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OPTIMIZATION AND EVOLUTIONARY CONTROL OF CHEMICAL REACTOR

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ABSTRACT
This work deals with using of evolutionary algorithm SOMA for static optimization of a batch reactor for the purpose to improve its behavior in uncontrolled state and for its subsequent evolutionary predictive control. The main aim of this work is to show that evolutionary algorithms are capable of successful optimization of very difficult and complex engineering problems. The importance of this problem is increasing with growing demand for special products made in batch reactors. The optimization gave the best solution, which markedly improved the performance of the reactor in comparison with original expert setting of reactor parameters. The optimized reactor was used in a simulation with predictive control by the evolutionary algorithms and excellent results were achieved
Keywords: Optimization, Evolutionary Algorithm, Control

1. INTRODUCTION
The optimization of batch processes has attracted attention in recent years [1,2] because it is a natural choice for reducing production costs, improving product quality, meeting safety requirements and environmental regulations. A wide variety of special chemicals, pharmaceutical products, and certain types of polymers are manufactured in batch operations. Batch processes are typically used when the production volumes are low, when isolation is required for reasons of sterility or safety, and when the materials involved are difficult to handle. From a process systems point of view, the key feature that differentiates continuous processes from batch and semi-batch processes is that continuous processes have a steady state, whereas batch and semi-batch processes do not [3,4].

2. DESCRIPTION OF THE REACTOR
The reactor has two physical inputs and one output (See Fig.1). Chemical FK (filter cake) flows into the reactor through the input denoted "Chemical FK", with parameters temperature-T_{FK}, mass flow rate-$\dot{m}_{FK}$ and specific heat-c_{FK}. The coolant flows into reactor through the second input denoted "Cooling medium", which is usually water of temperature T_{VP}, mass flow rate-$\dot{m}_V$ and specific heat-c_V. Cooling medium flows through the jacket inner space of the reactor, with volume related to mass-m_{VR}, and flows out through the second output, with parameters mass flow rate m_V, temperature-T_V and specific heat-c_V. At the beginning there is an initial batch inside the reactor with parameter mass-m_P. The chemical FK is then added to this initial batch, so the reaction mixture has total mass-m, temperature-T and specific heat-c_R, and also contains partially unreacted portions of chemical FK with concentration a_{FK}. The main aim of optimization is to achieve the processing of large amount of chemical FK in a short time. In general, the reaction which takes place in the reactor is highly exothermal. Hence, the most important parameter is the temperature of the reaction mixture. This temperature must not exceed 100°C because of safety aspects and product quality. The design of the reactor was based on standard methods and gives a proposal of reactor physical dimensions and parameters of chemical substances. These values are called expert parameters.

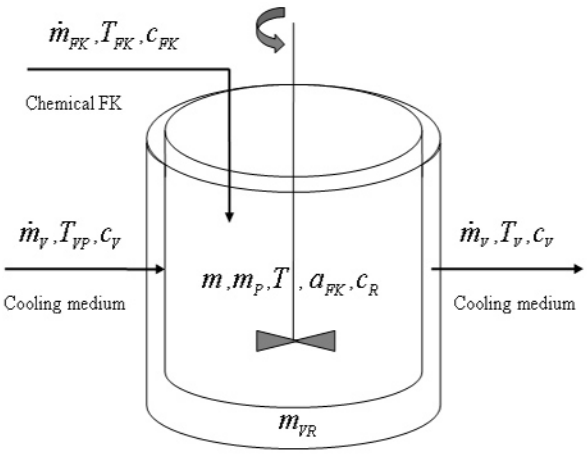

Figure 1. Scheme of reactor

2.1. Non-linear model of the reactor

Description of the reactor applies a system of four balance equations (1). The first expresses a mass balance of reaction mixture inside the reactor, the second a mass balance of the chemical FK, and the last two formulate enthalpic balances, namely balances of reaction mixture and cooling medium. Equation (2) represented by term "*k*", is written out here for simplified notation of basic equations (1).

$$\dot{m}_{FK} = m'[t] \tag{1}$$

$$\dot{m}_{FK} = m[t]\ a'_{FK}[t] + k\, m[t]\, a_{FK}[t]$$

$$\dot{m}_{FK} c_{FK} T_{FK} + \Delta H_r k\, m[t]\, a_{FK}[t] = K\, S\, (T[t] - T_V[t]) + m[t] c_R\, T'[t]$$
$$\dot{m}_V c_V T_{VP} + K\, S\, (T[t] - T_V[t]) = \dot{m}_V c_V T_V[t] + m_{VR} c_V\ T'_V[t]$$

$$k = A e^{-\frac{E}{RT[t]}} \tag{2}$$

3. STATIC OPTIMIZATION

The reactor described above, in the original set-up, gives unsatisfactory results. Concretely duration of one batch cycle is approx 25 000 sec and temperature of reaction mixture-*T* markedly exceeds the critical limit of 100°C (373.15 K). To improve reactor behavior, static optimization was performed using the algorithm SOMA [5]. In this optimization the point was to minimize the area arising as a difference between the desired and real temperature profile of the reaction mixture in a selected time interval. The required temperature was 97°C (370.15 K). The cost function that was minimized is given in (3), minimizing term which limits the maximum mass of one batch in (4). The optimization was repeated ten times to show and check robustness of used method.

$$f_{\cos t} = \sum_{t=0}^{t_1} |w - T[t]| + \sum_{t=0}^{t_1} a_{FK}[t] + pen.1 + pen.2 \tag{3}$$

$$pen.1 = \begin{cases} 0 & Max(T[\tau]) \le 323{,}15 \\ 50000 & else \end{cases} \quad \text{For } \tau \in \langle t_2, t_3 \rangle$$

$$pen.2 = \begin{cases} 0 & Max(T[\tau]) \le 373{,}15 \\ 50000 & else \end{cases} \quad \text{For } \tau \in \langle 0, t_3 \rangle$$

Where the time intervals were set for example as t_1 = 15000 s; t_2 =20000 s; t_3 =25000 s.

$$m[\mathrm{t}] \le m_{max} \tag{4}$$

This optimization proceeded with parameters shown in Tab. 1.

Table 1. Optimized parameters and comparison with expert set up

Parameter	Range	Expert setting	Optimized
$\dot{m}_{FK}$ [kg.s^{-1}]	0 - 640	0 - 3	0,1021
T_{VP} [K]	273.15 - 323.15	293.15	274.58
$\dot{m}_{V}$ [kg.s^{-1}]	0 - 10	1	4,67
m_{VR} [kg]	0 - 220	220	1159.7
d [m]	0.01 - 0.2	0.03	0.096
r [m]	0.5 - 2.5	0.78	1.017
h [m]	0.5 - 2.5	1.11	1.382
S [m^2]	-	7.35	12.08
V [m^3]	-	2.12	4.49
m_{p} [kg]	-	1810	3842.4
m_{FK} [kg]	-	640	1361.4

The results of optimization are shown in Fig.2. From these results it is obvious that the temperature of reaction mixture (RM) has moderately exceeded the critical value, but this was a simulation of uncontrolled reactor. This can be corrected by quality control of the batch process. Another fact not to be neglected is the shortened duration of the process and the improvement of reactor performance compared with the reactor set up by an expert (see Tab. 1).

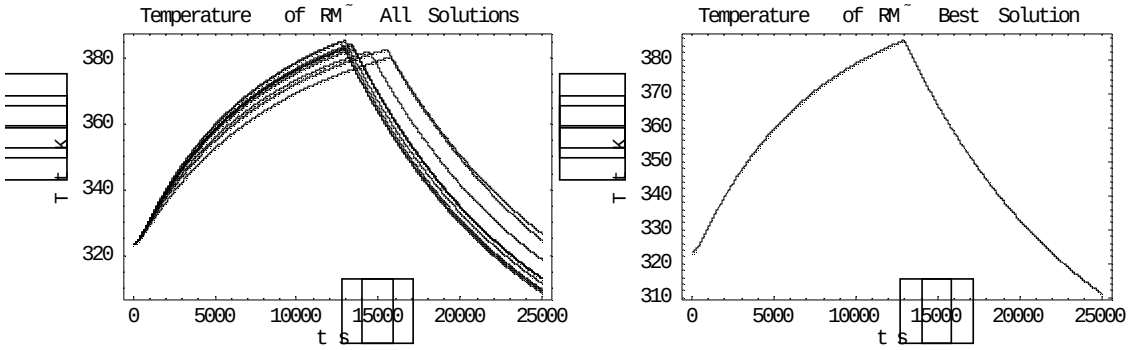

Figure 2.a) Results of static optimization b) The best solution – optimized reactor

4. EVOLUTIONARY CONTROL OF THE REACTOR

The main aim was the successful predictive control of optimized reactor by means of evolutionary algorithms. In this case the method was based on the control of the temperature by the controlled feeding of the input chemical FK - $\dot{m}_{FK}$ in range 0 - 5 [kg.s^{-1}]. The desired temperature was 96.85°C (370 K).The scheme of used control method is depicted in Fig. 3 and the cost function that was minimized is given in (5). Parameter set up for the control law was following N_1 = 1, N_2 =150 and N_u = 60. For results of predictive control see Fig.4.

$$J(N_1, N_2, N_u) = \sum_{j=N_1}^{N_2} [y(k+j) - w(k+j)]^2 + \sum_{j=1}^{N_u} \lambda(j)[\Delta u(k+j-1)]^2 \qquad (5)$$

Where: N_1 - Minimal prediction horizon, N_2 - Maximal prediction horizon, N_u - Control horizon,
λ - Weight for sequence of control actions

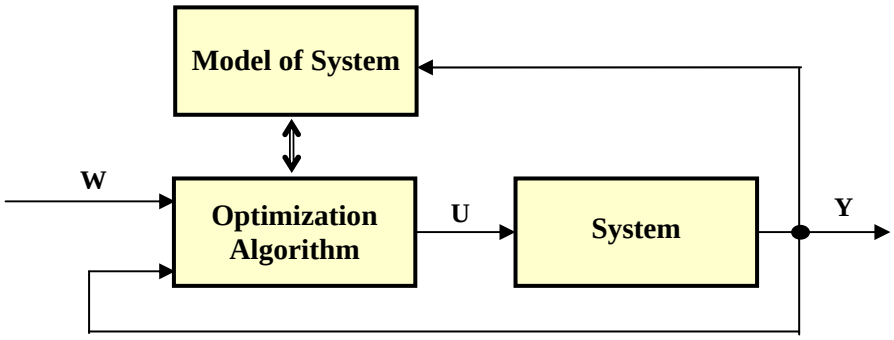

Figure 3. Predictive control scheme

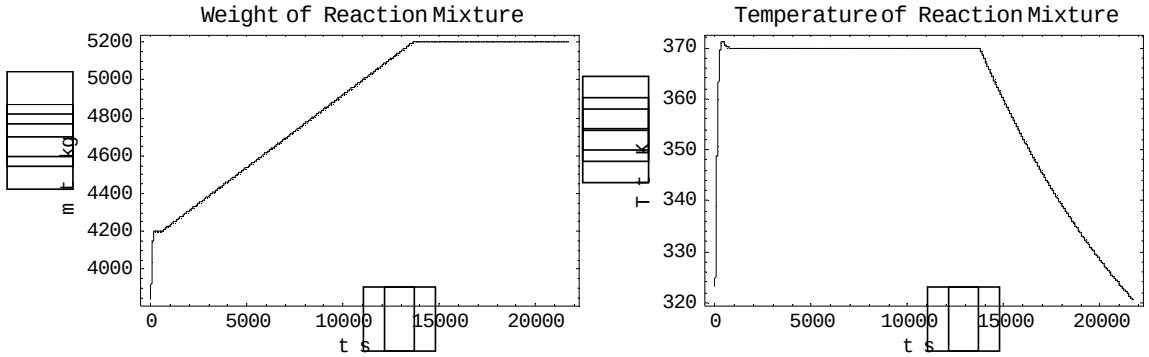

Figure 4.a) Results for predictive control - weight of RM b) Temperature of RM

5. CONCLUSION

Basic optimizations presented here were based on a relatively simple functional. For future research there is no problem in defining more complex functional including as subcriteria e.g., stability, costs, time-optimal criteria, controllability, etc. or their arbitrary combinations. Finally, on the basis of presented results it may be stated that the reactor parameters have been found by optimization which demonstrates performance superior to that of reactor set up by an expert. The optimized reactor was used in a simulation with predictive control by evolutionary algorithms and excellent results were achieved. Primarily the duration of batch cycle is shortened from 25000 s to 21000s and temperature does not exceed the restriction limit on whole simulation interval.

6. ACKNOWLEDGEMENT

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