Evolutionary Strategy for Feeding Trajectory Optimization of Fed-batch Reactors

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Abstract: Safe and optimal operation of complex production processes is one of the most important research and development problems in process engineering. This problem is the most relevant at the design of the optimal feeding profile of fed-batch chemical reactors due to the nonlinear and unstable dynamical behavior of the processes. This paper shows that how the optimal feeding policy can be determined in fed-batch reactors by sequential quadratic programming, classical evolutionary strategy (ES) and the advanced version of ES that is based on covariance matrix adaptation. A multi-objective function was created and the search space was constrained in case of all of the three applied algorithms. The switching times between states in the feeding trajectory and the feed rates in each state were manipulated to find the global minima of the objective function. To obtain the optimal feeding policy the first-principle model of a pilot fed-batch reactor was implemented in MATLAB and applied as a dynamic simulator of the process. Off-line optimization process was carried out in case of different dosing time distribution. As the results show a significant improvement can be achieved in process performance applying advanced ES based optimization algorithms to generate feeding trajectories.

Keywords: optimization, fed-batch reactor, quadratic programming, evolution strategy

1   Introduction

As optimal operating conditions of production processes are getting closer and closer to physical constraints, the development of knowledge based expert systems for supporting the operators to keep the operating conditions in this narrow range becomes more and more important [1, 2].

This problem is the most relevant at the design of the optimal feeding profile of fed-batch chemical reactors due to the nonlinear and unstable dynamical behavior of the involved processes, because in case of exothermic reactions thermal runaway can also occur [3-6]. Reactor runaway means a sudden and considerable change in the process variables that is a serious problem in many industrial

chemical processes, like oxidation and polymerization. For example in case of a highly exothermic reaction thermal runaway occurs when the reaction rate increases due to an increase in temperature, causing a further increase in temperature and hence a further increase in the reaction rate while the reactants are depleted.

Unfortunately the systems with low complexity are rare in production process, hence the analytical determination of optimal operation variables is rather complicated or in some cases it is impossible. An excellent summary of problems of the operation of batch and fed-batch reactors can be found in [7], where the author focuses on the safety, the product quality and the scale-up. To calculate the optimal temperature profile or the optimal feeding policy in such system a lot of optimization algorithm can be applied. Particle Swarm Optimization (PSO) algorithm is applied to estimate the optimal control feeding profile in a fed-batch fermentation process where heat effects have less importance in the changes of state-variables and cubic splines are used instead of linear ones to design a more smooth operation [8]. Different algorithms belonging to three main groups - Evolutionary Algorithms (EA), PSO and Differential Evolution (DE) - are applied to solve the same optimization problem and compared based on their performance in [9]. It is shown that PSO is the worst choice from the group of the compared optimization algorithms while they suggest applying DE algorithms instead of EA because of the fast convergence. These methods can be applied in those cases when the time of calculation is not an important aspect, e.g. to solve off-line or batch-to-batch optimization problems.

In this paper three optimization algorithms are used for the estimation of optimal feeding trajectory for a pilot-plant fed-batch reactor and the reached optimization performances are shown and compared at different distribution of feeding time. The paper is organized as follows: in Section 2 the applied optimization methods are briefly introduced; it is followed by the introduction of the investigated pilot-plant fed-batch system and its mathematical model. Further sections show the results and the comparison of optimization algorithms.

2   Applied Optimization Techniques

In these days sequential quadratic programming (SQP) methods are routinely applied to solve practical nonlinear programming problems. SQP methods are stabilized by a monotone line search procedure subject to a suitable merit function. In each iteration step of the SQP algorithm the solution of the quadratic program (QP) must be found. That makes the complex optimization problem simpler. The optimization algorithm has a quadratic objective function and applies linear constraints for manipulated variables. The SQP algorithm converges very rapidly, therefore it requires few iterations (hence few QP solutions) to find an

approximate solution with a good precision. The accuracy can be improved by using second derivatives in QP. The SQP algorithm is an appropriate approach to solve nonlinear optimization problems defined by the evaluation of functions and to calculate their derivatives is time consuming. Most industrial applications of SQP methods are found in optimization of mechanical structures [10-12].

The Evolutionary Algorithm (EA) is an optimization method which is based on the natural selection and survival of the fittest as it works in the biological world. EAs consistently perform well at approximating solutions for all types of problems because they do not make any assumption about the underlying fitness landscape that makes EAs applicable from different fields of engineering to social sciences [13]. EAs differ from more traditional optimization techniques in that they involve a search from a 'population' of solutions in each iteration step, instead of a single point. In each iteration step a competitive selection is made based on the 'fitness' value of solutions and the weak ones from the population are eliminated. The solutions with high fitness are 'recombined' with other solutions by swapping parts of a solution with another. Solutions are also 'mutated' by making a small change to a single element of the solution. Recombination and mutation are used to generate the new population of solutions that are diverted towards regions of the searching space where good solutions have already been seen.

However, it should be noted that EA has several different implementations: Evolutionary Programming (EP) which focuses on optimizing continuous functions without recombination, Evolutionary Strategy (ES) which focuses on optimizing continuous functions with recombination, Genetic Algorithm (GA) which focuses on optimizing general combinatorial problems and Genetic Programming (GP) which mainly evolves programs [10]. The selection of the proper technique and the tuning of the parameters of the selected technique require some knowledge about these techniques. In this article two different ES algorithms are applied to obtain the optimal feeding trajectory, a not modified one and an ES which applies covariance matrix adaptation (CMA) [14, 15].

Learning the covariance matrix in the CMA-ES is analogous to learning the inverse Hessian matrix in a quasi-Newton method. At the end, any convex-quadratic (ellipsoid) objective function is transformed into a spherical function. This can improve the performance on ill-conditioned and/or non-separable problems by orders of magnitude. The CMA-ES overcomes typical problems that are often associated with EAs, e.g. the poor performance on badly scaled and/or highly non-separable objective functions.

3   Fed-Batch Reactor and its Model

A highly exothermic reaction system was investigated and an optimal feeding policy was determined using SQP and ES techniques. First the investigated reactor and its first-principle model will be shortly introduced. The main product, 2-octanone is produced in a two-phase reaction system in a fed-batch reactor from 2-octanol. The 2-octanol is continuously fed into the organic phase, which does not exist before the start of the feeding. Hence, the organic phase is the dispersed one while the aqueous nitric acid phase where all the reaction steps take place is the continuous phase. The two phases are connected by the mass and heat transfer phenomena. Based on Castellan et al.'s work [16] which shows that the oxidation processes in room temperature mostly takes place according to ionic mechanism, Woezik and Westerterp [17] determined a reaction kinetic describing the way of oxidation of 2-octanol to form 2-octanone in nitric acid, which is proved to be feasible.

In the first step of this reaction mechanism the nitrosonium ion forms through this reaction:

$$HNO_3 + HNO_2 \rightleftharpoons NO^+ + NO_3^- + H_2O \tag{1}$$

The above reaction has a very long induction time, which can be shortened by adding a small amount an initiator like $NaNO_2$ to generate the necessary nitrous acid faster:

$$NaNO_2 + H_3O^+ \longrightarrow HNO_2 + Na^+ + H_2O \tag{2}$$

The nitrosonium ion forms only in the aqueous phase. It is followed by the oxidation of 2-octanol forming 2-octanone:

$$\tag{3}$$
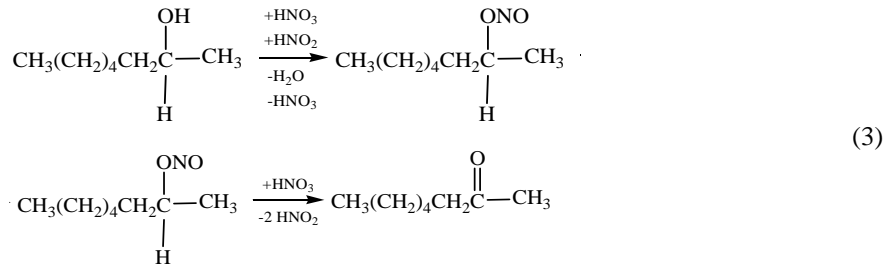
and the oxidation of 2-octanone producing different carboxylic acids:

$$\tag{4}$$
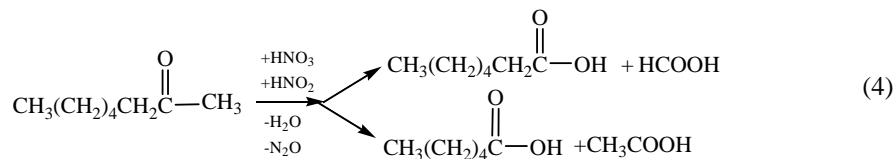
This process can be considered as an advanced benchmark problem in the field of process engineering. In [18] the control of this process has been analyzed, while in [19] the safety issues related to its operation were discussed. A report how the simulator of this process can be used in process engineering education has been published in [19], and from the viewpoint of this paper the most relevant work is published in, where the Hazard and Operability Analysis (HAZOP) of this process is developed also based on the application of process simulator.

Woezik and Westerterp introduced a mathematical model based on a simplified form of the kinetic introduced above to predict the dynamic behavior of the reactor [14]. In the next part just a brief introduction will be given about this model; a well detailed description can be found in [17, 18]. The simplified reaction mechanism:

$$A + B \rightarrow 2P + B \tag{5}$$

$$P + B \rightarrow X \tag{6}$$

where A is 2-octanol, B is nitrosonium ion, P is 2-octanone and X represents all the byproducts. The rate of reactions are calculated by the following equations

$$r_1 = \left(1 - \varepsilon_{org}\right) \cdot k_{eff,1} \cdot m_A \cdot c_A^{org} \cdot c_B^{aq} \tag{7}$$

$$r_2 = \left(1 - \varepsilon_{org}\right) \cdot k_{eff,2} \cdot m_P \cdot c_P^{org} \cdot c_B^{aq} \tag{8}$$

where the effective reaction rate constants are depend on the temperature and the acidity of the aqueous phase, ie.

$$k_{eff,i} = k_{eff,i}^0 \cdot \exp\left(-\frac{E_{A,eff,i}}{R \cdot T^R} - m_{H_0,eff,i} \cdot H_0 \right) \tag{9}$$

where the H_0 represents the Hammett-acidity function. To describe the concentration trajectories during the operation the following ordinary differential equations must be solved

$$\frac{d\left(V^R \cdot c_A^{org}\right)}{dt} = B^{R,in} \cdot c_{A,in} - r_1 \cdot V^R \tag{10}$$

$$\frac{d\left(V^R \cdot c_B^{aq}\right)}{dt} = V^R \cdot \left(r_1 - r_2\right) \tag{11}$$

$$\frac{d\left(V^R \cdot c_P^{org}\right)}{dt} = V^R \cdot \left(r_1 - r_2\right) \tag{12}$$

$$\frac{d\left(V^R \cdot c_X^{org}\right)}{dt} = V^R \cdot r_2 \tag{13}$$

$$\frac{d\left(V^R \cdot c_N^{aq}\right)}{dt} = -V^R \cdot \left(r_1 + r_2\right) \tag{14}$$

To describe the change in the temperature of the reactor and the jacket the following equations must be solved

$$\frac{dT^R}{dt} = \frac{1}{HC^R} \cdot \left(Q_r + Q_{in}^R - Q_{cool} + Q_{stir} - Q_{loss}\right) \tag{15}$$

$$\frac{dT^C}{dt} = \frac{1}{HC^C} \cdot \left(Q_{in}^C + Q_{cool}\right) \tag{16}$$

To illustrate the complex dynamical behavior of the process the following two experiments are performed. Trajectories of state-variables on Fig. 1 show the normal operation of the reactor when 2-octanone is the main product and the total quantity of byproducts is low. A small, only 3 °C change in the inlet temperature of the jacket results in a reactor runaway (see on Fig. 2). In this case byproducts are mainly generated during the operation while the conversion of 2-octanol is significantly decreased at the end of the operation. On Figs. 1 and 2 grey areas represent the instability region of the process. In another work we analyzed the stability of the model of this reactor using Ljapunov's indirect stability analysis method [20]. Our ultimate goal is to find an optimal feeding trajectory when reactor runaway doesn't occur.
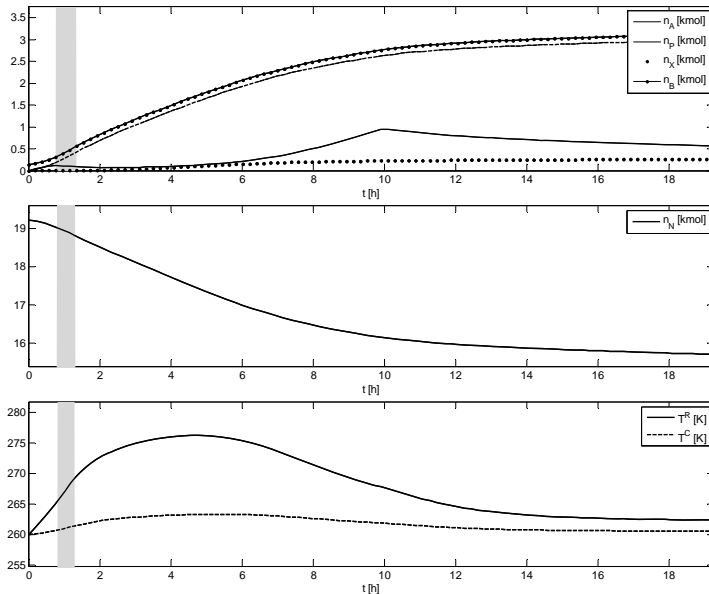

Figure 1
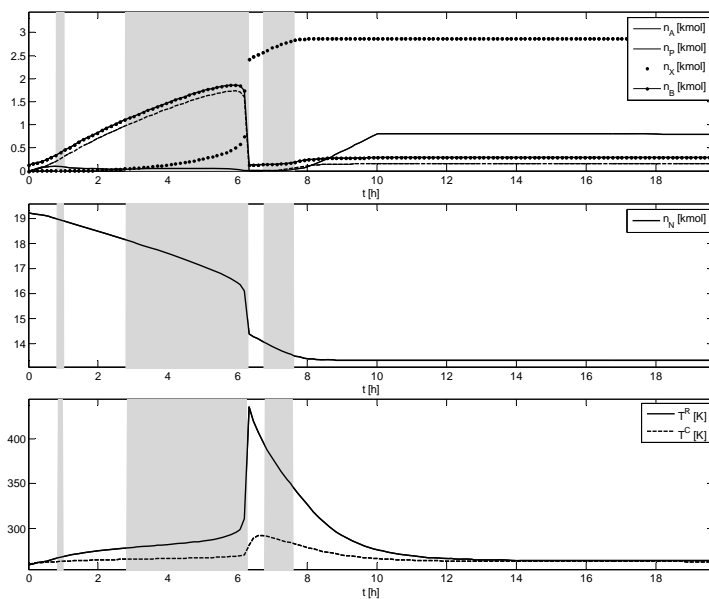
Trajectories of state variables (normal operation)

Figure 2

Trajectories of state variables (runaway occurs)

4　Optimization Results

In the objective function the purity of the product and the conversion of the 2-octanol was included with different weights. All the optimizations runs were stopped at the same tolerance for the change in objective function value. Initial values of the manipulated parameters were the same in every experiment.

Fig. 3 shows optimization results obtained with SQP. The feeding time domain is distributed into 4-9 parts. The value of the objective function can be seen next to the number of time segments. The first curve shows the trajectory of reactor temperature without optimization and applying constant feed rate. The best objective function value belongs to the fifth run, when the number of time segments is 8 while the worst belongs to the second run. As it shown the final value of the objective function is changing between -26.0 and -26.7 without convergence to any value of the objective function. As it can be seen in case of the second run (5 time segments) the algorithm can't find the global extrema. Only a small improvement can be achieved with the substitution of SQP with ES as it can be seen on Fig. 4. Otherwise, a significant difference can be noticed in the final value of the objective function at each run with the same time segments. The function value changes in a narrower range than previous one.
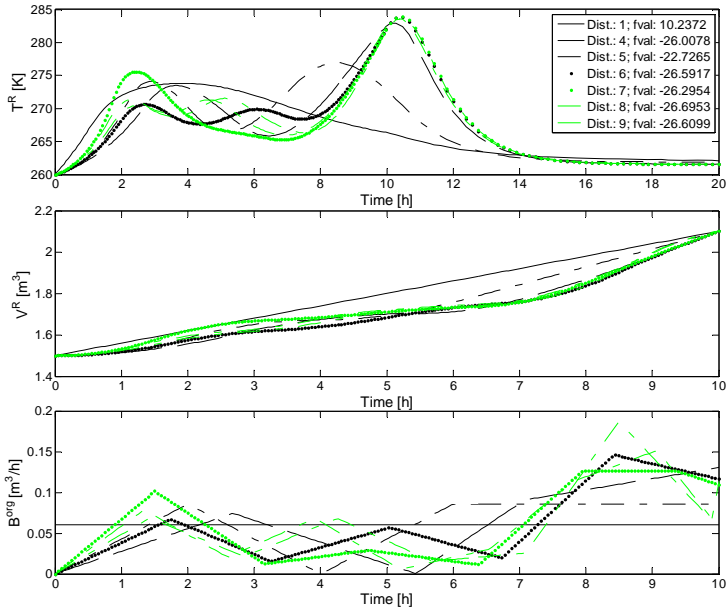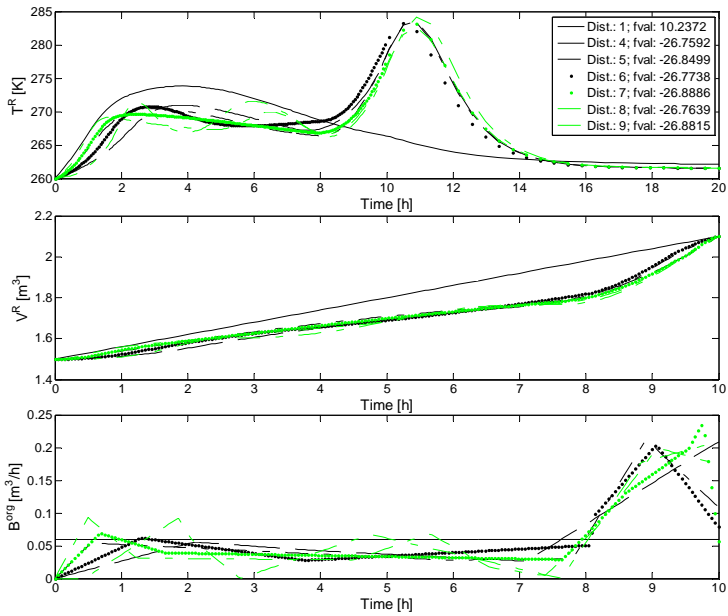
Figure 3

Optimization results with SQP

Figure 4

Optimization results with ES

The best results were obtained by the CMA-ES algorithm as it can be seen on Fig. 5. Beside to the 'highest' objective function values the CMA-ES prove the most reliable from the tested algorithms. The results for all methods are collected in Table 1. As it can be noticed two algorithms find the optimal number of the feeding time distribution at 8 and the other one at 7, thus it can be stated that it no need to further increase the distribution number in this optimization problem.
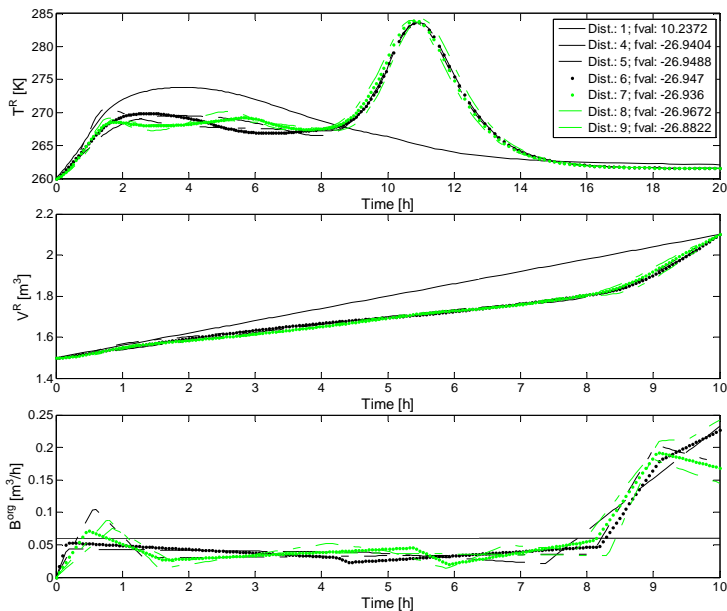

Figure 5

Optimization results with CMA-ES

Table 1

Optimization results with CMA-ES

Dist.	SQP	ES	CMA-ES
4	−26.0078	−26.7592	−26.9404
5	−22.7265	−26.8499	−26.9488
6	−26.5917	−26.7738	−26.9470
7	−26.2954	−26.8886	−26.9360
8	−26.6953	−26.7639	−26.9672
9	−26.6099	−26.8815	−26.8822

Conclusions

The operation of complex production processes is one of the most important research and development problems in process engineering. This problem is most relevant in the design of the optimal feeding profile of fed-batch chemical reactors

due to the nonlinear and unstable dynamical behavior of these processes. The optimal feeding profile was generated with SQP, ES and CMA-ES algorithms at different feeding time interval distribution. The obtained results show that the objective function value can't be significantly improved with ES and CMA-ES algorithms but the reliability of results is increased. The best results are achieved by the CMA-ES algorithm in the investigated optimization problem. From the structure of process model can be extracted some a priori information, which can be applied in the improvement of optimization performance and sped up the algorithm. In the following research the possible ways of utilizing this kind of extracted knowledge will investigated and will focus on how the extracted knowledge can be transformed into a set of constraints on the process variables and how these constraints can be applied in batch-to-batch optimization.

Acknowledgements

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