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PREDICTIVE FUNCTIONAL CONTROL OF TEMPERATURE IN A PHARMACEUTICAL HYBRID NONLINEAR BATCH REACTOR

These days, in times of recession, we are forced by competitiveness and the optimization of production to lower the costs of the temperature control in pharmaceutical batch reactors and increase the quantity and quality of the produced pharmaceutical product (active pharmaceutical substances). Therefore, a control algorithm is needed that provides us rapid and precise temperature control. This paper deals with the development of a control algorithm, where two predictive functional controllers are connected in a cascade for heating and cooling the content of the hybrid batch reactor. The algorithm has to be designed to cope with the constraints and the mixed discrete and continuous nature of the process of heating and cooling. The main goal of the control law is to achieve rapid and exact tracking of the reference temperature, good disturbance rejection and, in particular, a small number of heating and cooling medium switchings. The simulation results of the proposed algorithm gave a much better performance compared to a conventional cascade PI algorithm.

Keywords: batch processes, cascade control, predictive functional control, temperature control.

This paper deals with the development of a control algorithm for the temperature control of a batch reactor. According to some statistics, the use of batch-type processes, and hence the use of batch reactors, is about 50% of all production processes in industry today [1]. In most cases, these reactors can be used for the production of different types of products, and therefore their dynamics can vary widely from product to product.

Since the batch reactor is used for the preparation of solvents added to the production of active pharmaceutical substances, a rapid and precise temperature control of the reactor contents is essential. As described [2,3], good control - for processes with drastic changes in the prescribed temperature, a variety of uses of the reactor, the mixed continuous and discrete hybrid nature of the process behavior and the equipment - is hard to achieve. These days in times of recession, forced by competitiveness and the optimization of production costs, we need to lower the

costs of temperature control and increase the quantity and quality of the produced product. For this reason a conventional PI controller, which is the most commonly used in conventional practice, is not effective enough. Our goal is to improve the performance of the temperature control of the reactor contents by using advanced control algorithms. The control depends on the choice of the discrete heating-cooling medium and the continuous position of the analog valve. We are therefore dealing with a hybrid nonlinear system.

A lot of work and development has been done over the last thirty years in the fields of modeling, simulations and the temperature control of batch reactors. This is reflected in many published studies in the field of advanced control principles for the temperature control of batch reactors. A historical review of the development of control algorithms has been presented [4]. Surveys with examples and explanations of the theoretical and mathematical background for the following fields are given: optimal control [5-7], predictive control [8,9], adaptive control [10,11], nonlinear control [12-14] and fuzzy model-based controls [15,16]. Some of the advanced control algorithms are already used in industry, but most of them are present only in scientific research. From the conclusion of

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these studies, we can see that the use of advanced control algorithms - because of higher quality and quantity, combined with lower cost requirements - is increasingly necessary.

The most promising concepts in the field of adaptive control are reported [17-22]. The field of optimal control is represented [23-25] and the field of predictive control too [26-34]. In this article, for the temperature control of the batch reactor contents, the model predictive functional control (PFC) scheme is used [35-37]. PFC is one of the most frequently used predictive control schemes [38]. Due to its simplicity and good performance fuzzy and fuzzy adaptive versions of PFC were also proposed. The authors [39,40] use recursive fuzzy clustering to adapt the fuzzy model. In our case two PFC controllers connected in a cascade are used. The main advantage of this 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 the control law is to achieve fast and exact reference-temperature tracking and good disturbance rejection. What is more, the number of switchings and the consumption of the heating and cooling medium should be as small as possible.

For the development and testing of the PFC algorithm a good process model is needed. The authors [41-44] discuss the different types of batch reactors that are used in the chemical, biological, pharmaceutical and food industries. They also present different modeling techniques for these reactors. Our choice for the development and testing of the proposed algorithm is a theoretical model for the process of heating and cooling the reactor contents. In the literature a number of papers and books have been published that discuss the construction of a theoretical model. The basic theoretical models of a

batch reactor are described [45-47]. These works contain theoretical models for different types of batch reactors and the basis of the heat conduction between the reactor jacket, the reactor core and to the reactor surroundings. A detailed nonlinear theoretical model for the heating and cooling of a hybrid batch reactor was successfully developed [48]. For this reason we use this theoretical model for the development and testing of our algorithm.

The paper is organized in the following way: the second section describes the theoretical model of the batch reactor; the third section contains the temperature control of the reactor contents with the predictive functional control algorithm and a comparison between a conventional PI controller and the proposed algorithm. Finally, we give some concluding remarks.

THE HYBRID BATCH-REACTOR MODEL

The hybrid batch reactor [48] is made of stainless steel and serves for the preparation of solvents that are added to the production of drugs. The reactor capacity is 630 L. The temperature control (heating and cooling) of the reactor contents is performed *via* pipes wrapped around the wall of the reactor. The heating and cooling is done through these pipes with a heating-cooling medium (50% water and 50% glycol) at three different temperatures T_{in} : $T_{in1} = -25\text{ }^{\circ}\text{C}$, $T_{in2} = 5\text{ }^{\circ}\text{C}$ and $T_{in3} = 140\text{ }^{\circ}\text{C}$. The right medium for the temperature control is chosen according to the output of the control algorithm. The different input media cannot be mixed with each other. An additional adjustment from the control algorithm is made with an analog valve, which defines the amount of fresh water pumped into the reactor jacket.

The scheme of the hybrid batch reactor is shown in Figure 1.

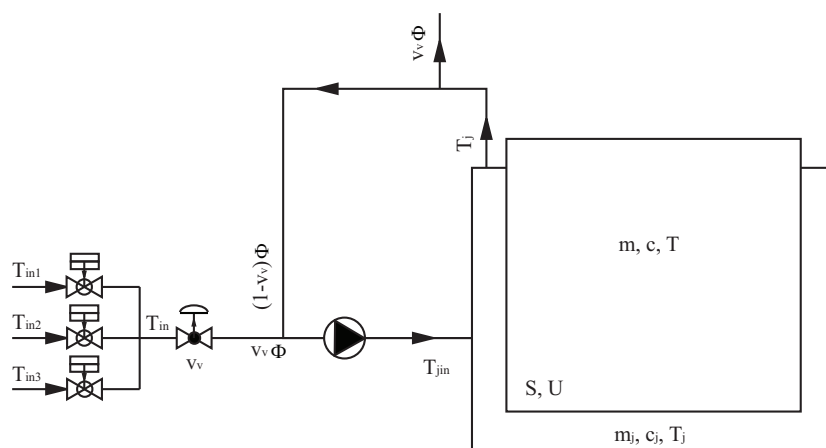


Figure 1. Scheme of the hybrid batch reactor.

The reactor core temperature, T , is controlled by the jacket's inlet temperature, T_{jin} , and the reactor jacket temperature, T_j . The authors [48] simplified the reactor jacket as a flat plate connected to the reactor core with the surface S . The heat transfer between the reactor core and the jacket is defined by the highly nonlinear overall thermal conductivity U , which is dependent of the reactors jacket temperature, T_j . The nonlinearities of this parameter are in detail described in the article mentioned above. While the parameters m and c define the mass and heat capacity of the reactor core contents, the parameters m_j and c_j define the mass and heat capacity of the medium mixture in the reactor jacket. Other parameters used in the theoretical model are: Φ the flow of the heating-cooling medium; v_v the position of the analog valve that represents the ratio between the fresh input heating-cooling medium T_{in} and the reflux of the heating-cooling medium T_j .

The theoretical model is defined by the first law of thermodynamics, the conservation of energy [42–44]:

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

$$m_j c_j \frac{dT_j}{dt} = \Phi c_j T_{jin} - \Phi c_j T_j - U(T_j) S (T_j - T) \quad (2)$$

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

The authors [48] determined that the process of heating and cooling of the reactor contents is highly nonlinear in terms of its parameters. Therefore, the authors developed a detailed nonlinear theoretical model, which was shown to very accurately describe the real plant.

Due to the nonlinearities of the theoretical model [48], we use this model for the development and for testing the advantages of a cascade predictive functional algorithm according to a conventional cascade PI algorithm. For all of the control development and testing purposes, the sampling time $T_s = 10$ s is used. All of the other model parameters values are given elsewhere [48].

PREDICTIVE FUNCTIONAL CONTROL ALGORITHM

For the control of the reactor core and jacket temperature we use two predictive functional control (PFC) algorithms connected in a cascade. While the internal loop controls the reactor jacket temperature, the external loop controls the reactor core temperature. The PFC algorithm in the state-space domain is

proposed [36,49,50]. The main idea of the PFC algorithm is to determine the future control action so that the predicted output trajectory coincides with the reference trajectory. The predicted output is calculated on the basis of the processes model in the state-space domain.

The goal of the control law is to achieve fast and exact tracking of the reference temperature of the reactor core. It is also very important to optimize the costs of the temperature control. For this reason the number of on/off valve switchings should be as small as possible. With this restriction we minimize the amount of heating-cooling medium that is used and extend the life cycle of the equipment.

Since the PFC algorithm is defined in discrete time domain, the theoretical model in continuous time domain should be discretized and the parameters of the model calculated at the operating point. The proper sampling time in our case is $T_s = 10$ s. The process of heating and cooling the reactor contents is described by two first-order processes for the reactor jacket and core temperatures in Eqs. (2) and (3). So the linearization is made by two first-order models in the state-space domain: the model for the reactor core temperature represented in Eq. (4) and the model for the reactor jacket temperature in Eq. (5):

$$T(k+1) = A_{mc}(k)T(k) + B_{mc}(k)T_j(k)$$

$$T(k) = C_{mc}(k)T(k) \quad (4)$$

$$T_j(k+1) = A_{mj}(k)T_j(k) + \begin{bmatrix} B_{mj}^1(k) & B_{mj}^2(k) \end{bmatrix} \begin{bmatrix} T(k) \\ T_{jin}(k) \end{bmatrix} \quad (5)$$

$$T_j(k) = C_{mj}(k)T_j(k)$$

where

$$A_{mc} = 1 - T_s \frac{U(T_{j0})S}{mc}, \quad A_{mj} = 1 - T_s \frac{U(T_{j0})S}{m_j c_j} - T_s \frac{\Phi}{m_j},$$

$$B_{mc} = T_s \frac{U(T_{j0})S}{mc}, \quad B_{mj}^1 = T_s \frac{U(T_{j0})S}{m_j c_j}, \quad B_{mj}^2 = T_s \frac{\Phi}{m_j},$$

$$C_{mc} = [1], \quad C_{mj} = [1]$$

and both input-output matrices are equal to zero.

For the parameters calculation the operating points for the reactor core temperature $T_0 = 50$ °C, for the reactor jacket temperature $T_{j0} = 50$ °C and for the reactor jacket inlet temperature $T_{jin0} = 50$ °C were chosen. Changes of the different temperatures around the operating point do not give significant changes in the model.

For the control the following predictive functional control law u in a general case can be obtained in a similar manner as in literature [49]:

$$u(k) = \eta^{-1}((1 - a_r^H)(w(k) - y_p(k)) + y_m(k) - C_m A_m^H x_m(k)) \tag{6}$$

where $\eta = C_m(A_m^H - I)(A_m - I)^{-1}B_m$, A_m is the state matrix, B_m is the input matrix, C_m is the output matrix, a_r is the parameter of the reference model, H is the coincidence horizon, w is the reference signal, y_p is the current process output, y_m is the process model output and x_m is the state of the process model.

This control law is realizable if the process is stable, controllable and observable ($\eta \neq 0$). This means that the PFC control law in its common form can be implemented only for open-loop stable systems. The stability is proven [50]. 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 ρ of the controlled system ($H \geq \rho$).

Based on the proposed control, we develop an algorithm where two predictive functional controllers are connected in a cascade. First, the predictive control law w_{T_j} is calculated, as given in Eq. (7). w_{T_j} is the desired temperature of the reactor jacket needed to achieve the reference temperature w_T in the reactor core. w_{T_j} is constrained between -25 and 140 °C. In the second step, the constrained predictive control law $w_{T_{jin}}$ is calculated, as given in Eq. (9). $w_{T_{jin}}$ is the desired temperature of the reactor jacket inlet needed to achieve the reference jacket temperature w_{T_j} (Eq. (7)) in the reactor jacket. $w_{T_{jin}}$ is also constrained between -25 and 140 °C.

$$w_{T_j}(k) = \eta_{mc}^{-1}((1 - a_{rc}^H)(w_T(k) - T(k)) + T_{mc}(k) - C_{mc} A_{mc}^H x_{mc}(k)) \tag{7}$$

$$T_{mc}(k + H_c) = C_{mc}(A_{mc}^H x_{mc}(k) + (A_{mc}^H - I)(A_{mc} - I)^{-1} B_{mc} T_j(k)) \tag{8}$$

where $\eta_{mc} = C_{mc}(A_{mc}^H - I)(A_{mc} - I)^{-1}B_{mc}$, a_{rc} is the parameter of the reactor core reference model, H_c is the coincidence horizon for the reactor core temperature, T is the current temperature in the reactor core, T_{mc} is the predicted temperature for the reactor core and x_{mc} is the state of the process model that defines the dynamics between the reactor jacket temperature and the reactor core temperature.

$$w_{T_{jin}}(k) = \eta_{mj}^{-1}((1 - a_{rj}^H)(w_{T_j}(k) - T_j(k)) + T_{mj}(k) - C_{mj} A_{mj}^H x_{mj}(k)) \tag{9}$$

$$T_{mj}(k + H_j) = C_{mj}(A_{mj}^H x_{mj}(k) + (A_{mj}^H - I)(A_{mj} - I)^{-1} B_{mj}^2 T_{jin}(k)) \tag{10}$$

where $\eta_{mj} = C_{mj}(A_{mj}^H - I)(A_{mj} - I)^{-1}B_{mj}^2$, a_{rj} is the parameter of the reactor jacket reference model, H_j is the coincidence horizon for the reactor jacket temperature, T_j is the current temperature of the reactor jacket, T_{mj} is the predicted temperature for the reactor jacket and x_{mj} is the state of the process model that defines the dynamics between the reactor jacket temperature and the reactor jacket inlet temperature.

The basic control scheme of the PFC algorithm described above is shown in Figure 2, where G_j is the process of heating and cooling the reactor jacket, G_c is the process of heating and cooling the reactor core:

$$g_c = \eta_{mc}^{-1}(1 - a_{rc}^H) \tag{11}$$

$$L_c(z) = \eta_{mc}^{-1}(1 - a_{rc}^H)(zI - A_{mc})^{-1} B_{mc}$$

$$g_j = \eta_{mj}^{-1}(1 - a_{rj}^H) \tag{12}$$

$$L_j(z) = \eta_{mj}^{-1}(1 - a_{rj}^H)(zI - A_{mj})^{-1} B_{mj}$$

In the end the decision logic for the choice of the input heating-cooling medium is defined. First, the position of the mixing valve is calculated from Eq. (1) as follows:

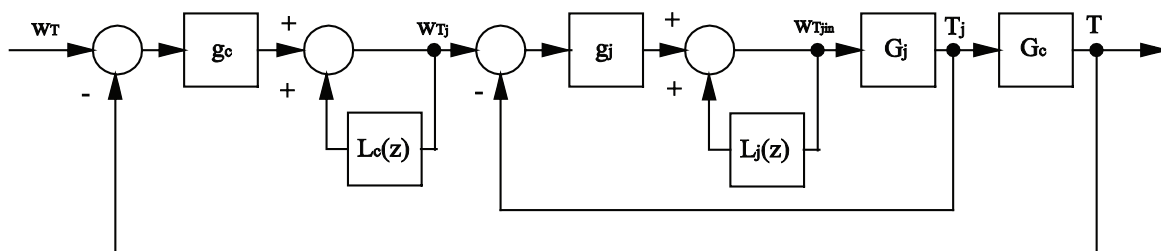


Figure 2. Basic control scheme of the PFC algorithm.

$$v_v(k) = \frac{w_{T_{jin}}(k) - T_j(k)}{T_{in}(k) - T_j(k)} \quad (13)$$

So the decision logic (DL) is defined as follows:

$$\text{if } T_{in}(k) = T_{in1} \text{ and } v_v(k) < -\delta \\ \text{then } T_{in}(k+1) = T_{in2} \quad (14)$$

$$\text{if } T_{in}(k) = T_{in2} \text{ and } v_v(k) < -\delta \text{ then} \\ T_{in}(k+1) = T_{in3} \quad (15)$$

$$\text{if } T_{in}(k) = T_{in2} \text{ and } v_v(k) > 1 + \delta \text{ then} \\ T_{in}(k+1) = T_{in1} \quad (16)$$

$$\text{if } T_{in}(k) = T_{in3} \text{ and } v_v(k) < -\delta \text{ then} \\ T_{in}(k+1) = T_{in2} \quad (17)$$

In the decision rules, the parameter δ defines the dead zone involved in the switchings of the heating-cooling medium. With the included switching we redesign the control scheme of the PFC algorithm (Figure 3).

Before testing the proposed algorithm we include some limitations in the switchings between the heating-cooling media. First, it is important that only one medium at a time is used. We have also to consider the equipment's protection against deformation due to large temperature changes in the reactor jacket. Therefore, no direct heating-cooling medium change from T_{in1} to T_{in3} and vice versa is allowed. To optimize the cooling of the reactor core we consider that the medium T_{in1} is used only if the reactor core temperature is below 30 °C. This limitation stems from the fact that the heat transfer between the reactor jacket and the core is much smaller because of the thick film that is formed on the walls inside the reactor jacket, as described in the section for the theoretical model.

Control with the proposed algorithm

The proposed PFC algorithm was tested by simulating the theoretical model of the batch reactor. The main goal of the study was to achieve rapid and

exact reference-temperature tracking and a good disturbance rejection. It is also very important that the number of switchings of the heating-cooling medium stays as small as possible. This minimizes the amount of heating-cooling medium that is used and extends the equipment's life cycle.

In the simulation we assume some disturbances as with the real process. There is a disturbance on the prefabricated heating-cooling mediums T_{in} . Due to the sensor noise, we consider disturbances in the reactor jacket temperature, T_j , and the reactor core temperature, T . The initial values are for the reactor jacket temperature $T_j(0) = 0$ °C, the reactor core temperature $T(0) = 0$ °C and the mass of the reactor contents is $m(0) = 550$ kg. We also consider the addition of 80 kg of solvent with a temperature of 10 °C at time $t = 400$ min.

In the next step, the initialization of the predictive functional control algorithm is given. The parameters of the reference trajectories are $a_r = 0.8212$, $a_{qj} = 0.7141$; and the prediction horizons for the reactor core and jacket are $H = 13$ and $H_j = 2$. The dead zone of the switchings of the heating-cooling medium is chosen to be $\delta = 20$.

The simulation results are shown in Figures 4-7. Figure 4 shows the batch reactor core temperature T and the changing reference temperature, w_T , Figure 5 shows the batch reactor jacket temperature, T_j , Figure 6 shows the temperature of the chosen heating-cooling medium, T_{in} , and Figure 7 shows the position of the continuous valve.

Finally, a comparison between the results using the proposed algorithm and a conventional controller is given. For the temperature control of the batch reactor in the comparison we chose two conventional PI controllers, connected in a cascade. Different sets of PI parameters were compared. While a "rapid" PI results in rapid reference-temperature tracking and many heating-cooling medium switchings, a "slow" PI results in less heating-cooling medium switchings but much slower reference-temperature tracking. For the sake of comparison, we adjusted the parameters so that the PI controller achieved approximately the same reference-temperature tracking performance and

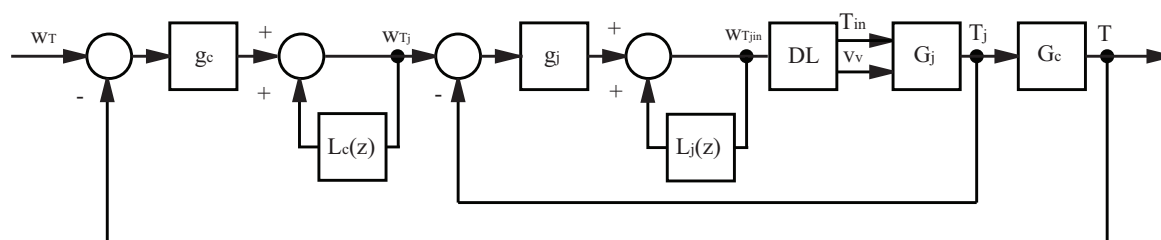


Figure 3. Temperature control scheme for the batch reactor.

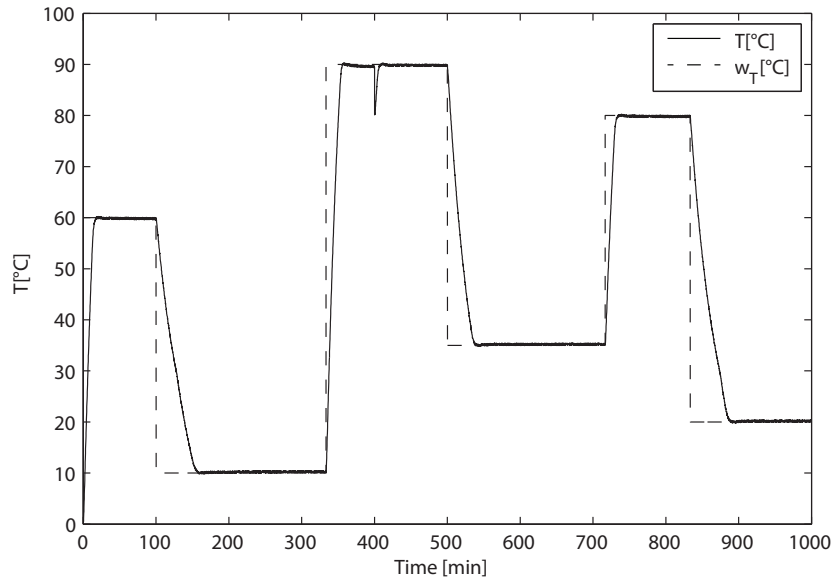


Figure 4. Control of the reactor core temperature with the proposed algorithm.

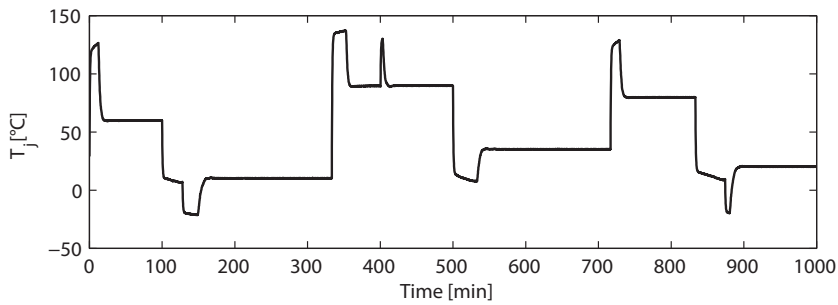


Figure 5. Reactor jacket temperature (PFC).

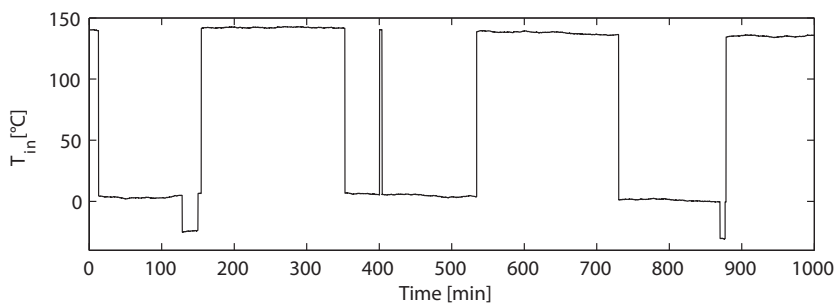


Figure 6. Temperature of the heating-cooling medium (PFC).

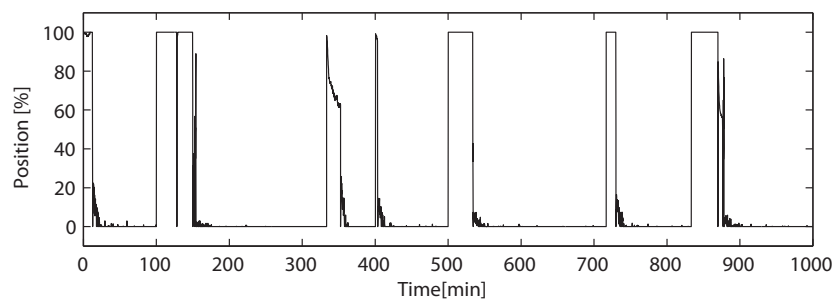


Figure 7. Position of the continuous valve (PFC).

disturbance rejection as the proposed algorithm. The parameters for the conventional cascade controller are: for the external PI controller (proportional gain is $k_{cp} = 12.5$ and integral gain is $k_{ci} = 25$) and for the internal PI controller (proportional gain is $k_{cp} = 2.5$ and integral gain is $k_{ci} = 660$). The dead zone of the switchings of the heating-cooling medium is the same as with the proposed algorithm $\delta = 20$.

As seen from the simulation results using the proposed control algorithm (Figures 4-7) and with the PI control algorithm (Figures 8-11), both control

approaches give us good reference-temperature tracking and a rapid disturbance rejection. The control performance is measured with the root-mean-square deviation for both algorithms (Eq. (18)):

$$RMSD = \sqrt{\frac{\sum_{i=1}^n (w_T(i) - T(i))^2}{n}} \quad (18)$$

where $n = 6000$ is the number of measurements.

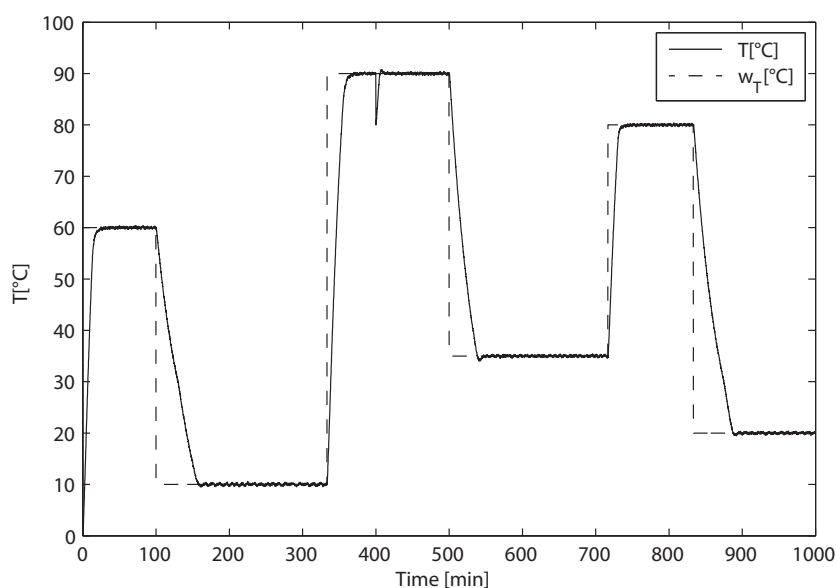


Figure 8. Control of the reactor core temperature with conventional PI controller connected in a cascade.

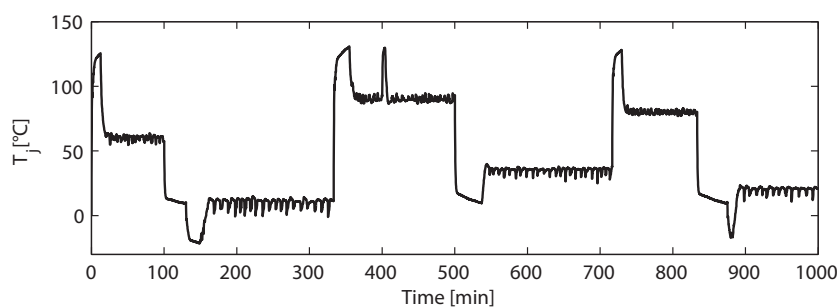


Figure 9. Reactor jacket temperature (PI).

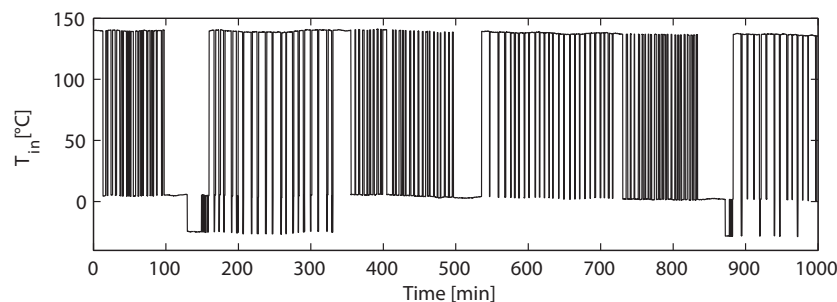


Figure 10. Temperature of the heating-cooling medium (PI).

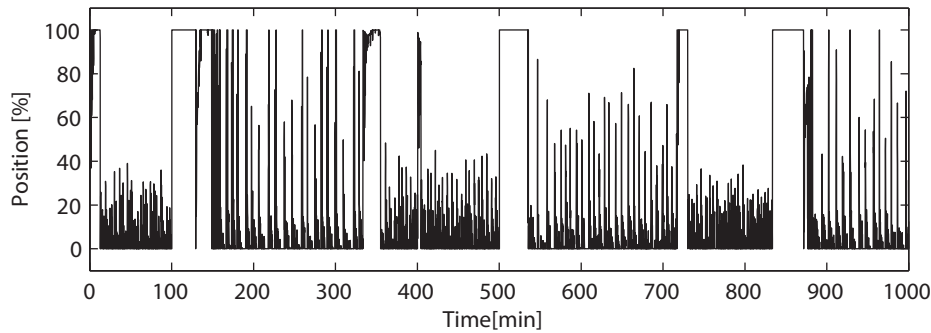


Figure 11. Position of the continuous valve (PI).

The result for the proposed control algorithm is $RMSD_{PFC} = 5.012$ °C and for the PI control algorithm $RMSD_{PI} = 5.347$ °C. We can conclude that the proposed algorithm ensures a slightly better performance than the PI control approach. However, the most significant difference is that the number of heating-cooling medium switchings with the proposed algorithm is only 12 (Figure 6), while with the PI algorithm we have to deal with 336 (Figure 10) switchings. The greater number of heating-cooling medium switchings also means many more switchings of the three on/off valves, which decreases the life cycle of the actuators. To sum up, the switchings of the three on/off valves from open to closed or *vice versa* happens only 24 times using the proposed algorithm. On the other hand, when using the PI algorithm, the switchings happen 672 times. This means that the proposed algorithm decreases the number of switchings of the on/off valves by 96% compared to the PI algorithm, ensuring a comparable reference-tracking performance.

Another indicator for the longevity of the equipment is the total movement (TM) of the analog valve that is calculated in Eq. (19). The total movement for the proposed algorithm is 32.89, whereas for the PI algorithm it is 364.62. Again, the proposed algorithm reduces the movement of the analog valve by 91%, compared to the PI algorithm:

$$TM = v_v(1) + \sum_{i=2}^n |(v_v(i) - v_v(i-1))| \quad (19)$$

The quantity of the used medium (UM) for both control approaches is calculated with Eq. (20):

$$UM = \sum_{i=1}^n \Phi(T_{jin}) v_v(i) T_s \quad (20)$$

The calculated amount of heating-cooling medium spent to control the reactor core temperature for the proposed algorithm was $UM_{PFC} = 27.5$ m³ and for the PI algorithm $UM_{PI} = 34.0$ m³.

From these results we can conclude that the proposed algorithm results in a slightly better performance, a saving of 23.6% on the costs for the heating-cooling medium, a more than 10-fold increase in the life cycle of the analog valve and a more than 20-fold extension of the life cycle of the on/off valves. The PI controller could probably be better tuned by searching the parameters space for better parameters, but this is in general a very time consuming procedure. This is also one of the advantages of the PFC - it is tuned more properly and faster than the PI controller.

CONCLUSION

The main goal of the study was to develop a control algorithm that allows rapid and exact reference-temperature tracking, good disturbance rejection and a minimal number of heating-cooling medium switchings.

For the temperature control the predictive functional control algorithm connected in a cascade was chosen. The obtained results have shown that the proposed algorithm for the temperature control of the reactor content meets the desired criteria. According to the other advanced control principles the main advantage of the proposed control algorithm is in the analytical expression of the control law, which enables its use in real-time control and implemented on low-cost hardware. The comparison between the control with the proposed algorithm and the control with the conventional PI controller shows us better performance, which significantly reduces the number of switchings of the heating-cooling medium and the analog valve movement. This decreases the costs of the temperature control by using less heating-cooling medium and extends the life cycle of the equipment.

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NAUČNI RAD

PREDIKTIVNA FUNKCIONALNA KONTROLA TEMPERATURE U FARMACEUTSKOM HIBRIDNOM NELINEARNOM ŠARŽNOM REAKTORU

U današnje vreme recesije, kompetitivnost i optimizacija proizvodnje zahtevaju smanjenje troškova kontrole temperature u farmaceutskim šaržnim reaktorima i povećanje kvantiteta i kvaliteta farmaceutskog proizvoda (aktivna supstanca). Zbog toga je potreban algoritam koji obezbeđuje brzu i preciznu kontrolu temperature. Ovaj rad se bavi razvojem algoritma kontrole u kome su dva prediktivna funkcionalna kontrolora vezana u kaskadu za zagrevanje i hlađenje reakcione smeše hibridnog šaržnog reaktora. Ovaj algoritam mora da savlada ograničenja i mešanu diskretno-kontinualnu prirodu procesa zagrevanja i hlađenja. Glavni cilj kontrolnog sistema je da se postigne brzo i tačno praćenje referentne temperature, dobro odbacivanje poremećaja i, naročito, mali broj promena zagrevanje/hlađenje. Rezultati simulacije razvijenog algoritma ukazuju na bolje performace u poređenju sa konvencionalnim PI algoritmom.

Ključne reči: šaržni procesi, kaskadna kontrola, prediktivna funkcionalna kontrola, temperaturna kontrola.