Semi-batch reactor predictive control using MATLAB fmincon function compared to SOMA algorithm

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Abstract: - In this paper the usability of the self-organizing migrating algorithm (SOMA) in a nonlinear system predictive control area is studied. Two approaches to model predictive control applied on a nonlinear system are compared here. Firstly, the SOMA was used to minimize the objective function, secondly, the *fmicon* function included in the MATLAB optimization toolbox was used for the same. 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 input data used here to simulate the process were obtained from the real chemical exothermic process.

Key-Words: - Semi-batch reactor; predictive control; MATLAB software; SOMA algorithm, nonlinear system, exothermic reaction

1 Introduction

Control of nonlinear systems brings challenges in the controller design. The current availability of powerful computing technologies enables application of complex computational methods. One of such complex method is also the self-organizing migrating algorithm (SOMA). This algorithm can be used for various optimization problems solving. Such optimization task to solve could be also the model predictive control (MPC). Here suitable algorithm minimizes an objective function which is based on the responses from a real system model and the real system itself. Minimizing the objective function using SOMA is studied here and the comparison with the MATLAB *fmincon* function minimization is also done to evaluate the SOMA control ability. Results obtained by the simulation means are than evaluated using suitable criterion which was defined for that purpose. The real process model on which the simulations are performed comes from leather waste recycling technology. Block diagram of this procedure named an enzymatic dechromation can be seen in the Figure 1.

An enzymatic dechromation is a waste free technology which 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 a strongly exothermic oxidation-reduction reaction which can be controlled by the chromium sludge (the waste produced by leather industry) into the hot reaction blend of chromium sulphate acid dosing [1]. The system itself, an exothermic semi-batch reactor, exhibits nonlinear behavior.

2 The nonlinear system to be controlled

2.1 Semi-batch process

As was already mentioned, the nonlinear system here represents the exothermic semi-batch reactor in which the chromium leather waste is recycled. 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 reactor is filled with initial filling given by the solution of chemicals without the chromium sludge (filter cake). The sludge is fed into the reactor 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

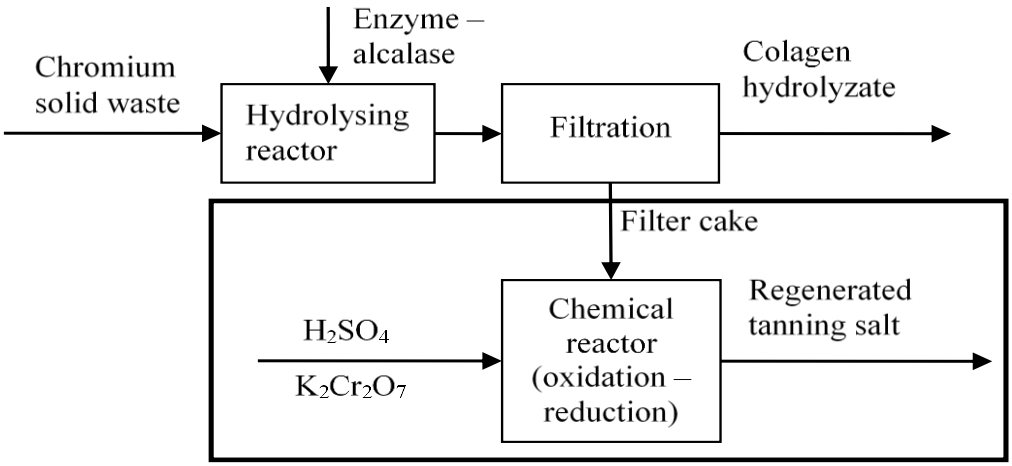

Fig. 1. Chromium waste recycling procedure

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.

2.2 System mathematical model

Based on the balanced equations (the mass and heat balance), system mathematical model was derived [2]. The equations describing the system are displayed here (Eq. 1-4):

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

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

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

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

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} are 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 are 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}, ΔHr = 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).

2.3 System constrains and other limits

The maximum reactor filling is limited by its volume to m = 2450 kg 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 373.15 K; this temperature value holds also for the coolant (water) but it is not so critical in this case as shown by further experiments.

3 Control of the system

Our nonlinear system here represents a chemical reactor. The state of art of chemical reactors control presents for example Luyben in [3] and [4], control and monitoring of batch reactors also describes Caccavale et al. in [5]. Generally, it can be stated that chemical reactors controllers use various control methods, such as PI controllers, adaptive control methods [6-8], robust approaches [9], predictive control and the like [10-19]. The model predictive control [20-22] [23-25] 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 [26-27]. Some review of the recent state can be found for example in [28].

3.1 Model predictive control

Two different approaches to the model predictive control of the given system are introduced in this paper. At first, the model predictive controller uses SOMA algorithm for the optimization of the control sequence. This methodology ensues from model predictive control method [29] while it uses same value of the control signal for whole control horizon in order to reduce computational demands of the controller. Secondly, the classic MPC controller, which uses Matlab Optimization Toolbox *fmincon* function, was used.

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 (Eq. 5) over a specified future time horizon [30]:

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

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 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 applied. 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.

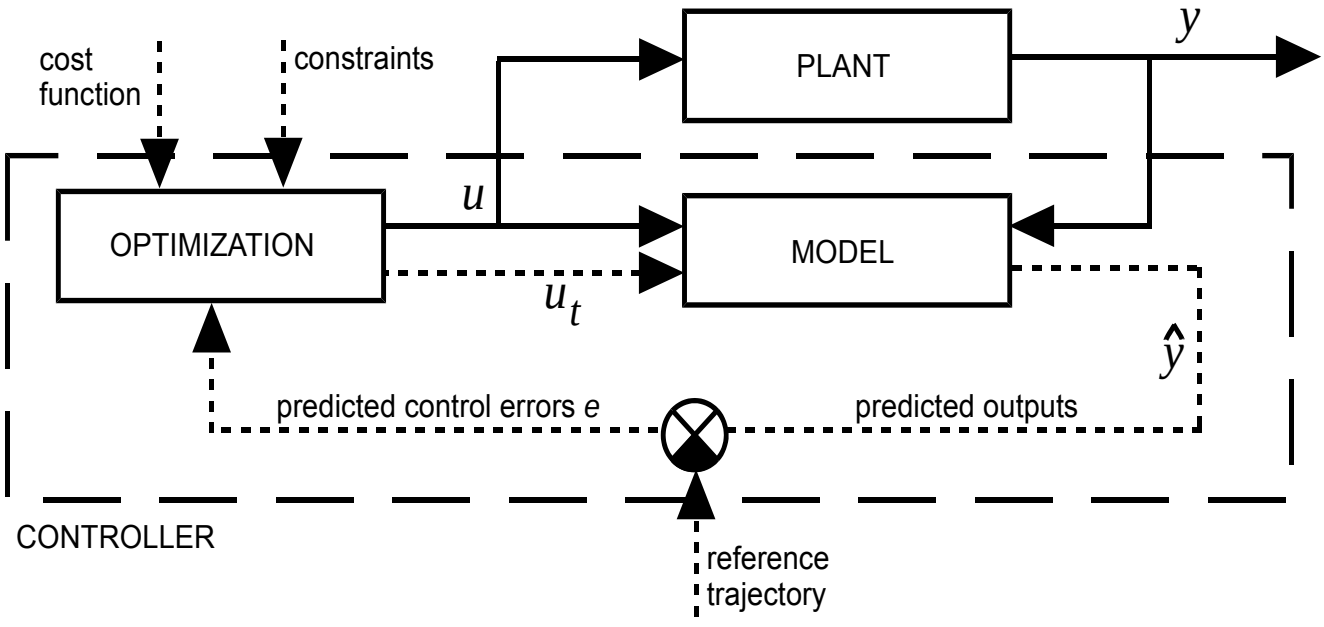

Fig. 2. Basic structure of the model predictive controller

3.2 Model predictive control using SOMA

3.2.1 SOMA algorithm

The Self-Organizing Migrating Algorithm (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.

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 [31-33], while interesting comparison to with simulated annealing and differential evolution is provided by Nolle et al. in [34].

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 socalled 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 [35]. 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. SOMA shows these attributes as well. Because of this, it is more appropriate to classify SOMA as a memetic algorithm.

3.2.2 SOMA simulations

Simulations 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 [35].

Seven different simulations using SOMA algorithm were performed. First three 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.

Table 1. SOMA controller settings.

	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

The control horizon (N_u) actually means the time interval, for which the actuating variable (F_1) 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 the lower value 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.

Graphical output of SOMA7 (the optimal settings) simulation is depicted in Figure 3. The two most important dependencies are here – the inreactor temperature and the chromium sludge

dosing development. As was already mentioned, the temperature has to stay under critical point 373.15 K. The chromium sludge dosing shouldn't embody any rapid changes.

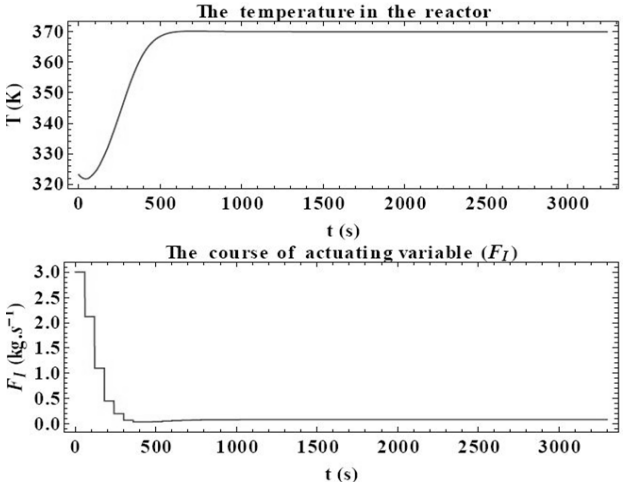

Fig. 3. Results of SOMA7 simulations.

3.3 Conventional MPC approach

This part was simulated using Matlab/Simulink, where the standard Matlab Optimization Toolbox function *fmincon* with receding control strategy was implemented. The *fmincon* function used trust-region-reflective algorithm [36].

To get the similar settings as in the SOMA case (the constant control action for the whole length of the control horizon N_u = 60), the sample time was set to 60s. The control horizon N_u and the prediction horizon N_2 were set to 10. The rest of the controller design remained same – the predictor was based on the white box model described by equations (1 – 4), objective function used by MATLAB was also the same (5).

The first set of simulations showed that the control did not provide acceptable results. The permanent control error and/or controlled variable overshoot where not satisfactory here. It was found that the problems were located mainly in the beginning of the control process. The controller took enormous control actions there. This strange behaviour was result of reaction kinetics and strongly exothermic reaction combination. Even small concentration growth of the chromium sludge (the increase in actuating variable) causes steep rise of the temperature, but the reaction kinetics can cause a response delay to the dosing.

To prevent this unwanted behaviour, new criterion based on the criterion (5) was defined. This enhanced criterion was able to penalize values of the control signal in the process start part. Also, at the same time the penalization has to decrease taperingly. The new enhanced criterion is described by equations (6-7) and the controller settings are placed in table 2.

Table 2. Matlab controller settings.

	λ	ρ	γ	γ_c	N_1	N_2	N_u
MLB1	1	100	0	0	1	10	10
MLB2	1	100	2000	100	1	10	10
MLB3	1	100	2000	200	1	10	10
MLB4	1	100	1500	100	1	10	10

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

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

The parameter γ_c defines here the speed of the decrement in γ. In this way we can influence the speed of the chromium sludge dosing, the actuating value. We can say that γ parameter defines penalization of the control signal, while the ratio γ/γ_c specifies the length of the penalization interval. Too high γ parameter or γ/γ_c ratio caused delays or oscillations (the settings MLB2 in Table 2). On the other hand, small γ/γ_c ratio led to overshoots of the temperature (the settings MLB3 in Table 2). The best result obtained using this approach was obtained for MLB4 settings and is displayed in Figure 4.

3.4 Results comparison

Results of the best SOMA and MATLAB simulations were selected for the comparison. To compare the control error, the criterion function S_y was defined (Eq. 8):

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

Other criterion S_u (Eq. 9) was defined to monitor the speed of the control signal changes. From the practical view, the monitoring of it is very important, because lifetime of the mud pump

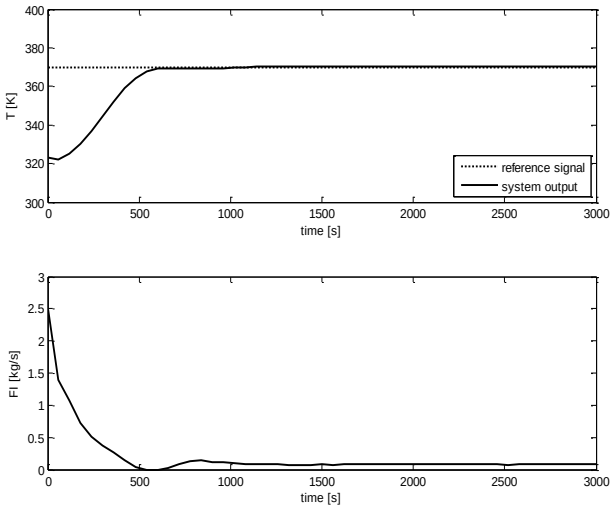

Fig. 4. MATLAB simulations results.

(actuator) that injects the chromium sludge to the reactor would be shortened significantly in case of steep changes.

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

The number of steps computed for the criterions S_y and S_u is defined by t_f and was set to 50 steps.
Observed were also the maximum overshoot of the output value y_{max} and the time of the reaction (dosing) t_b.

For the reason that the plant is strongly 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 (chromium sludge dosing) t_b. The heating up and maintaining the system temperature usually takes about 3000s and after that only cooling is performed.

In fact, there was not significant difference in the temperature overshoots between the SOMA and MATLAB, they were quite similar. Anyway, as can be seen in Table 3 the result obtained by SOMA was a bit better. Also the results provided by criterion S_y were in both cases close. The lower value is better value in case of S_y and again the SOMA control quality prevailed. The time of dosing achieved by SOMA was shorter approximately for one minute (58 seconds).
On the other hand, the MATLAB gave better results for the S_u criterion. The SOMA value 2.3200 was higher than the 1.5500 MATLAB value. The actuating device would last longer without servicing in MATLAB case.

Table 3. Final comparison.

	S_y [K^2]	S_u[kg^2·s^{-2}]	y_{max}[K]	t_b[s]
SOMA7	$9.257 \cdot 10^3$	2.3200	370.174	3242
MLB4	$1.033 \cdot 10^4$	1.5500	370.236	3300

4 Conclusion

Both the SOMA and MATLAB were able to control our complex nonlinear process here, but there were some differences. A surprising difference emerged when the MATLAB was not able to provide satisfactory control results using the same objective function as SOMA algorithm did. The controlled variable (the in-reactor temperature) showed an overshoot unfortunately. That is why the purpose function had to be changed for the MATLAB simulations. After this change, the comparison was made from four points of view. Firstly, the value of the in-reactor temperature overshoot and the related quality of the inreactor 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. Although the results were similar, SOMA showed generally better results than MATLAB. The results show that the nonlinear system can be successfully controlled by evolutionary algorithms.

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