OPTIMIZATION AND CONTROL OF BATCH REACTOR BY EVOLUTIONARY ALGORITHMS

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ABSTRACT

This work deals with using a method of artificial intelligence, namely the evolutionary algorithm SOMA, for static optimization of a chemical batch reactor, for the purpose to improve its behavior in uncontrolled state and predictive control. The importance of this problem is increasing with growing demand for special products made in batch reactors. The optimizations has been performed in several ways, each one for another set of reactor parameters or another cost function. The optimization gave the best solution, which improved the performance of the reactor. All the important results of each optimization are discussed continuously and at the end of the paper too. The optimized reactor was used in a simulation with predictive control by the evolutionary algorithms and excellent results were achieved.

INTRODUCTION

Chemical industry produces a whole range of products through physical and chemical reactions. Successful mastering of the chemic-technological process requires its quantitative and qualitative assessment. This is particularly necessary in the cases where an introduction of automatic control systems of technological procedures is under consideration. In order to prevent computer-control modernization of existing and future processes becoming an end in itself, it is necessary to proceed in individual stages.

The most important stage is an analysis of the manufacturing system, which in most cases comprises simulating calculations based on a realistic understanding of physic-chemical mechanisms through which initial raw materials are converted into the required product. These calculations then reveal key points of the technological process which by their nature enforce changes and adjustments of the technological procedure so that potential automation produces the required effect, i.e. a quality product at minimal production costs.

Generally it may be stated that key technological points are chemical reactors. Designing optimal reactor parameters including control constitutes one of the most complex tasks in process engineering. The situation is particularly complicated by the fact that the precise mechanism of chemical reaction kinetics is very often unknown. For this reason it is necessary to carry out extensive measurements of input and output concentration dependencies of components on time, temperature, etc. These quite complex kinetic models, verified of course by experimental measurements, are subsequently linearized employing various methods, which enables to apply already developed control methods to these models.

Disregarding the petrochemical field, attention of chemical industry is mostly given to raw materials for producing macromolecular materials, i.e. plastics. High-molecular compounds arise through two types of reactions, polymeration and polycondensation. What is essential for designing algorithms controlling such reactions is the fact that the majority of these reactions are exothermic, i.e. releasing heat. From the viewpoint of economy, productivity of the chemical reactor is usually demanded to be in a certain respect maximal, and final-product quality to be as required. Reactor productivity depends on reaction rate, which usually increases exponentially with increasing temperature.

At first sight it seems that an exothermal character of a reaction is very advantageous. This conclusion is true to a certain extent, nevertheless, as with all, it also has limitations regarding both safety and quality (e.g. product quality may be degraded with increased temperature).

This is particularly true if the main reaction is accompanied with undesired side reactions whose rates also increase exponentially with temperature. Hence, it is apparent that the principal controlled quantity in exothermal reactions is temperature of reaction mixture. Therefore, models presented in this work are based on entalpic balances enabling relevant simulations.

Characteristics of batch processes

The optimization of batch processes has attracted attention in recent years (Aziz et al. 2000), (Silva et al. 2003) because, in the face of growing competition, it is a natural choice for reducing production costs, improving product quality, meeting safety requirements and environmental regulations. Batch and semi-batch processes are of considerable importance in the fine chemicals industry. 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

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low, when isolation is required for reasons of sterility or safety, and when the materials involved are difficult to handle. In batch operations, all the reactants are charged in a tank initially and processed according to a pre-determined course of action during which no material is added or removed. In semi-batch operations, a reactant may be added with no product removal, or a product may be removed with no reactant addition, or a combination of both. 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 (Srinisavan 2000 et al. 2002a and 2000b)

DESCRIPTION OF REACTOR

This work used a mathematical model of reactor shown in Fig.1. This chemical reactor was designed for chemic-technological process of leather manufacturing waste processing, which is a huge ecologic problem world-wide. Successful determination of the reactor optimal parameters and improved control of the whole process will help to elaborate a propose of technological plant, which will be able to satisfy economical and quality requirements.
The reactor has two physical inputs (one for chemical substances and one for cooling medium) and one output (cooling medium). Equations (1) and (2) represent the mathematical model of the reactor.

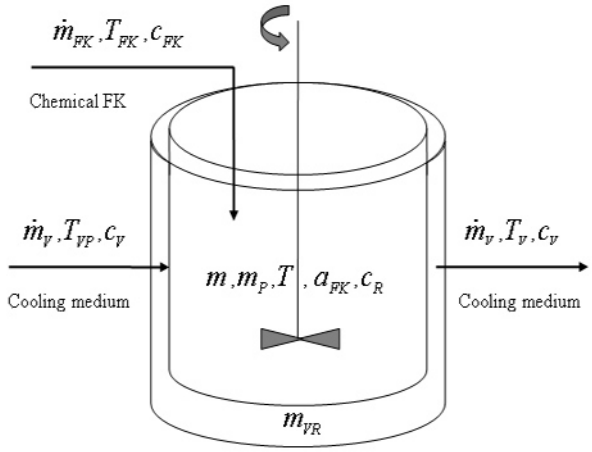

Fig.1 Scheme of reactor

Chemical FK flows into the reactor through the input denoted “Chemical FK”, with parameters temperature T_{FK}, mass flow rate 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 m_V and specific heat c_V.
Cooling medium flows through jacket inner space of reactor, with volume related to mass flow rate m_{VR}, and flows out through second output, with parameters mass flow rate m_V, temperature T_V and specific heat c_V.
At the beginning of the process 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 inside the reactor has total mass m, temperature T and specific heat c_R and also contains partially unreacted portions of chemical FK described by parameter concentration a_{FK}.
This technique partially allows controlling the temperature of reaction mixture by the controlled feeding of the input chemical FK
The main objective of optimization is to achieve the processing of large amount of chemical FK in very short time. An exothermal reaction described by relationships (1) – (3) takes place in the reactor.
In general, this reaction 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 quality of processing,
Designing the reactor was based on standard chemical-technological methods and gives a proposal of reactor physical dimensions and parameters of chemical substances. These values are called in this work **expert parameters**. The objective of this part of the work was to perform a simulation and optimization of the given reactor.

Non-linear model of reactor

Description of the reactor applied a system of four balance equations (2). 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 entalpic balances, namely balances of reaction mixture and cooling medium. Equation (1), in which (2) is represented by term “k”, is written out here for simplified notation of basic equations.

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

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

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

$$\dot{m}_V c_V T_{VP} + K\, S\,(T[t] - T_V[t]) = \dot{m}_V c_V T_V[t] + m_{VR} c_V\, T'_V[t]$$

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

After modification into standard form, balance equations are obtained in form (3)

$$m'[t] = \dot{m}_{FK} \tag{3}$$

$$a'_{FK}[t] = \frac{\dot{m}_{FK}}{m[t]} - A\, e^{-\frac{E}{RT[t]}}\, a_{FK}[t]$$

$$T'[t] =$$

$$= \frac{\dot{m}_{FK} c_{FK} T_{FK}}{m[t] c_R} + \frac{A\, e^{-\frac{E}{RT[t]}}\, \Delta H_r\, a_A[t]}{c_R} - \frac{K\, S\, T[t]}{m[t] c_R} + \frac{K\, S\, T_V[t]}{m[t] c_R}$$

$$T'_V[t] = \frac{\dot{m}_V T_{VP}}{m_{VR}} + \frac{K\, S\, T[t]}{m_{VR} c_V} - \frac{K\, S\, T_V[t]}{m_{VR} c_V} - \frac{\dot{m}_V T_V[t]}{m_{VR}}$$

Parameters for this reactor and initial conditions (a_{FK0}, T_{V0}, T_0, m_0,….) have been specified by expert, giving both physical dimensions as well as parameters of individual chemical substances. These were used to simulate the behavior of this reactor. It is evident from Fig.2, that reactor behavior in compliance with parameters thus specified by expert is not quite satisfactory during the processing of one batch. The duration of the processing of one batch is given by the time from the start of the process till the reaction mixture cools down to its initial temperature T_0.
The behavior of the reactor was simulated using five different values of batching the chemical FK into the reaction mixture (from the range of 0 – 3 $kg.s^{-1}$).
$\dot{m}_{FK}$ = (0,05 (violet) ; 0,1 (green) ; 0,5 (blue) ; 1 (red) ; 3 (black)) $kg.s^{-1}$.

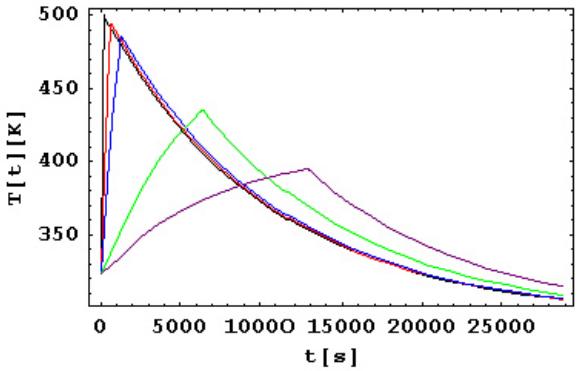

Fig.2 Behavior of the reactor set up by means of expert parameters

Facts that follow from the simulation of this strongly exothermal reaction are as follows:

1. Duration of one batch cycle is approx 25 000 sec

2. Temperature of reaction mixture T markedly exceeds critical limit of 100°C (373,15 K), even in case of simulation with lowest value of batching chemical FK into the reactor.

As these are very serious, multifold repeated static optimizations by means of SOMA algorithm has been performed, and this led to finding the reactor parameters with which the reactor behavior is much more acceptable.

Optimizing algorithm

Optimization algorithms are a powerful tool for solving many problems in engineering practice. They are usually applied when solving a given problem analytically is impossible or unrealistic. When properly implemented, they can be employed in such manner that even frequent user's intervention in work of the respective plant where they are applied is unnecessary.
This contribution consider the use of optimization algorithm SOMA. Numerous results have shown SOMA is a viable algorithm that can be used to solve many practical as well as theoretical problems. (Zelinka 2004)

STATIC OPTIMIZATION OF REACTOR

The reactor described above, in the original set-up, gave unsatisfactory results. To improve reactor behavior, static optimization was performed using the algorithm SOMA. The optimization was performed by the following three basic methods.

1. Optimization of batching value $\dot{m}_{FK}$
2. Optimization of batching value $\dot{m}_{FK}$ together with process parameters of the cooling medium
3. Optimization that covered all previous optimized parameters, and including also optimization of reactor geometry and cooling area.

Each optimization was repeated ten times just in case, and separate figures present time plots of all important variables collected together in order to emphasize optimizing robustness, including courses of time evolutions from all ten simulations. The behavior of the best reactor was shown with the last optimization. A discussion on particular optimization cases follows in the sections below.

Optimization of batching value

In this optimization the point was to minimize the area arising as a difference between the required and real temperature profile of the reaction mixture in a selected time interval, which was the duration of a batch cycle. The required temperature was 97°C (370,15 K). The cost function that was minimized is given in (5), minimizing term which limits the maximum mass of one batch in (6)

$$f_{cost} = \sum_{t=0}^{t} \left| w - T[t] \right| \tag{5}$$

$$m[t] \leq m_{max} \tag{6}$$

The simulation results are presented in Fig.3. The optimization algorithm obviously found the best value for batching so that the critical temperature was not exceeded. Nevertheless, the duration of the batch cycle was not shortened so the performance of the reactor could not be improved without more effective cooling of the reaction mixture. Thus the next step was the second optimization covering process parameters of the cooling medium, but preserving the geometry of the reactor.

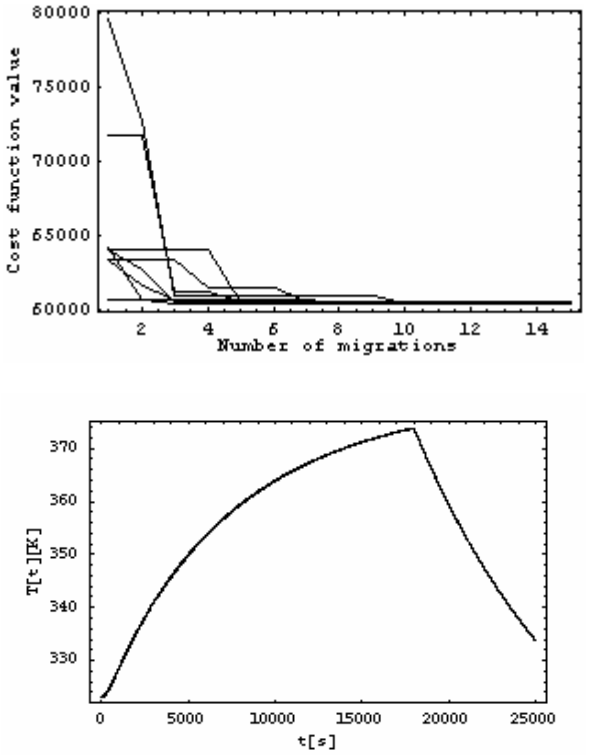

Fig.3 Results of optimization of batching value

Optimization of batching value and process parameters of cooling medium

Optimization proceeded in the second case with the parameters that are shown in Tab.1.
The actual functional that was minimized was the same as in the first case (5), minimizing term also the same as in previous case, which limits the maximum mass of one batch, is presented in (6). Another restriction terms were the ranges of optimized parameters (see Tab. 1.).
The results of simulations are presented in Fig.4. As can be seen, this optimization again found a good value for batching so that the critical temperature was not exceeded. Nevertheless, the opposite consequence was reached than required shortening duration of batch cycle and increasing the performance of reactor. The optimization found a relatively high value of the input cooling medium temperature. That essentially means that chemical reaction was started faster and required temperature was reached in shorter time. This fact corresponds to the selected minimization functional (5), but on the other side cooling of reaction mixture was very slow after filling up the reactor and thus termination of reaction. As a result of these facts the third optimization included the optimization of reactor geometry and the minimized functional had to be changed to achieve reasonable balance between the demands of fast start of chemical reaction, critical temperature and fast cooling to initial temperature and hence to increase the performance of reactor.

Tab.1 Optimized reactor parameters

Parameter	Range
$\dot{m}_{FK}$ [kg.s^{-1}]	0 – 640
T_{VP} [K]	253,15 – 323,15
$\dot{m}_{V}$ [kg.s^{-1}]	0-10

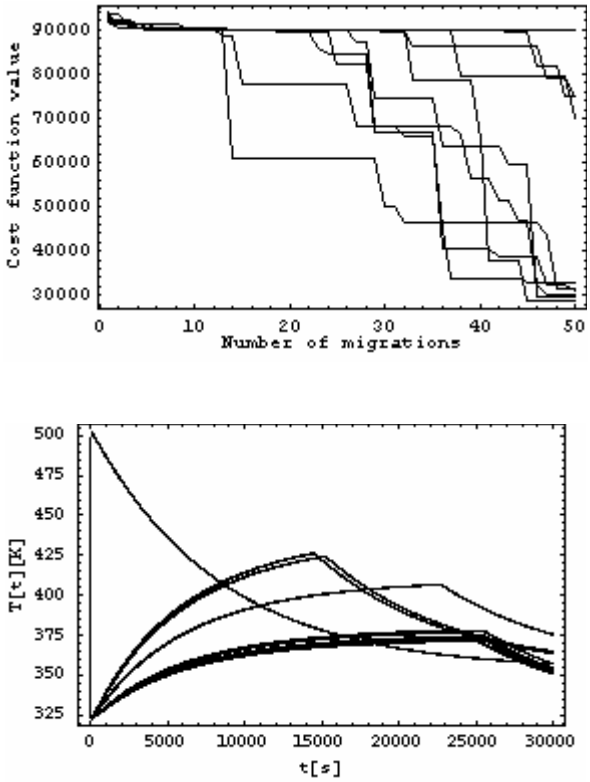

Fig.4 Results of optimization of batching value and process parameters of cooling medium

Optimization of process parameters and the reactor geometry

This optimization proceeded with parameters that are shown in Tab.2.

Tab.2 Optimized reactor parameters

Parameter	Range
$\dot{m}_{FK}$ [kg.s^{-1}]	0 – 640
T_{VP} [K]	273,15 – 323,15
$\dot{m}_V$ [kg]	0 – 10
m_{VR} [kg]	220
r [m]	0,5 – 2,5
h [m]	0,5 – 2,5

As a result of last two simulations the actual functional that was minimized was changed to (7). It was divided into three time intervals and also two penalizations (8) and a special part were added. This special part ensures rapid reaction of the whole batch of chemical FK hence very low value of concentration a_{FK} of partly unreacted portions of chemical FK in reaction mixture.
The first penalization helps to find solutions in which the temperature of reaction mixture cools down fast to its initial state, and the process duration is shortened. The second corresponds to the critical temperature condition.

$$f_{\cos t} = \sum_{t=0}^{t_1} |w - T[t]| + \sum_{t=0}^{t_1} a_{FK}[t] + pen.1 + pen.2 \qquad (7)$$

$$pen.1 = \begin{cases} 0 & Max(T[\tau]) \le 323{,}15 \\ 50000 & else \end{cases}$$
$$\text{for } \tau \in \langle t_2, t_3 \rangle \qquad (8)$$

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

where the time intervals were set for example as:
t_1 = 15000 s; t_2 =20000 s; t_3 =25000 s
The minimizing term, presented in (6), is also the same as in the previous case, which limits the maximum mass of one batch. Another restriction terms were the ranges of optimized parameters (see Tab. 2.). Moreover, many parameters were interrelated due to the optimization of the reactor geometry. The relation between m, m_{FK} and m_P was given by relationship (9).

$$m = m_p + m_{FK} \qquad (9)$$

The stechiometric ratio is given by (10).

$$m_P = 2{,}82236 m_{FK} \qquad (10)$$

The relationship between the optimized volume of reactor and the mass of added chemical FK is given by (11). Then substituting to (10) gives the mass of initial batch in reactor.

$$m_{FK} = \frac{\rho_p \rho_{FK} V}{2{,}82236 \rho_{FK} + \rho_p} \qquad (11)$$

The results of this optimization are shown in Figs.5 and 6. Fig.6 demonstrates the behavior of a selected reactor where predictive control was applied using algorithm SOMA. From these results it is obvious that the temperature of reaction mixture moderately exceeded the critical value, but this was a simulation of uncontrolled reactor. This can be corrected by a quality control of the batch process. Another fact not to be neglected is the shortened duration of process and the improvement of reactor performance compared with the reactor set up by an expert (see Tab.3).

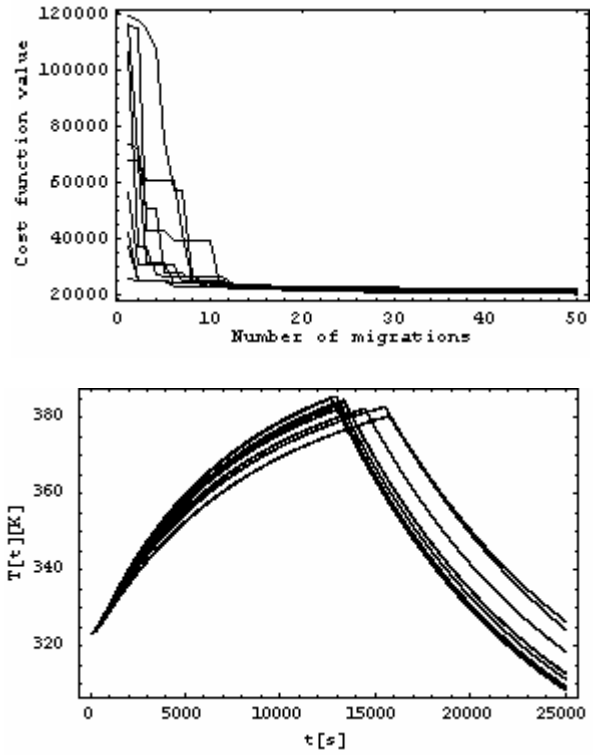

Fig.5 Results of optimization of process parameters and reactor geometry

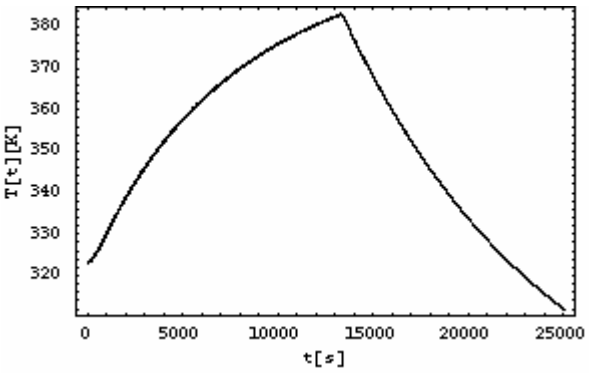

Fig.6 Reaction mixture temperature profile for the best optimized reactor

CONCLUSION

This report describes a chemical reactor (Fig.1). After a general introduction and description of chemistry of the relevant reaction, this part discusses a nonlinear model constructed on the basis of physic-mathematical analysis
(equations (1–3) including an illustrations of reactor behavior based on parameters set up by an expert (see Fig.2)).
Based on the obtained results, it may be claimed that the behavior of an uncontrolled reactor gives quite unsatisfactory results, which may be overcome through static optimization of a given reactor. The quality of results produced by the optimizations depends not only on the problem being solved but also on how a given functional is defined. Its construction may comprise not only optimization of a basic criterion but also optimization of subcriteria capable of improving optimization quality.
Basic optimizations presented here were based on a relatively simple functional. Unless the experimenter is limited by technical issues when searching for optimal parameters, there is no problem in defining more complex functional including as subcriteria e.g., stability, economic costs, time-optimal criteria, controllability, etc. or their arbitrary combinations. However, complexity of such functional indirectly implies the application of advanced software such as Mathematica or Matlab.
The advantage of parallel optimization (in the context of evolutionary algorithms – i.e. "simultaneously" seeking X possible solutions and selecting the best) lies in the fact that unless an optimal solution is found, one usually obtains suboptimal solutions, which are usually not too distant from the true optimum.
Differences between both reactors are best to be seen in Tab.3. The first part shows the parameters of reactor designed by an expert, and the second part shows the parameters obtained through static optimization. In Tab.3, the internal radius of reactor is expressed in parameter r and is related to cooling area "S" The parameter d represents the distance between the outer and inner jacket and the parameter h represents the height of the reactor. The meaning of the other parameters is quite obvious from the table.

Tab.3 Difference between reactor designed by an expert and the optimized reactor

Parameter	Expert setting	Optimized
$\dot{m}_{FK}$ [kg.s^{-1}]	0 - 3	0,1021
T_{VP} [K]	293,15	274,58
$\dot{m}_{V}$ [kg]	1	4,67
m_{VR} [kg]	220	1159,7
d [m]	0,03	0,096
r [m]	0,78	1,017
h [m]	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

Finally, on the basis of presented results it may be stated that the reactor parameters has been found by optimization which demonstrates performance superior to that of reactor set up by an expert.

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