)$$

$$\boldsymbol{\theta}_i(k) = \boldsymbol{\theta}_i(k-1) + \sigma_i(k)(y_{fi}(k) - \boldsymbol{\psi}_{fi}^{T}(k)\boldsymbol{\theta}_i(k-1)), \quad i = 1, 2 \quad (31)$$

where $\mathbf{P}_i(k)$, $i = 1, 2$, denotes the covariance matrix ($\mathbf{P}_1(k) \in R^{3\times3}$, $\mathbf{P}_2(k) \in R^{2\times2}$), $\boldsymbol{\theta}_i(k)$, $i = 1, 2$, denotes the vector of the identified or estimated process parameter, γ_i, $i = 1, 2$, denotes the forgetting factor, and $\mathbf{I}_1(k) \in R^{3\times3}$ and $\mathbf{I}_2(k) \in R^{2\times2}$ are unity matrices. This means that two recursive identification algorithms are running in parallel, to estimate the process parameters $\boldsymbol{\theta}_1(k)$ and $\boldsymbol{\theta}_2(k)$.

Using the recursive least-squares algorithm, we are faced with the problem of the covariance matrix $\mathbf{P}_i(k)$, $i = 1, 2$, when there is not enough excitation. In that case, the covariance matrix is exponentially increasing if the forgetting factor $\gamma_1 < 1$, $i = 1, 2$. This problem, which is called *bursting*, is solved by calculating the recursive algorithm only in the case of a satisfied excitation criterion,

$$\boldsymbol{\psi}_{fi}^{T}(k)\mathbf{P}_i(k-1)\boldsymbol{\psi}_{fi}(k) > k_{DZ}(1-\gamma_i),\ i = 1, 2 \quad (32)$$

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

3. Predictive Functional Control Algorithm

In this section, the well-known basic algorithm of predictive functional control is introduced.[19,23] The algorithm is used mainly because of its efficiency and simple design. The simplicity is most important, because of its implementation into the programmable logic controller. The algorithm is developed in state-space where the process is described with the following state-space model representation

$$x(k+1) = Ax(k) + Bu(k), \quad y_m(k) = Cx(k) \quad (33)$$

where $x_m(k)$ stands for the model states.

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 constant future manipulated variables ($u(k) = u(k+1) = ... = u(k+H-1)$). This strategy is known as mean-level control. The H-step-ahead prediction of the plant output is estimated in eq 34,

$$y_m(k+H) = C(A^{H}x(k) + (A^{H} - \mathbf{I})(A - \mathbf{I})^{-1}Bu(k)) \quad (34)$$

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

The reference model is given by the following difference equation

$$x_r(k+1) = a_r x_r(k) + b_r w(k)$$
$$y_r(k) = c_r x_r(k) \quad (35)$$

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

$$c_r(1-a_r)^{-1}b_r = 1 \quad (36)$$

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

$$y_r(k+H) = a_r^{H}y_r(k) + (1 - a_r^{H})w(k) \quad (37)$$

where a constant and bounded reference signal ($w(k+i) = w(k)$, $i = 1, ..., H$) 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, eq 37 is first rewritten as

$$w(k+H) - y_r(k+H) = a_r^{H}(w(k) - y_r(k)) \quad (38)$$

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

$$y_p(k+H) = w(k+H) - a_r^{H}(w(k) - y_p(k)) \quad (39)$$

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.,

$$\Delta_p = \Delta_m \quad (40)$$

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 $y_p(k)$

$$\Delta_p = y_r(k+H) - y_p(k) \quad (41)$$

Taking into account the idea of perfect tracking of the reference trajectory ($y_p(k+i) = y_r(k+i)$, $i = 0, 1, ..., H$) and substituting eq 39 into eq 41 yields

$$\Delta_p = y_p(k+H) - y_p(k) = w(k+H) - a_r^{H}(w(k) - y_p(k)) - y_p(k) \quad (42)$$

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

$$\Delta_m = y_m(k+H) - y_m(k) \quad (43)$$

Substituting eqs 42 and 43 into eq 40 and using eqs 39 and 34, the following control law can be obtained,

$$u(k) = \eta^{-1}[(1 - a_r^{H})(w(k) - y_p(k)) + y_m(k) - CA^{H}x(k)] \quad (44)$$

where

$$\eta = C(A^{H} - \mathbf{I})(A - \mathbf{I})^{-1}B \quad (45)$$

Note that the control law (eq 44) 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.[22] 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 ref 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 equal to the relative order of the controlled system, ρ ($H \geq \rho$), as proposed.

3.1. Predictive Functional Control Law for Fed-Batch Reactor. The algorithm of predictive functional control is basically internal model control design with the process models given in the state-space domain. The state-space representation of the process model is obtained from the transfer functions, $G_m(z)$ and $G_{mj}(z)$. Assuming the observability of the process plant, both transfer functions, $G_m(z)$ and $G_{mj}(z)$, are transformed to the observable canonical form.

The obtained state-space model in the case of $G_m(z)$ is given as follows

$$A_m = \begin{bmatrix} 0 & a_0 \\ 1 & a_1 \end{bmatrix}, \quad B_m = \begin{bmatrix} b_0 \\ 0 \end{bmatrix}, \quad C_m = [0 \;\; 1] \tag{46}$$

and in the case of $G_{mj}(z)$, it is the following,

$$A_{mj} = \begin{bmatrix} 0 & a_0 \\ 1 & a_1 \end{bmatrix}, \quad B_{mj} = \begin{bmatrix} -b_0 \\ b_1 \end{bmatrix}, \quad C_{mj} = [0 \;\; 1] \tag{47}$$

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

The state-space equivalents of the transfer functions $G_{mj}(z)$ and $G_m(z)$ are now given as follows:

$$x_{mj}(k+1) = A_{mj}x_{mj}(k) + B_{mj}T^m_{jin}, \quad T^m_j(k) = C_{mj}x_{mj}(k) \tag{48}$$

$$x_m(k+1) = A_m x_m(k) + B_m T^m_{jin}, \quad T^m(k) = C_m x_m(k) \tag{49}$$

4. Supervisory Predictive Functional Control for a Fed-Batch Reactor

The control algorithm in the case of a fed-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, $T_j(k)$, which should not exceed T_{jmax}, 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 maximal values and the minimal and maximal rates of the valve. The time constant of the mixing valve is taken into account by the proposed identification of the process dynamics.

The control is obtained by calculating the predictive functional law for the input jacket temperature, T^r_{jin}, which acts as the indirect control variable. The actual control variables υ_C, υ_H, and υ_M are after that, taking into account the desired indirect control variable T^r_{jin} and the constraint jacket temperature, $T_j(k)$, calculated at the supervisory level. 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 indirect predictive control law, $T^u_{jin}(k)$, is calculated as given next,

$$T^u_{jin}(k) = \eta_m^{-1}[(1 - a^H_r)(T^r(k) - T(k)) + T^m(k) - C_m A^H_m x_m(k)] \tag{50}$$

$$\eta_m = C_m(A^H_m - \mathbf{I})(A_m - I)^{-1}B_m \tag{51}$$

where $T(k)$ stands for the current core temperature and $x_m(k)$ and $T^m(k)$ are, respectively, the states and the output of the process model, which defines the reactor core dynamics.

In the second step, the constrained predictive control law $T^c_{jin}(k)$ is calculated as follows,

$$T^c_{jin}(k) = \eta_{mj}^{-1}[(1 - a^H_r)(T_{jmax} - T_j(k)) + T^m_j(k) - C_{mj}A^H_{mj}x_{mj}(k)]$$
$$\eta_{mj} = C_{mj}(A^H_{mj} - \mathbf{I})(A_{mj} - \mathbf{I})^{-1}B_{mj} \tag{52}$$

where $T_j(k)$ stands for the current jacket temperature and $x_{mj}(k)$ and $T^m_j(k)$ are, respectively, the states and the output of the process model, which defines the reactor jacket dynamics.

In the third step, the prediction of the jacket temperature is calculated using the unconstrained control law $T^u_{jin}(k)$,

$$T^m_j(k+h) = C_{mj}[A^h_{mj}x_{mj}(k) + (A^h_{mj} - \mathbf{I})(A_{mj} - \mathbf{I})^{-1}B_{mj}T^u_{jin}(k)] \tag{53}$$

where $h \geq \rho_{in}$ denotes the prediction horizon of the internal model and ρ_{in} stands for the 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 $T^u_{jin}(k)$ and the constrained control $T^c_{jin}(k)$ in the following way,

$$\text{if } T^m_j(k+h) - T^m_j(k) \leq T_{jmax} - T_j(k) \text{ then } T^r_{jin}(k) = T^u_{jin}(k)$$
$$\text{if } T^m_j(k+h) - T^m_j(k) > T_{jmax} - T_j(k) \text{ then } T^r_{jin}(k) = T^c_{jin}(k) \tag{54}$$

where the jacket input temperature, $T^r_{jin}(k)$, acts as the required 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, $T^r_{jin}(k)$, given in eq 54. The position of the on/off valves ($\upsilon_{CH}(k)$) is defined on the supervisory level by introducing the decision logic, which is as follows,

$$\text{if } T^r(k) - T(k) < \delta_e \text{ then } \upsilon_{CH}(k) = -1 \text{ else } \upsilon_{CH}(k) = 1 \tag{55}$$

where $T^r(k)$ stands for the reference reactor core temperature and δ_e defines the switching threshold ($\delta_e = -1$ °C). The switched system, in general, does not inherit the properties of the individual subsystems; a well-known example is that switching among globally exponentially stable subsystems could lead to instability.[13] The switched linear system is exponentially stable if the individual subsystems are exponentially stable and for the *dwell-time* switching signals.[17] The stability of switching systems can be proven by using LaSalle's invariance principle, and by using this principle, one can deduce the asymptotic stability using multiple Lyapunov functions as proposed in ref 10.

By taking into account eq 2, where $T_{in}(k)$ is defined by the position of the on/off valves, and eq 11, the actual control variable, $\upsilon_M(k)$, is calculated as follows:

$$v_M(k) = \frac{T_{jin}^r(k) - T_j(k)}{T_{in}(k) - T_j(k)} \tag{56}$$

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 [−0.002, 0.002]).

5. Simulation Results

The adaptive supervisory predictive functional control algorithm was tested on a fed-batch reactor by means of a simulation. The study was meant to show the potential of the proposed approach for further real applications using fed-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, and the 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 $T_s = 20$ s, and the initial covariance matrices are equal to $\mathbf{P}_1(0) = 100\mathbf{I}_3$ and $\mathbf{P}_2(0) = 100\mathbf{I}_2$. The vectors of the estimated process parameters were initialized as $\boldsymbol{\theta}_{11} = \boldsymbol{\theta}_{22} = 1$, and the other parameters were equal to zero. The forgetting factors of the identification algorithms were set to $\gamma_1 = \gamma_2 = 0.999$, and the factor of the dead zone was set to $k_{DZ} = 0.1$. The initialization of the generalized predictive control algorithm was the following: $H = 10$, $h = 200$, and $a_r = 0.925$.

In the simulated experiment, the initial mass in the reactor's core equals $m(0) = 400$ kg, the conduction surface $S(0) = 2$ m^2, the heat capacity $c(0) = 4200$ J kg^{-1} K^{-1}, and the mass in the jacket equals $m_j = 200$ kg. The reactor is fed with an additional ingredient ($m_{f1} = 200$ kg, $c_{f1} = 4200$ J kg^{-1} K^{-1}, $T_{f1} = 17$ °C) at the time $t_1 = 8000$ s, and with the second additional ingredient ($m_{f2} = 300$ kg, $c_{f2} = 4200$ J kg^{-1} K^{-1}, $T_{f2} = 17$ °C) at the time $t_2 = 25\,000$ 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 $\boldsymbol{\theta}$ is obtained by recursive identification.

The prescribed temperature profile is the following: the ingredient of the reactor should first be heated to 40 °C (in this phase, the first additive is added); at the time 15 000 s, the temperature is changed to 50 °C (in this phase, the second additive is added); and at time 35 000 s, the temperature is cooled down to the outer temperature, which equals 17 °C.

In Figure 3, the output signal, $T(k)$, the jacket temperature, $T_j(k)$, and the reference signal, $T_{ref}(k)$, are shown in the upper subplot and the position of the mixing valve is shown in the lower subplot. The algorithm succeeds in controlling the temperature $T(k)$ in the tolerance intervals that are required, as well as when the additional ingredients are fed in the reactor, and also the temperature $T_j(k)$ remains constrained inside the prescribed limits. Only during the switch-on procedure does it overcome the upper constraint. In the stationary state, the discrete valve for hot water is open ($v_{CH} = 1$) together with the mixing valve v_M being slightly open, because of the energy loss in the surroundings. The switching of the discrete valves is minimal, as required. In Figures 4 and 5, the time courses of the identified process parameters $\boldsymbol{\theta}_{11}$, $\boldsymbol{\theta}_{12}$, $\boldsymbol{\theta}_{13}$, $\boldsymbol{\theta}_{21}$, and $\boldsymbol{\theta}_{22}$ are shown. The process parameters, $\boldsymbol{\theta}_{ij}$, 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 $\boldsymbol{\theta}_{22}$, as seen in Figure 5). In these situations, the excitation of the system is large enough to fulfill eq 32 and trigger the recursive identification.

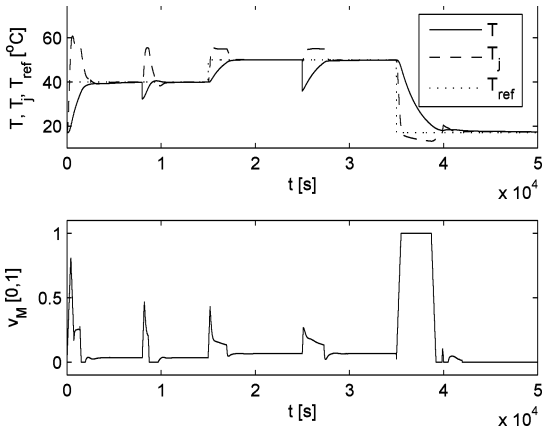

Figure 3. Control of the fed-batch reactor ($T(k)$, $T_j(k)$, $T^r(k)$) and the position of the mixing valve v_M.

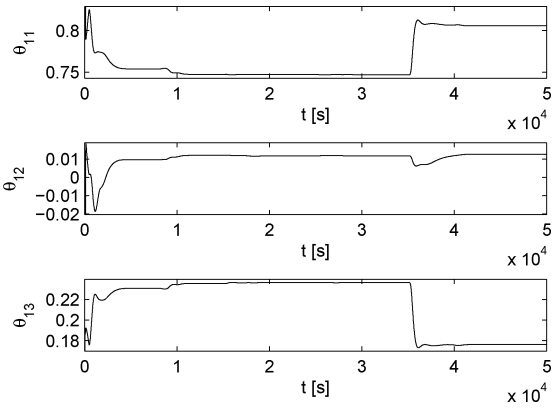

Figure 4. Identified process parameters $\boldsymbol{\theta}_{11}$, $\boldsymbol{\theta}_{12}$, and $\boldsymbol{\theta}_{13}$.

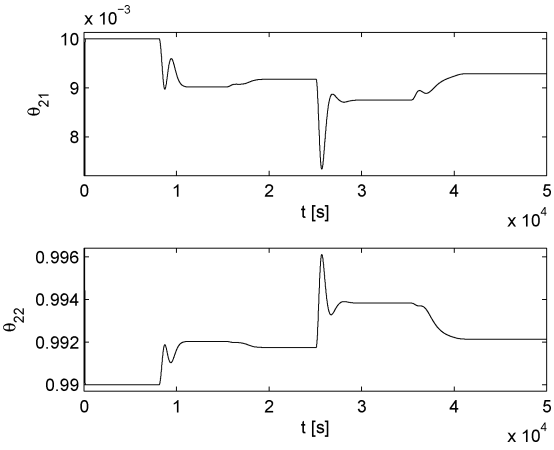

Figure 5. Identified process parameters $\boldsymbol{\theta}_{21}$ and $\boldsymbol{\theta}_{22}$.

In Figure 6, the switching between the unconstrained control law (ucl) and the constrained control law (ccl) is presented in the upper two subplots, and in the lower subplot, the switching of the on/off valves is shown with variable v_{CH}. The detail of the required position of the continuous mixing valve v_M and the actual position of the mixing valve are shown in Figure 7. Although the shown dynamics of the mixing valve is really very slow (the opening and closing times of the valve are 500 s), the obtained results of the temperature control are of sufficient quality. The simulation study was realized to study the possible use of the proposed adaptive supervisory control algorithm in the real application where the actuators have really very slow dynamics. Using the simulation study, the implementation of an adaptive predictive functional control algorithm was justified. It has been shown that the obtained results meet the desired

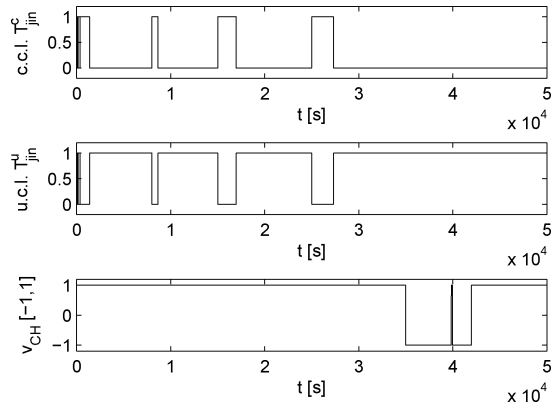

Figure 6. Switching between the unconstrained control law (ucl) and the constrained control law (ccl) and the switching of the on/off valves (v_{CH}).

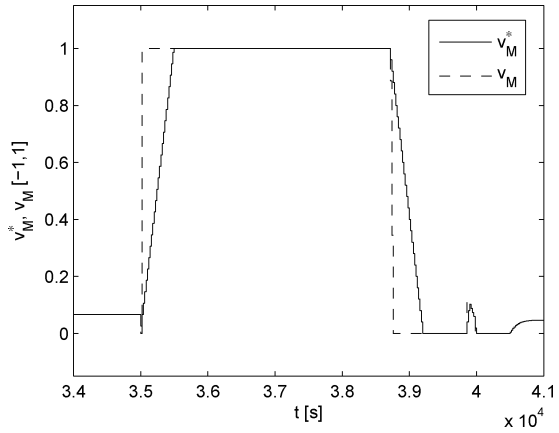

Figure 7. Desired, v_M, and current position, v^*_M, of the mixing valve.

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.

6. Conclusion

In this paper, an adaptive supervisory predictive functional control algorithm was tested to control the temperature in a reactor's core. The fed-batch reactor is an example of a hybrid process because of the discrete and continuous actuators that are used. The continuous actuator has very slow dynamics, which causes some problems in control. The continuous control with supervision is used to control the process. A simulation study was carried out to elaborate the possible use of the proposed adaptive supervisory predictive control algorithm in the real application. Using the simulation study, the implementation of an 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.

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