Evolutionary Strategy-based Feeding Profile 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 most relevant at the design of the optimal feeding profile of fed-batch chemical reactors due to the nonlinear and unstable dynamical behavior of these 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 multiple objective function was created and the search space is constrained in case all 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 multiple objective function. To obtain the optimal feeding policy the first-principle model of a pilot fed-batch reactor was implemented into MATLAB and applied as dynamic simulator of the process. An off-line optimization process was carried out at different number of feeding 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

While optimal operating conditions of production processes are getting closer and closer to physical constraints, more and more important is the development of knowledge based expert systems for supporting the operators to keep the operation conditions in this narrow range [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 these processes, because in case of exothermic reactors thermal runaway can also be occur [3-6]. Reactor runaway means a sudden and considerable change in

the process variables that is a serious problem in many chemical industrial technologies, like oxidation processes and polymerization technologies. 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 simple complexity are rare in production process, hence the analytically determination of optimal operation variables is more complicated or in some cases it is impossible. To calculate the optimal temperature profile or the optimal feeding policy in such system a lot of optimization algorithm can be applied. In this paper three optimization algorithms are used in estimation of optimal feeding trajectory for a pilot-plant fed-batch reactor and the reached optimization performances are shown and compared at different number of feeding time distribution.

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 comparing 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 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, meaning that it requires few iterations (hence QP solves) 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 problem defined by the evaluation of functions and to calculate their derivatives is time consuming. Most industrial applications of SQP methods are found in mechanical structural optimization [7-9].

The Evolutionary Algorithm (EA) is an optimization method which based on the natural selection and survival of the fittest as it works in the biological world. EAs consistently perform well approximating solutions to all types of problems because they do not make any assumption about the underlying fitness landscape, hence it makes EAs applicable from different fields of engineering to social sciences [10]. EAs differ from more traditional optimization techniques in that they involve a search from a ‘population’ of solutions in each iteration step, not

from a single point. In each iteration step a competitive selection is made based on the 'fitness' value of solutions and the poor ones from the population are eliminated. The solutions with high fitness are 'recombined' with other solutions by swaping 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.

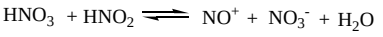
However, it should be noted that EA has several implementations: Evolutionary Programming (EP) which focuses on optimizing continuous functions without recombination, Evolutionary Strategy (ES) which focuses on optimizing continuous functions with recombination, Genetic Algorithm (GA) which focuses on 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) [11, 12].

Learning the covariance matrix in the CMA-ES is analogous to learning the inverse Hessian matrix in a quasi-Newton method. In the end, any convex-quadratic (ellipsoid) objective function is transformed into the 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

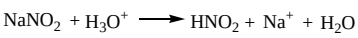
A highly exothermic reaction system was investigated and an optimal feeding policy was determined using SQP and ES techniques. In first the investigated reactor and its first-principle model will be shortly introduced. The main product, 2-octanone is produced in a two-phase reaction system in a fed-batch reactor from 2-octanol. The 2-octanol is continuously feeding into the organic phase, which does not exist before the start of the feeding. Hence, the organic phase is the dispersed 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 [13] which shows that the oxidation processes in room temperature mostly play according to ionic mechanism, Woezik and Westerterp [14] determined a reaction kinetic for 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:



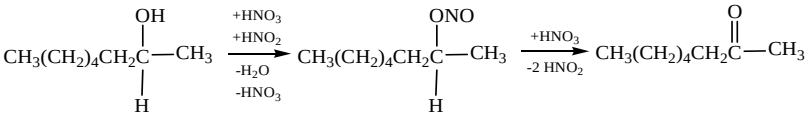
(1)

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:



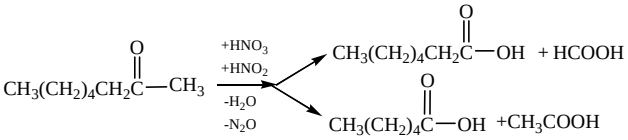
(2)

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



(3)

and the oxidation of 2-octanone producing different carboxylic acids:



(4)

Woezik and Westerterp introduced a mathematical model based on a simplified form of the introduced kinetic above to predict the dynamic behavior of the reactor [14]. In the next part just a briefly introduction will be given about this model a well detailed description can be read in [14, 15].

This process can be considered as an advanced benchmark problem in the field of process engineering. In [15] the control of this process has been analyzed, while in [16] 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 [16], 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.

The mathematical model of the system was worked out by Woezik and Westerterp [14]. They introduced a mathematical model based on a simplified form of the introduced kinetic above to predict the dynamic behavior of the reactor. 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. In the next part just a briefly introduction will be given about this

model a well detailed description can be read in [14, 15]. 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 dependent with the temperature and the acidity of the aqueous phase so

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

in which 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 can be seen on Fig. 1 show the normal operation of the reactor when 2-octanone is the main product and the summarized quantity of byproducts is low. Due to only 5 °C change in the inlet temperature of the jacket reactor runaway occurs (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 during the process. In our other work the stability of the model of this reactor is analyzed using Ljapunov's indirect stability analysis method. So our purpose is to find an optimal feeding trajectory when reactor runaway doesn't occur.

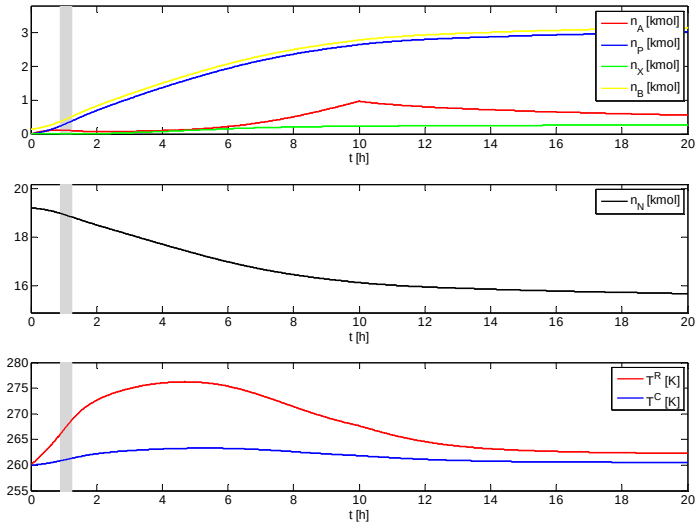


Figure 1
Trajectories of state variables (normal operation)

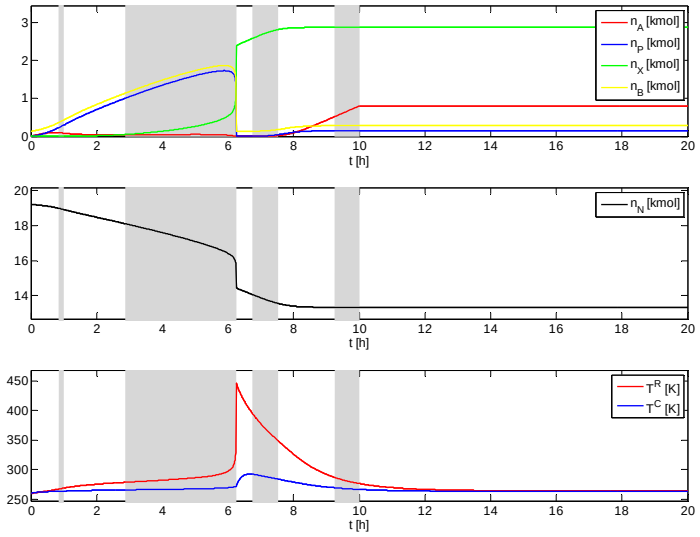


Figure 2
Trajectories of state variables (runaway occurs)

3 Optimization Results

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

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 distribution. 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 time distribution 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 it focuses on anywhere except the second run.

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. The function value changes in a narrower range than previously but it doesn't focus anywhere too.

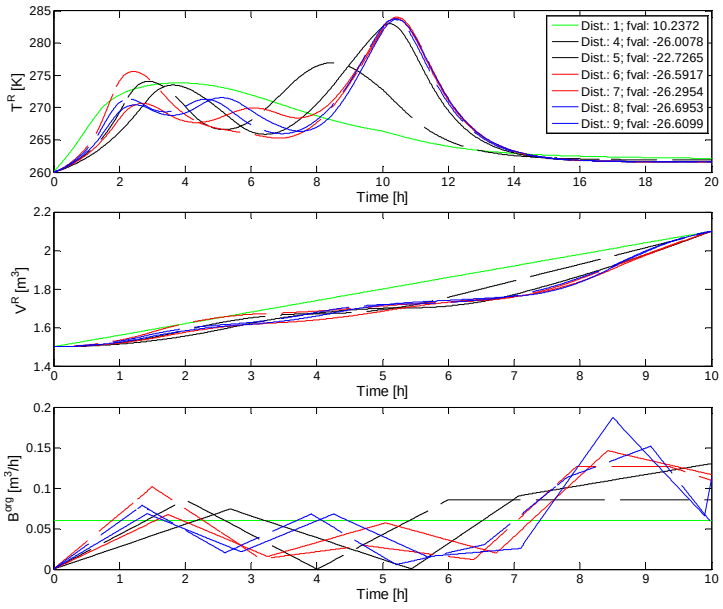


Figure 3
Optimization results with SQP

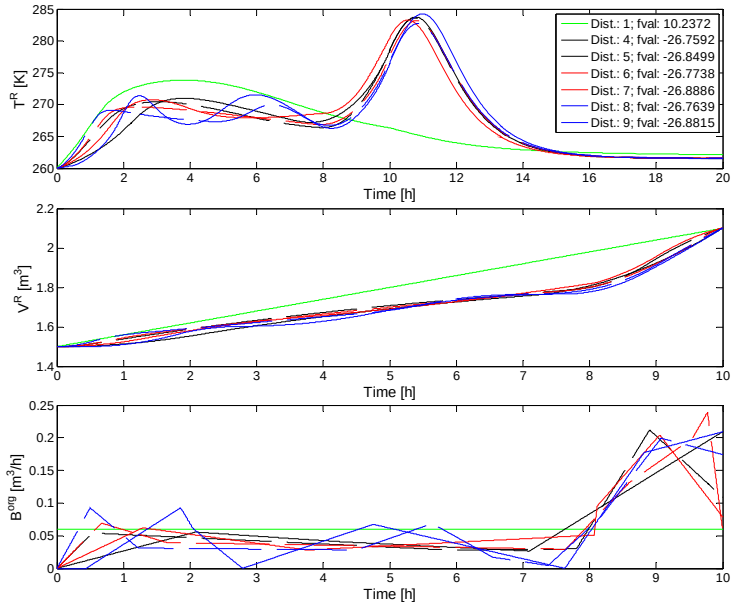


Figure 4
Optimization results with ES

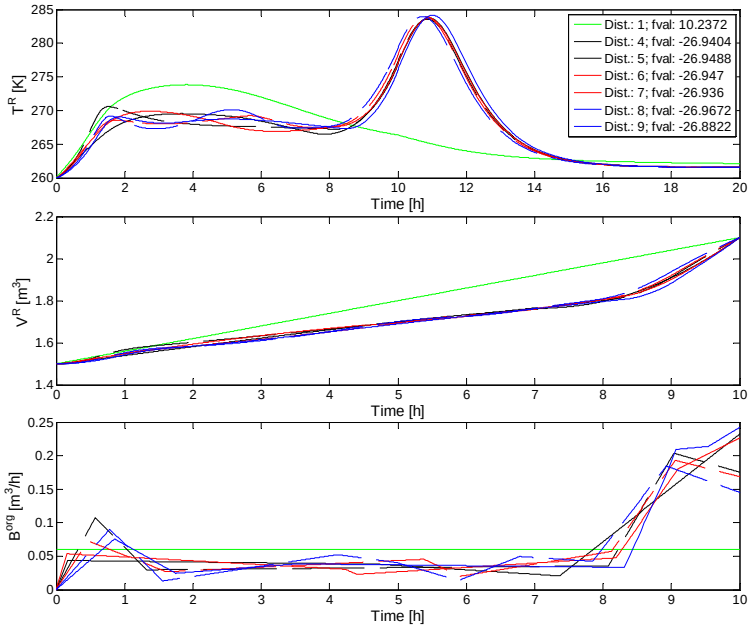


Figure 5
Optimization results with CMA-ES

The best results were obtained by the CMA-ES algorithm as it can be seen on Fig. 5. Next to the 'highest' objective function values the CMA-ES prove the most reliable from the tested algorithms. All the results 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, so it can be mentioned that it no need to increase the distribution number in this optimization problem.

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 at 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 algorihtms but the reliability of results is increased. The best results are achieved by the CMA-ES algorithm in the investigated optimization problem. Further research 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.

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