SELF - ORGANIZING MIGRATING ALGORITHM IN MODEL PREDICTIVE CONTROL: CASE STUDY ON SEMI-BATCH CHEMICAL REACTOR

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Abstract

Control of complex nonlinear systems brings challenges in the controller design. One of methods how to cope with this challenge is the usage of advanced optimization methods. This work presents application of self-organizing migrating algorithm (SOMA) in control of the semi-batch reactor. The reactor is used in chromium recycling process in leather industry. Because of the complexity of this semi-batch reactor control, the model predictive control (MPC) approach is used. The MPC controller includes self-organizing migrating algorithm (SOMA) for the optimization of the control sequence.

KeywordsModel Predictive Control; SOMA; Chemical reactor; Exothermic reaction; Mathematical modelling

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1. Introduction

In the industrial processing, there are a lot of different techniques used today. But all have a common goal - to bring maximum profit at minimum cost. Nowadays the situation is even more complicated by the necessity of unwanted by-products or/and products after their lifetime disposal. Of course this brings additional costs, which must be taken into account when pricing the final product. Priority is given mainly to non-waste technologies and recycling technologies.

One of such waste free technologies is an enzymatic dechromation. This technology recycles waste originated during chrome tanning process and also waste generated at the end of the final product lifetime (used leather goods).
Part of the recycling process includes also an oxidation-reduction reaction which is strongly exothermic and can be controlled by the chromium filter sludge into the hot reaction blend of chromium sulphate acid dosing [1]. Optimization of this process control is studied in this paper.

Nomenclature

A	[s^{-1}]	pre-exponential factor
c_C	[$J \cdot kg \cdot K^{-1}$]	specific heat capacity of the cooling water
c_I	[$J \cdot kg \cdot K^{-1}$]	specific heat capacity of the reaction component input
E	[$J \cdot mol^{-1}$]	activation energy
F_I	[$kg.s^{-1}$]	mass flow rate of the reaction component input
F_C	[$kg.s^{-1}$]	mass flow rate of the cooling water
ΔH_r	[$J \cdot kg^{-1}$]	reaction heat
J		performance criterion
K	[$kg \cdot s^{-3} \cdot K^{-1}$]	conduction coefficient
k		discrete time step
m_B	[kg]	initial mass filling of the reactor
m_C	[kg]	weight of the cooling water in the cooling system
N_u		control horizon
N_1		prediction horizon beginning
N_2		prediction horizon end
R	[$J \cdot mol^{-1} \cdot K^{-1}$]	gas constant
S	[m^2]	heat transfer surface
S_u		control signal changes criterion function
S_y		control error criterion function
T	[K]	reactor content temperature
T_C	[K]	output temperature of the cooling water
T_I	[K]	temperature of the reaction component input
T_{CI}	[K]	input temperature of the cooling water
u		control action (controller output)
u_t		tentative control signal
y		system output signal
$\hat{y}$		system model response
γ_c		speed of the γ decrement
y_r		desired target value of the output signal (desired response)
λ		weight of the future control errors sum
ρ		weight of the control action sum

2. Semi-batch chemical reactor

Process itself runs in a semi-batch chemical reactor. The chemical reactor is a vessel with a double wall filed with a cooling medium. It has a filling opening, a discharge outlet, cooling medium openings and a stirrer. The scheme of the reactor is depicted in the Fig. 1.

The scheme shows a reactor with initial filling m_B [kg] given by the solution of chemicals without the chromium sludge (filter cake). The sludge is fed into the reactor by F_I [$kg.s^{-1}$] to control the developing heat since the temperature has to stay under a certain critical level ($T(t) < 373.15K$), otherwise the reactor could be destroyed. On the other hand it is desirable to utilize the maximum capacity of the reactor to process the maximum amount of waste in the shortest possible time (higher temperature is desirable). Therefore an optimal control strategy has to find a trade-off between these opposite requirements.

The feed rate is limited by the reactor walls heat transfer. The reaction is exothermic so the rising heat must be removed. The rate of heat transfer depends on three factors [2]:

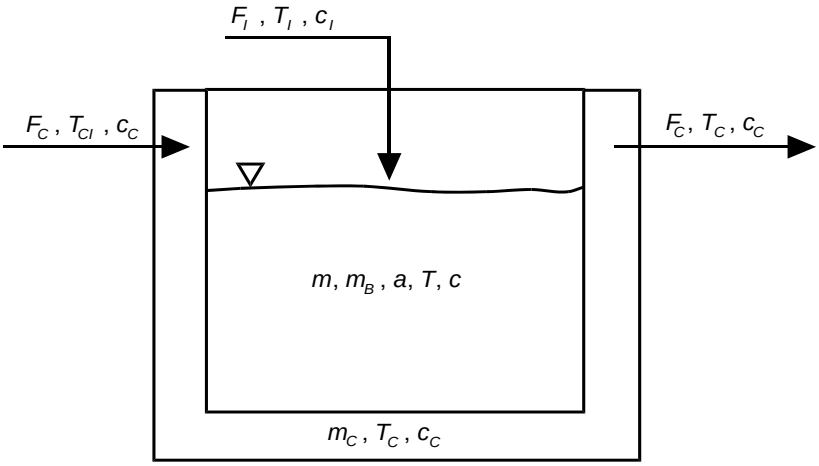

Fig. 1. Semi-batch reactor scheme

1. The temperature difference between the reaction liquid and the jacket coolant. The latter depends on the coolant flow rate, the inlet coolant temperature, and the heat-transfer rate. 2. The overall heat-transfer coefficient, which depends on agitator mixing in the vessel and the flow rate of coolant in the jacket. 3. The heat-transfer area. If jacket cooling is used, the effective heat-transfer area in a fed-batch reactor varies during the course of the batch directly with the volume of liquid in the vessel.

Due to the complexity of the reaction mixture and the difficulties to perform on-line composition measurements, control of batch and fed-batch reactors is essentially a problem of temperature control. The temperature profile in batch reactors usually follows three-stages [3]: (i) heating of the reaction mixture until the desired reaction temperature, (ii) maintenance of the system at this temperature and (iii) cooling stage in order to minimize the formation of by-products. Any controller used for the reactor control must be able to overcome these different stages.

3. Mathematical model

The above mentioned reactor can be described by the mathematical model shown below. Under usual simplifications, based on the mass and heat balance, the following 4 nonlinear ordinary differential equations can be derived [4]:

$$\frac{\mathrm{d}\,m(t)}{\mathrm{d}\,t} = F_I \tag{1}$$

$$\frac{\mathrm{d}\,a(t)}{\mathrm{d}\,t} = \frac{F_I[1-a(t)]}{m(t)} - A\cdot e^{-\frac{E}{R\cdot T(t)}}\cdot a(t) \tag{2}$$

$$\frac{\mathrm{d}\,T(t)}{\mathrm{d}\,t} = \frac{F_I\cdot c_I\cdot T_I}{m(t)\cdot c} + \frac{A\cdot e^{-\frac{E}{R\cdot T(t)}}\cdot \Delta H_r\cdot a(t)}{c} - \frac{K\cdot S\cdot T(t)}{m(t)\cdot c} + \frac{K\cdot S\cdot T_C(t)}{m(t)\cdot c} - \frac{T(t)F_I}{m(t)} \tag{3}$$

$$\frac{\mathrm{d}\,T_C(t)}{\mathrm{d}\,t} = \frac{F_C\cdot T_{CI}}{m_C} + \frac{K\cdot S\cdot T(t)}{m_C\cdot c_C} - \frac{K\cdot S\cdot T_C(t)}{m_C\cdot c_C} - \frac{F_C\cdot T_C(t)}{m_C} \tag{4}$$

Individual symbols have the following meaning: m is the total weight of reaction components in the reactor, a is the mass concentration of the reaction component in the reactor, c = 4500 J·kg·K^{-1} is the specific heat capacity of the reactor content and T its temperature. F_I, T_I = 293.15 K and c_I = 4400 J·kg·K^{-1} is the reaction component input mass flow rate, temperature and specific heat capacity. F_C = 1 kg·s^{-1}, T_{CI} = 288.15 K, T_C, c_C = 4118 J·kg·K^{-1} and m_C = 220 kg is the cooling water mass flow rate, input temperature, output temperature, specific heat capacity and weight of the cooling water in the cooling system of the reactor, respectively. Other constants: A = 219.588 s^{-1}, E = 29967.5087 J·mol^{-1}, R = 8.314 J·mol^{-1}·K^{-1}, ΔH_r = 1392350 J·kg^{-1}, K = 200 kg·s^{-3}·K^{-1}, S = 7.36 m^2.

The fed-batch reactor use jacket cooling, but the effective heat-transfer area (S = 7.36 m^2) in the mathematical model was treated as constant, not time varying. The initial amount of material placed in the reactor takes about two-thirds of the in-reactor volume and the reactor is treated as ideally stirred, so we can do this simplification.
Variables F_I, F_C, T_I, T_{CI}, can serve as manipulated signals. However, from practical point of view, only F_I and F_C are usable. The T_I or T_{CI} temperature change is inconvenient due to the economic reasons (great energy demands).3.1.

3.1 Technological limits and variables saturation

Maximum filling of the reactor is limited by its volume to m = 2450kg approximately. The process of the chromium sludge feeding F_I has to be stopped by this value. Practically, the feeding F_I can vary in the range $F_I \in \langle 0;3 \rangle$ kg.s^{-1}. As stated in the system description, the temperature *T(t)* must not exceed the limit 373.15K ; this temperature value holds also for the coolant (water) but it is not so critical in this case as shown by the further experiments.

4. SOMA algorithm

The Self-Organizing Migrating Algorithm is used for the above mentioned system optimization. SOMA algorithm can be used for optimizing any problem which can be described by an objective function. This algorithm optimizes a problem by iteratively trying to improve a candidate solution, i.e. a possible solution to the given problem. The SOMA has been successfully utilized in many applications [5-7], while interesting comparison to with simulated annealing and differential evolution is provided by Nolle et al. in [8].

SOMA is based on the self-organizing behavior of groups of individuals in a “social environment”. It can be classified in two ways – as an evolutionary algorithm or as a so-called memetic algorithm. During a SOMA run, migration loops are performed causing individuals repositioning as in evolutionary algorithm. The position of the individuals in the search space is changed during a generation, called a ‘migration loop’. Individuals are generated by random according to what is called the ‘specimen of the individual’ principle. The specimen is in a vector, which comprises an exact definition of all those parameters that together lead to the creation of such individuals, including the appropriate constraints of the given parameters. [9]. On the other hand, no new ‘children’ are created in the common ‘evolutionary’ way. The category of memetic algorithms covers a wide class of meta-heuristic algorithms. We can say that memetic algorithms are classified as competitive-cooperative strategies showing synergetic attributes. [10]. SOMA shows these attributes as well. Because of this, it is more appropriate to classify SOMA as a memetic algorithm.

5. Control of the reactor

Despite the fact that various reactors have been widely used in the chemical industry for decades, the efficient reactor control still encounters many difficulties. There have been published a lot of works dealing with the reactor control approaches. Good introduction to chemical reactors provides for example [11] or [12]. The state of art of chemical reactors control presents Luyben in [13] and [14], control and monitoring of batch reactors describes Caccavale et al. in [15]. Generally, it can be stated that chemical reactors controllers uses various control methods, such as PI controllers, adaptive control methods, robust approaches, predictive control and the like [16-25]. The model predictive control [26-28] belongs to the one of the most popular and successful approaches for semi-batch reactors control. However, this methodology brings some difficulties in finding optimal control sequence especially when complex nonlinear model is utilized. Interesting way how to cope with the optimization problem offers the usage of evolutionary algorithms [29], [30].

In this paper two different approaches to the model predictive control of the given plant are introduced. At first, the model predictive controller that uses self-organizing migrating algorithm for the optimization of the control sequence is presented. This methodology ensues from model predictive control method [3] while it uses same value of the control signal for whole control horizon. This modification was applied in order to reduce computational demands of the controller. The classic MPC controller, which uses Matlab Optimization Toolbox for obtaining the optimal control sequence, is used as the comparative method. This MPC controller computes the control sequence at every sampling period but only first value is applied.

5.1. Notation

From the systems theory point of view the reactor manipulated variables here are input flow rates of the chromium sludge F_I and of the coolant F_C. Input temperatures of the filter cake T_I and of the coolant T_{CI} can be alternatively seen as disturbances. Although the system is generally MIMO, it is assumed just as a single input – single output (SISO) system in this chapter. Thus, the only input variable is the chromium sludge flow rate F_I and the coolant flow rate F_C is treated as a constant. This input variable, often called control action, is in the control theory denoted as u. The output signal to be controlled is again the temperature inside the reactor T. The output signal is usually in the control theory denoted as y and consequently the desired target value of the output signal as y_r.

5.2. Model predictive control

The main idea of MPC algorithms is to use a dynamical model of process to predict the effect of future control actions on the output of the process. Hence, the controller calculates the control input that will optimize the performance criterion J over a specified future time horizon [31]:

$$J(k)=\lambda\cdot\sum_{i=N_1}^{N_2}\left(y_r(k+i)-\hat{y}(k+i)\right)^2+\rho\cdot\sum_{i=1}^{N_u}\left(u_t(k+i-1)-u_t(k+i-2)\right)^2 \tag{5}$$

where k is discrete time step, N_1, N_2 and N_u define horizons over which the tracking error and the control increments are evaluated. The u_t variable is the tentative control signal, y_r is the desired response and $\hat{y}$ is the network model response. The parameters λ and ρ determine the contribution that the sums of the squares of the future control errors and control increments have on the performance index.

Typically, the receding horizon principle is implemented, which means that after the computation of optimal control sequence only the first control action is implemented. Then, the horizon is shifted forward one sampling instant and the optimization is again restarted with new information from measurements. Simplified structure of the MPC control strategy is depicted in the figure 2.

5.3. Model predictive control using SOMA

All simulations with algorithm SOMA were performed in the Mathematica 8.0 software. Here the algorithm SOMA was used for the cost function (5) minimization and was set as follows: Migrations = 25; AcceptedError = 0.1; NP = 20; Mass = 3; Step = 0.3; PRT = 0.1; Specimen = {0.0, 3.0, 0.0}; Algorithm strategy was chosen All To One. First two parameters serve for the algorithm ending. Parameter "Migrations" determines the number of migration loops, "AcceptedError" is the difference between the best and the worst individuals (algorithm accuracy). If the loops exceed the number set in "Migrations" or "AcceptedError" is larger than the difference between the best and the worst individuals, the algorithm stops. Other parameters influence the quality of the algorithm running. "NP" is the number of individuals in the population (its higher value implicates higher demands on computer hardware and can be set by user), "Mass" is the individual distance from the start point, "Step" is the step which uses the individual during the algorithm, "PRT" is a perturbation which is similar to hybridizing constant known from genetic algorithms or differential evolutions. "Specimen" is the definition of an exemplary individual for whole population. For details see [9].

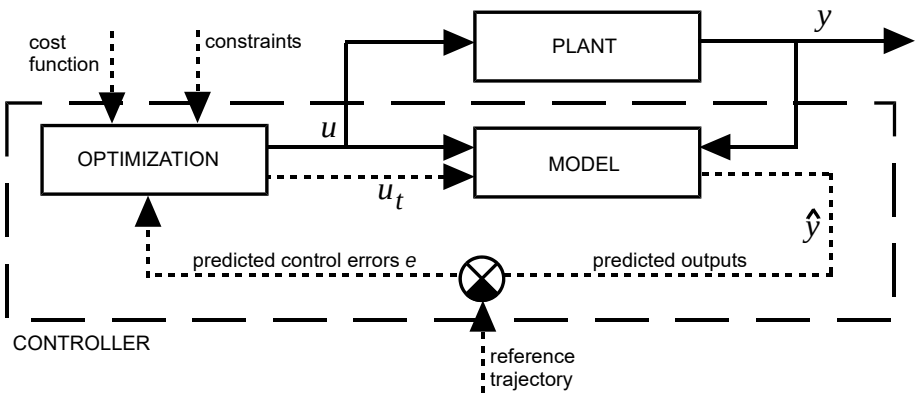

Fig. 2. Basic structure of the model predictive controller

There were performed seven different simulations using SOMA algorithm described in this section. First tree simulations (SOMA1 – SOMA3) were done to study the control horizon N_u influence, next three (SOMA4 – SOMA6) the prediction horizon N_2 influence and the last one (SOMA7) is the simulation with an optimal setting. All settings can be seen in Table 1.

	λ	ρ	N_2	N_u
SOMA1	1	1	300	30
SOMA2	1	1	300	60
SOMA3	1	1	300	90
SOMA4	1	1	200	60
SOMA5	1	1	280	60
SOMA6	1	1	360	60
SOMA7	1	1	320	60

Table 1. SOMA controller settings

Graphical output of SOMA7 (the optimal settings) simulation is depicted in figure 3. Only two most important dependencies are shown – the in-reactor temperature and the chromium sludge dosing development. As was already

said, the temperature has to stay under critical point 373.15K. The chromium sludge dosing shouldn't embody any rapid changes.

The control horizon (N_u) actually means the time interval, for which the actuating variable (F_I) has constant value. It is generally better to set it as short as possible because of more rapid influence on the system, but on the other hand it increases the computing time during the calculations. So it is necessary to find the control horizon value, which balance between these two requirements.

The prediction horizon (N_2) determines how forward controller knows the system behavior. If the horizon is too short, the controller doesn't react in time and the system may become uncontrollable. Long horizon means again the more demanding computation, i.e. the need of more powerful computer hardware.

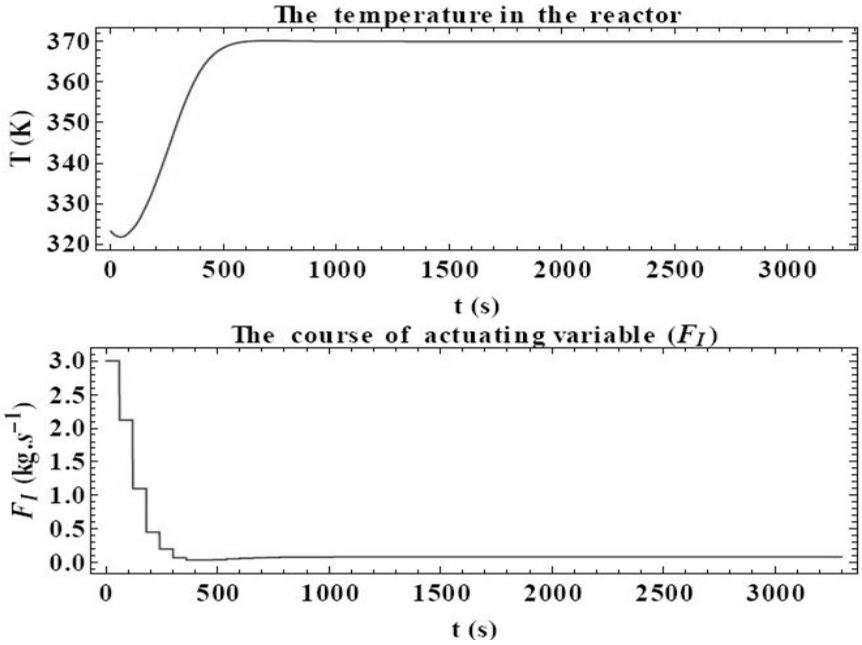

Fig. 3. Results of SOMA7 simulations

5.4. Conventional model predictive approach

The comparative method is based on the classical MPC strategy described in the part 5.2. The optimization box (see figure 2) utilizes standard Matlab Optimization Toolbox function `fmincon` and receding control strategy was implemented. The `fmincon` function used trust-region-reflective algorithm [32].

For the reason that the compared controllers SOMA applied the same control action for whole length of the control horizon N_u= 60 (with the sample time = 1s), the sample time of the comparative controllers was set to 60s. The control horizon N_u was set to 10 as well as the prediction horizon N_2. The rest of the controller design remained same – the predictor was based on the white-box model described by equations (1 – 4), cost function of MPC was the same.

The control loop was simulated using Matlab/Simulink, the controller was built-in as the Matlab M-File and predictor used Matlab S-Function technology.

	λ	ρ	γ	γ_c	N_1	N_2	N_u
MPC1	1	100	0	0	1	10	10
MPC2	1	100	2000	100	1	10	10
MPC3	1	100	2000	200	1	10	10
MPC4	1	100	1500	100	1	10	10

Table 2. Settings of the controllers

However, such controller (Table 2 MPC1 settings) that follows equation (5), did not provide acceptable results. It was not possible to avoid either the overshoot of the in-reactor temperature or the permanent control error using the control configuration. It results from simulations that the biggest problem comes in the very beginning of the control, when the control error is the highest and the controller performs enormous control actions. This is caused by the fact that the reaction is strongly exothermic and even small concentration of the filter cake causes steep rise of the temperature.

Thus, the enhancement of the criterion (5) that penalizes values of the control signal in the beginning of semi-batch process was necessary. Also, at the same time the penalization has to decrease taperingly (6-7):

$$J(k)=\lambda\cdot\sum_{i=N_1}^{N_2}\left(y_r(k+i)-\hat{y}(k+i)\right)^2+\rho\cdot\sum_{i=1}^{N_u}\left(u_t(k+i-1)-u_t(k+i-2)\right)^2+\gamma(k)\cdot\sum_{i=1}^{N_u}u_t(k+i) \tag{6}$$

$$\gamma(k)=\gamma(k)-\gamma_c \tag{7}$$

where γ_c is the parameter which defines the speed of the decrement in γ. This enhancement brought possibility to influence more intensely the speed of dosing of the filter cake with two parameters. In other words γ parameter defines the level of penalization of the control signal, while the ratio $\gamma/\gamma c$ specifies the length of the penalization interval. However, too high γ parameter or γ/γ_c ratio caused unavailing delays or oscillations (the settings *MPC2* in Table 2). On the other hand, small γ/γ_c ratio led to overshoots of the temperature (the settings *MPC3* in Table 2). The best result which was obtained using this approach was obtained for *MPC4* settings and is presented in figure 4.

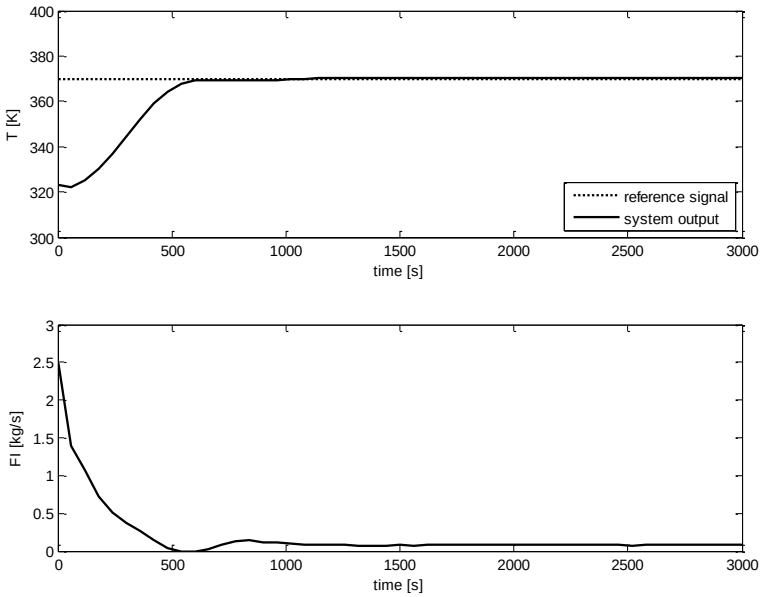

Fig. 4. Control of the semi-batch reactor using MPC4 controller

6. Comparison

The best representatives of the two different approaches were selected to be compared in this section. In order to describe the control error the criterion function S_y was defined:

$$S_y=\sum_{i=1}^{t_f}\left(y_r(i)-y(i)\right)^2 \tag{8}$$

T he criterion S_u describes the speed of the control signal changes. Monitoring of it is very important, because lifetime of the mud pump that injects the filter cake solution to the reactor would be significantly shortened due to steep changes of delivery.

$$S_u=\sum_{i=1}^{t_f}\left(u(i+1)-u(i)\right)^2 \tag{9}$$

The t_f defines number of steps for that are the criterions S_y and S_u computed. In this paper the t_f was set to 50 steps, because only the first 3000 seconds provide information about control. The dosing (control) commonly finishes shortly after 3000s and after that only cooling is performed.

For the reason that the plant is very exothermic and it is very sensitive to the exceeding of the desired value of the temperature (y_r = 370K), it was necessary to observe the maximum overshoot of the output value y_{max}. Furthermore, it is essential to observe the time of the reaction (dosing) t_b.

As can be seen from Table 3, the in-reactor temperature overshoots were in both cases quite similar. Nevertheless, the overshoot obtained by using SOMA algorithm is a little bit lower. As far as the criterion S_y, we need as low value as possible - the lower value the better. Even if the results were again close, the SOMA provided the lower value, which means that quality of the control was better too. The time of dosing achieved by SOMA was shorter approximately for one minute (58 seconds).

The only criterion which was better in MPC control was the S_u. Here the value 2.3200 is quite higher than 1.5500. For the actuating device it means higher loading and shorter lifetime.

	S_y	S_u	y_{max}	t_b
controller	K^2	$kg^2 \cdot s^{-2}$	K	s
SOMA7	$9.2571 \cdot 10^3$	2.3200	370.1740	3242
MPC4	$1.0333 \cdot 10^4$	1.5500	370.2358	3300

Table 3. Comparison of the controllers

7. Conclusion

The paper presented comparison of two approaches to semi-batch process model predictive control. Firstly, the Self Organizing Migrating Algorithm implemented in Mathematica software was used for cost function optimization. Secondly, as the comparative method model predictive controller implemented in Matlab was selected. This controller used built-in function fmincon from Matlab Optimization Toolbox instead of SOMA. It can be concluded that both algorithms provided applicable results. Nevertheless, SOMA provided slightly faster semi-batch process. What is more, the comparative method based on Matlab Optimization Toolbox required modification of the cost function in order to obtain appropriate control.

The comparison itself was made from four points of view. Firstly, the value of the in-reactor temperature overshoot and the related quality of the in-reactor temperature course were observed. Secondly, the time of processing which is important for effectiveness of a real plant and also the course of the actuating signal that is important from the practical point of view were monitored.

The paper showed that Self Organizing Migrating Algorithm successfully improved the control performance of the selected plant. It can be concluded that evolutionary algorithms should be considered as good way how to optimize control sequence in model predictive control, especially in case of complex nonlinear systems.

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