

INVESTIGATION ON OPTIMIZATION OF PROCESS PARAMETERS AND CHEMICAL REACTOR GEOMETRY BY EVOLUTIONARY ALGORITHMS

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ABSTRACT

The present work aims to employ evolutionary algorithms (EAs) to optimize an industrial chemical process. A unique combination of the simplified fundamental theory and direct hands-on computer simulation is used to present the modeling of a dynamic chemical engineering process in a highly understandable way. The main aim is to use them for analysis of dynamical system behaviour, especially of a given chemical reactor. A non-linear mathematical model is required to describe the dynamic behaviour of batch process; this justifies the use of evolutionary method of the EAs to deal with this process. Two algorithms - differential evolution and self-organizing migrating algorithm are used in this investigation. Differential Evolution is an evolutionary optimization technique which is exceptionally simple, significantly faster & robust at numerical optimization and is more likely to find a function's true global optimum. SOMA is also robust algorithm in sense of global extreme searching. In this way, in order to optimize the process, the EAs code is coupled with the rigorous model of the reactor. Both algorithms (SOMA, DE) have been applied 100 times in order to find the optimum of process parameters and the reactor geometry. The results show that the EAs are used successfully in the process optimization.

INTRODUCTION

Evolutionary algorithms derived by observing the process of biological evolution in nature, have proven to be a powerful and robust optimizing technique in many cases (Gross B.; Roosen P. 1998). In computer science evolutionary computation is a subfield of artificial intelligence (more particularly computational intelligence) that involves combinatorial optimization problems (Wikipedia encyclopedia).

Since the 60s, several approaches (genetic algorithms, evolution strategies etc.) have been developed which apply evolutionary concepts for simulation and

optimization purposes. Also in the area of multiobjective programming, such approaches (mainly genetic algorithms) have already been used (Evolutionary Computation 3(1), 1–16)(Thomas Hanne 2000).

Evolutionary algorithms such as evolution strategies and genetic algorithms have become the method of choice for optimization problems that are too complex to be solved using deterministic techniques such as linear programming or gradient (Jacobian) methods. The large number of applications (Beasley (1997)) and the continuously growing interest in this field are due to several advantages of EAs compared to gradient based methods for complex problems (Ivo F. Sbalzarini, Sibylle Muller and Petros Koumoutsakos, 2000).

The optimization of dynamic process has received growing attention in recent years because it is essential for the process industry to strive for more efficient and agile manufacturing in face of saturated market and global competition (T. Backx, O. Bosgra 2000).

In chemical engineering, evolutionary optimization has been applied by the author and others to system identification (Pham and Coulter, 1995; Moros, 1996); a model of a process is built and its numerical parameters are found by error minimization against experimental data. Evolutionary optimization has been widely applied to the evolution of neural networks models for use in control applications (e.g. Li & Haubler, 1996).

In this paper, the methods of artificial intelligence by evolutionary algorithms - SOMA and DE are presented for optimizing chemical engineering processes, particularly those in which the evolutionary algorithm is used for static optimization of a chemical batch reactor to improve its parameter. Consequently, it is used to design geometry technique equipments for chemical reaction. The method was used to optimize the design of the growth chamber, and was found to be in good agreement with the observed growth rate results.

The area of reactor network synthesis currently enjoys a proliferation of contributions in which researchers from various perspectives are making efforts to develop systematic optimization tools to improve the performance of chemical reactors. The contributions reflect on the increasing awareness that textbook knowledge and heuristics (Levenspiel, 1962), commonly employed in the development of chemical

reactors, are now deemed responsible for the lack of innovation, quality, and efficiency that characterizes many industrial designs.

From an economic viewpoint, final-product of the required quality demands a certain respectable maximal productivity of a chemical reactor. The reactor productivity depends on reaction rate, which usually increases exponentially with rising temperature.



Figure 1: Batch reactor with single external cooling jacket

DESCRIPTION OF A REACTOR

This work uses a mathematical model of a reactor shown in Figure 2. From constructional standpoint, the acts about the vessel with double side for cooling medium and is further equipped with stirrer for mixing reactionary mixtures.

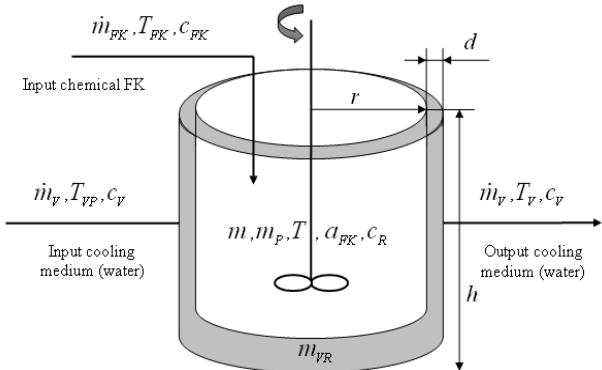


Figure 2: Batch reactor

Reactor disposes by two physical inputs. First input denoted "Input Chemical FK " is chemical dosing into reaction about mass flow rate \dot{m}_{FK} , temperature T_{FK} and specific heat c_{FK} . Second input denoted "Input cooling medium" is water drain into the reactor double side with mass flow rate \dot{m}_v , temperature T_{vp} and specific heat c_v . This coolant further traverses among - jacketed through space of reaction and his total weight in this space is m_{VR} . Coolant after it gets off the exit reaction denoted "output cooling medium" about mass flow rate \dot{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 . Reactionary mixture then has total mass m , temperature T , specific heat c_R and stirs till the time chemicals FK described by parameter concentration a_{FK} .

Non-linear model of reactor

Description of the reactor applies a system of four balance equations (1). The first one 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. Equations (1), where for simplified notation of basic equations (2) is represented by term "k".

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

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

$$\begin{aligned} \dot{m}_{FK}c_{FK}T_{FK} + \Delta H_r km[t]a_{FK}[t] &= \\ = KS(T[t] - T_V[t]) + m[t]c_R T'[t] & \end{aligned} \quad (1)$$

$$\dot{m}_V c_V T_{VP} + KS(T[t] - T_V[t])$$

$$= \dot{m}_V c_V T_V[t] + m_{VR} c_V T'_V[t]$$

$$k = Ae^{-\frac{E}{RT[t]}} \quad (2)$$

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

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

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

$$T'[t] = \frac{\dot{m}_{FK} c_{FK} T_{FK}}{m[t] c_R} + \frac{Ae^{-\frac{E}{RT[t]}} \Delta H_r a_A[t] - KST[t]}{c_R} - \frac{KST_V[t]}{m[t] c_R} \quad (3)$$

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

The design of 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 participation expert parameters. The objective of this part of the work is to perform a simulation and optimization of the given reactor.

Therefore into system equations (3) were instated constants:

$$A = 219,588 \text{ s}^{-1}, E = 29967,5087 \text{ J.mol}^{-1}, R = 8,314 \text{ J.} \text{mol}^{-1} \cdot \text{K}^{-1}, c_{FK} = 4400 \text{ J.kg. K}^{-1}, c_V = 4118 \text{ J.kg. K}^{-1}, c_R = 4500 \text{ J.kg. K}^{-1}, \Delta H_r = 1392350 \text{ J.kg}^{-1},$$

$$K = 200 \text{ kg.s}^{-3} \cdot \text{K}^{-1},$$

Next parameters, that are important for calculations are:

- Geometric dimension of the reaction: $r[\text{m}]$, $h[\text{m}]$
- Density of chemicals: $\rho_p = 1203 \text{ kg.m}^{-3}$,
- $\rho_{FK} = 1050 \text{ kg.m}^{-3}$.
- Stoichiometric rate chemical:

$$m_p = 2,82236 \cdot m_{FK}$$

OPTIMIZATION OF PROCESS PARAMETERS AND THE REACTOR GEOMETRY

We illustrate the design approach using the batch reaction system shown in Figure. 1. The main aim in this example is finding the optimization of process parameters and the reactor geometry. Here, it is a optimization of batching value m_{FK} together with process parameters of the cooling medium and including also reactor geometry and cooling area.

Mathematical problems

In this optimization was founded optimized parameters with one another linked ,so that heat transfer surface, volume, and hence also mass mixtures of reaction was mutually in relation. Heat transfer surface S have relation:

$$S = 2\pi rh + \pi r^2 \quad (4)$$

Where r is radius and h is high of the space reactor (see Figure.2)

Volume of vessel of rector applies to relation:

$$V = \pi r^2 h \quad (5)$$

Total mass of mixtures in the reaction is initial batch inside the reactor with parameter mass m_p a mass input chemical m_{FK} , that:

$$m = m_p + m_{FK} \quad (6)$$

The stechiometric ratio is given by (7).

$$m_p = 2,82236 m_{FK} \quad (7)$$

Total volume of mixtures in the reaction equal sum of volume initial mixtures in the reaction and volume of FK:

$$V = V_p + V_{FK} = \frac{m_p}{\rho_p} + \frac{m_{FK}}{\rho_{FK}} \quad (8)$$

The relationship between the optimized volume of reactor and the mass of added chemical FK is given by (8). Then substituting to (7) gives the mass of the initial batch in the reactor.

$$m_{FK} = \frac{\rho_p \rho_{FK} V}{2,82236 \rho_{FK} + \rho_p} \quad (9)$$

In this example, the optimization was then added parameter thickness d of vessel, which have relation that:

$$m_{VR} = \rho_V S d \quad (10)$$

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 (CF) that was minimized is given in (11):

$$f_{cost} = \sum_{t=0}^T |w - T[t]| \quad (11)$$

The CF has been calculated in general from the distance between desired state and actual system output.

Static optimization of reactor

The above described reactor, in the original set-up, gives unsatisfactory results. To improve reactor behavior, static optimization was performed using the algorithms SOMA and DE. In this work the optimization was performed by the following optimization of batching value reactor's parameters geometry.

Used Algorithm and Parameter Setting

For the experiments described here, stochastic optimisation algorithms, such as Differential Evolution (DE) (Price, 1999) and Self-Organizing Migrating Algorithm (SOMA) (Zelinka, 2004), had been used. Alternative algorithms, like Genetic Algorithms (GA) and Simulated Annealing (SA), are now in process, and results are hoped to be presented soon. Main reason why DE and SOMA has been used comes from contemporary state in chemical engineering and EAs use. Since now has been done some research with attention on use of EAs in chemical engineering optimization, including DE. This participation has to show that applicability of relatively new algorithms is also positive and can lead to applicable results, as was shown for example in Zelinka (2001), which has been done under 5th EU project RESTORM (acronym of Radically Environmentally Sustainable Tannery Operation by Resource Management) and main aim was to use EAs in chemical engineering processes. True is also that there is a plenty of other heuristic like particle swarm (Liu, Liu, Cartres, 2007), scatter search (Glover, Laguna, Martí, 2003), memetic algorithms, simulated annealing (Kirkpatrick, Gelatt, Vecchi, 1983), etc. and

according to No Free Lunch theorem (Wolpert, Macready, 1997) is clear that each heuristic would be less or more applicable on example presented here. DE and SOMA has been also used because authors have satisfactorial experiences with both algorithms. Very brief description is as follows.

Differential Evolution (Price, 1999) is a population-based optimization method that works on real-number coded individuals. For each individual $x_{i,G}$ in the current generation G , DE generates a new trial individual $x'_{i,G}$ by adding the weighted difference between two randomly selected individuals $x_{1,G}$ and $x_{2,G}$ to a third randomly selected individual $x_{3,G}$. The resulting individual $x'_{i,G}$ is crossed-over with the original individual $x_{i,G}$. The fitness of the resulting individual, referred to as perturbated vector $u_{i,G+1}$, is then compared with the fitness of $x_{i,G}$. If the fitness of $u_{i,G+1}$ is greater than the fitness of $x_{i,G}$, $x_{i,G}$ is replaced with $u_{i,G+1}$, otherwise $x_{i,G}$ remains in the population as $x_{i,G+1}$. Differential Evolution is robust, fast, and effective with global optimization ability. It does not require that the objective function is differentiable, and it works with noisy, epistatic and time-dependent objective functions. Pseudocode of DE is:

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1. Input :  $D, G_{\max}, NP \geq 4, F \in (0,1], CR \in [0,1]$ , and initial bounds :  $\bar{x}^{(lo)}, \bar{x}^{(hi)}$ .
2. Initialize :  $\begin{cases} \forall i \leq NP \wedge \forall j \leq D : x_{i,j,G=0} = x_j^{(lo)} + rand_j[0,1] \cdot (x_j^{(hi)} - x_j^{(lo)}) \\ i = \{1,2,\dots,NP\}, j = \{1,2,\dots,D\}, G = 0, rand_j[0,1] \in [0,1] \end{cases}$ 
3. While  $G < G_{\max}$ 
    4. Mutate and recombine :
        4.1  $r_1, r_2, r_3 \in \{1,2,\dots,NP\}$ , randomly selected, except :  $r_1 \neq r_2 \neq r_3 \neq i$ 
        4.2  $j_{rand} \in \{1,2,\dots,D\}$ , randomly selected once each  $i$ 
        4.3  $\forall j \leq D, u_{j,i,G+1} = \begin{cases} x_{r_j,G} + F \cdot (x_{r_j,G} - x_{r_j,r_2,G}) & \text{if } (rand_j[0,1] < CR \vee j = j_{rand}) \\ x_{r_j,G} & \text{otherwise} \end{cases}$ 
    5. Select
         $\bar{x}_{i,G+1} = \begin{cases} \bar{u}_{i,G+1} & \text{if } f(\bar{u}_{i,G+1}) \leq f(\bar{x}_{i,G}) \\ \bar{x}_{i,G} & \text{otherwise} \end{cases}$ 
     $G = G + 1$ 

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SOMA is a stochastic optimization algorithm that is modelled on the social behaviour of co-operating individuals (Zelinka, 2004). It was chosen because it has been proved that the algorithm has the ability to converge towards the global optimum (Zelinka, 2004). SOMA works on a population of candidate solutions in loops called migration loops. The population is initialized randomly distributed over the search space at the beginning of the search. In each loop, the population is evaluated and the solution with the highest fitness becomes the leader L. Apart from the leader, in one migration loop, all individuals will traverse the input space in the direction of the leader. Mutation, the random perturbation of individuals, is an important operation for evolutionary strategies (ES). It ensures the diversity amongst the individuals and it also provides the means to restore lost information in a population. Mutation is different in SOMA compared with other ES strategies. SOMA uses a parameter called PRT to achieve perturbation. This parameter has the same effect

for SOMA as mutation has for GA. The PRT Vector defines the final movement of an active individual in search space.

The randomly generated binary perturbation vector controls the allowed dimensions for an individual. If an element of the perturbation vector is set to zero, then the individual is not allowed to change its position in the corresponding dimension. An individual will travel a certain distance (called the path length) towards the leader in n steps of defined length. If the path length is chosen to be greater than one, then the individual will overshoot the leader. This path is perturbed randomly. For an exact description of use of the algorithms see (Price, 1999) for DE and (Zelinka, 2004) for SOMA. Pseudocode of SOMA is:

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Input:  $N, Migrations, PopSize \geq 2, PRT \in [0,1], Step \in (0,1], MinDiv \in (0,1],$ 
PathLength  $\in [0,5]$ , Specimen with upper and lower bound  $x_j^{(hi)}, x_j^{(lo)}$ 
Initialization  $\begin{cases} \forall i \leq PopSize \wedge \forall j \leq N : x_{i,j,Migrations=0} = x_j^{(lo)} + rand_j[0,1] \cdot (x_j^{(hi)} - x_j^{(lo)}) \\ i = \{1,2,\dots,PopSize\}, j = \{1,2,\dots,N\}, Migrations=0, rand_j[0,1] \in [0,1] \end{cases}$ 
While  $Migrations < Migrations_{\max}$ 
    While  $t \leq PathLength$ 
        if  $rnd_j < PRT$  pak  $PRTVector_j = 1$  else  $0, j = 1, \dots, N$ 
     $\forall i \leq PopSize, x_{i,j}^{ML+1} = x_{i,j,start}^{ML} + (x_{i,j}^{ML} - x_{i,j,start}^{ML}) PRTVector_j$ 
         $f(x_{i,j}^{ML+1}) = \begin{cases} f(x_{i,j}^{ML}) & \text{if } f(x_{i,j}^{ML}) \leq f(x_{i,j,start}^{ML}) \\ f(x_{i,j,start}^{ML}) & \text{else} \end{cases}$ 
     $t = t + Step$ 
     $Migrations = Migrations + 1$ 

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The control parameter settings have been found empirically and are given in Tab. 1 (SOMA) and Tab. 2 (DE). The main criterion for this setting was to keep the same setting of parameters as much as possible and of course the same number of cost function evaluations as well as population size (parameter PopSize for SOMA, NP for DE). Individual length represents number of optimized parameters, see Tab. 3.

Table 1: SOMA parameter setting

	A
PathLength	3
Step	0.41
PRT	0.1
PopSize	20
Migrations	50
MinDiv	-1
Individual Length	6
CF Evaluations	6951

Table 2: DE parameter setting

	A
NP	20
F	0.9
CR	0.2
Generations	200
Individual Length	6
CF Evaluations	4000

EXPERIMENTAL RESULTS

Due to the fact that EAs are partly of stochastic nature, a large set of simulations has to be done in order to get data for statistical data processing. Both algorithms (SOMA, DE) have been applied 100 times in order to find the optimum of process parameters and the reactor geometry. All important data has been visualized directly or/and processed for graphs demonstrating performance of both algorithms. Estimated parameters and their diversity (minimum, maximum and average) are depicted in Figure. 3 -Figure. 6 . From those pictures it is visible that results from both algorithms are comparable. For the demonstration are graphically the best solutions shown in Figure. 8, 10 and Figure. 12. There is shown time dependence of a_{FK} and T from both algorithms. The best values of parameter setting are recorded in Tab.3 & Tab. 4. On Figure. 7 - Figure. 22 are for example shown records of all 100 simulations and the best solutions of all 100 simulations (Fig. 7-14 for DE and Figure. 15-22 for SOMA).

The simulation results are sometimes different due to observed parameter since it depends on the number of migration loops. Furthermore, global minimum process function is corresponding to the oxies “z” of cost function, but it is the difference between the required state (stabilized fixed point) and the real system output on the whole simulation interval t .

Table 3: Optimized reactor parameters and their range inside which has been optimization done

Parameter	Range
\dot{m}_{FK} [kg.s-1]	0 – 500
r [m]	0.3 – 3.0
h [m]	0.5 – 3.5
T_{VP} [K]	273.15 – 323.15
\dot{m}_V [kg.s-1]	0-10
d [m]	0.03 – 0.1

Table 4: The best values of optimized parameters by SOMA and DE

Parameter	SOMA	DE
\dot{m}_{FK} [kg.s-1]	0.00545104	0.042049
r [m]	0.322817	0.543594
h [m]	0.50696	1.86628
T_{VP} [K]	315.873	294.718
\dot{m}_V [kg.s-1]	7.94792	9.94168
d [m]	0.0848451	0.0563635

Parameter diversity for repeated simulations

Results visualised on Figure. 7 – 22 are also numerically recorded in Tab. 5 for DE and Tab. 6 for SOMA.

Table 5: Estimated parameters for DE

Parameter	Min	Avg	Max
\dot{m}_{FK} [kg.s-1]	0.020	0.154	0.460
r [m]	0.318	1.754	2.996
h [m]	0.512	1.740	3.492
T_{VP} [K]	293.219	304.565	322.652
\dot{m}_V [kg.s-1]	2.349	9.227	9.997
d [m]	0.0300	0.0410	0.0834

Tab.6: Estimated parameters for SOMA

Parameter	Min	Avg	Max
\dot{m}_{FK} [kg.s-1]	0.005	0.025	0.077
r [m]	0.300	0.580	2.069
h [m]	0.500	1.583	3.415
T_{VP} [K]	293.326	307.351	322.321
\dot{m}_V [kg.s-1]	4.00591	8.386	9.998
d [m]	0.0300	0.0546	0.0968

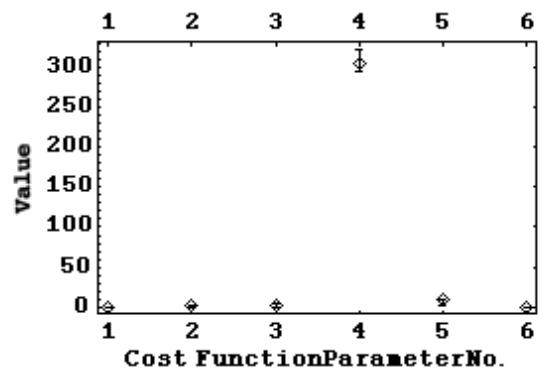


Figure 3: Parameter variation (DE)

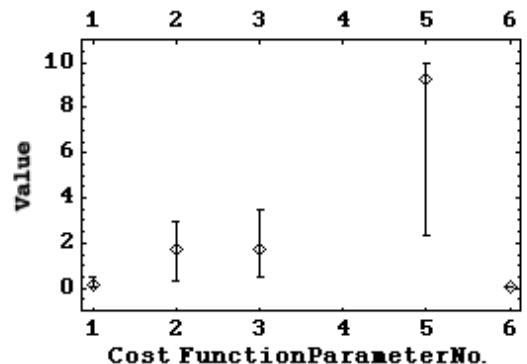


Figure 4: Parameter variation (DE) – detail

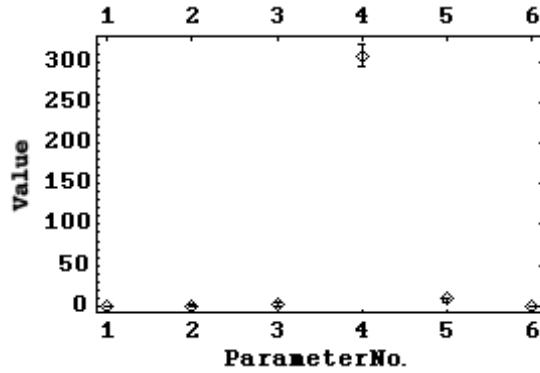


Figure 5: Parameter variation (SOMA)

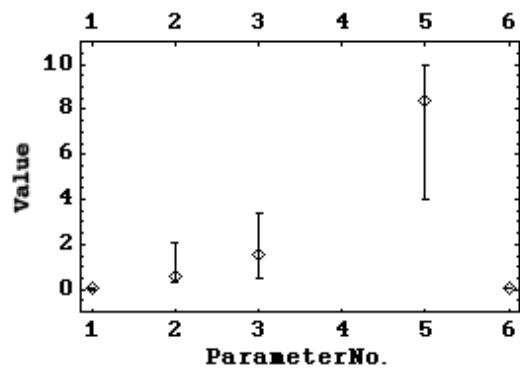


Figure 6: Parameter variation (SOMA) – detail

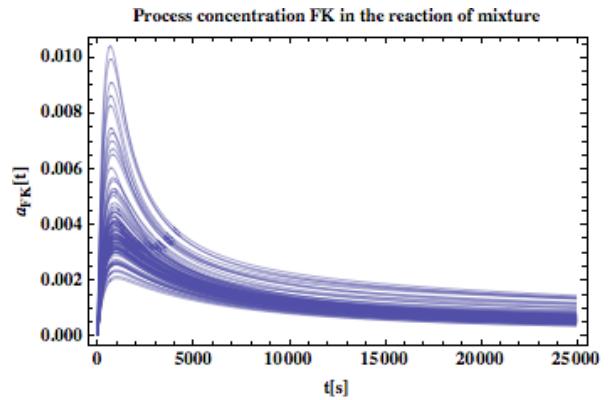


Figure 9: 100 simulations for aFK (DE)

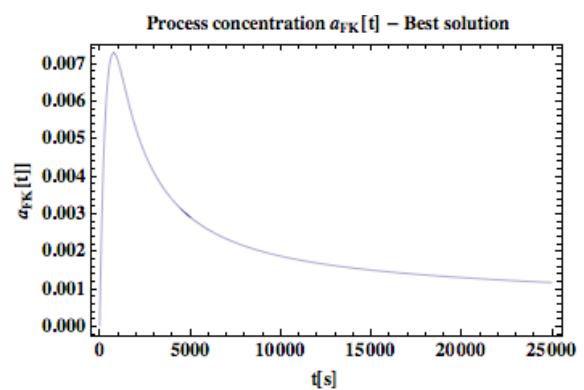


Figure 10: The best solution for aFK (DE)

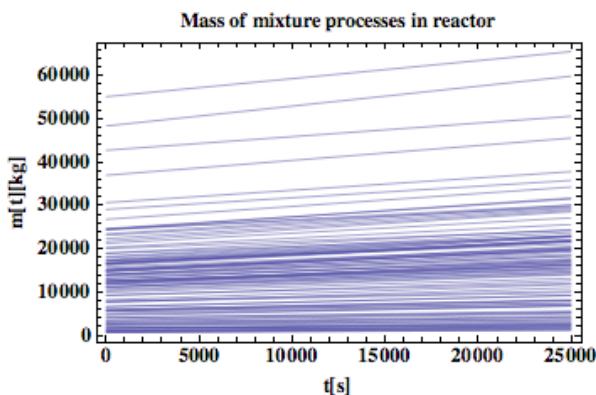


Figure 7: 100 simulations for m (DE)

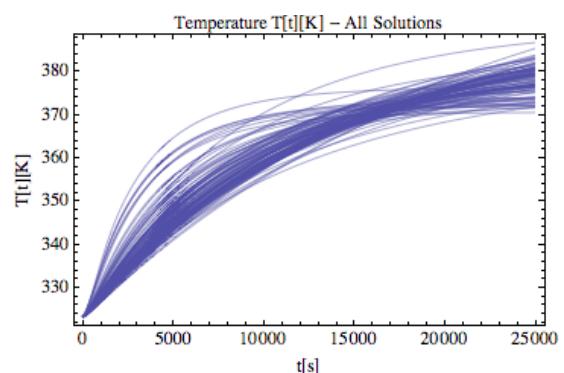


Figure 11: 100 simulations for T (DE)

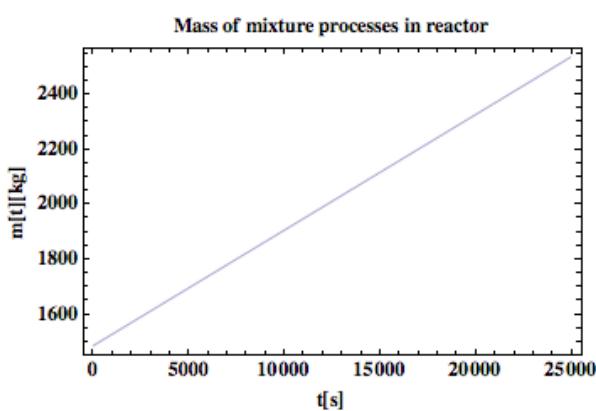


Figure 8: The best solution for m (DE)

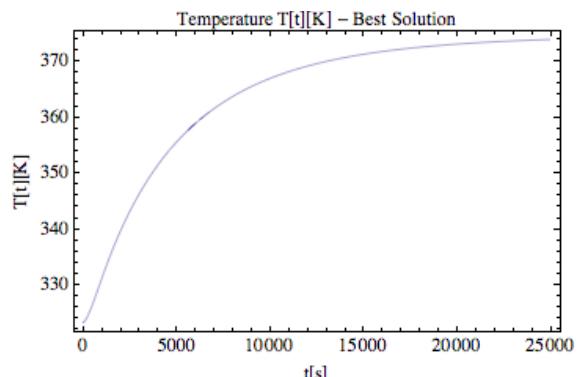


Figure 12: The best solution for T (DE)

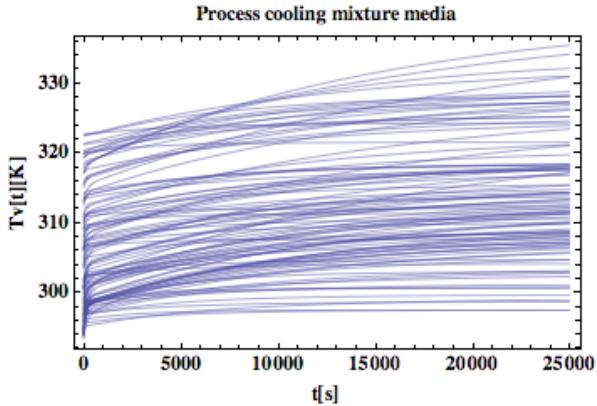


Figure 13: 100 simulations for TV (DE)

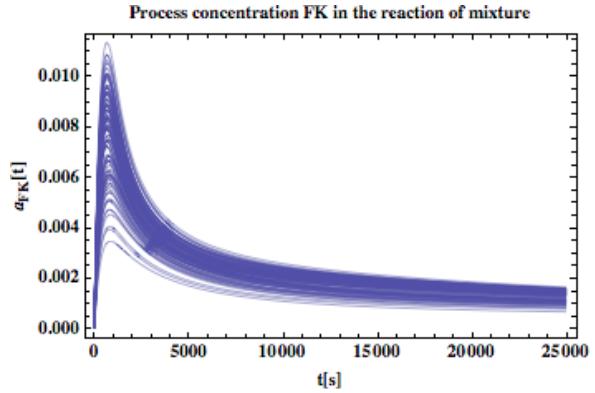


Figure 17: 100 simulations for aFK (SOMA)

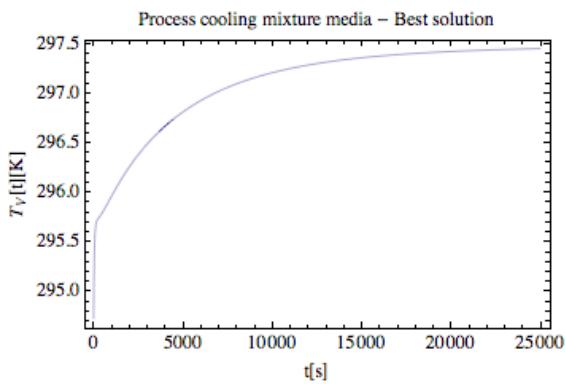


Figure 14: The best solution for TV (DE)

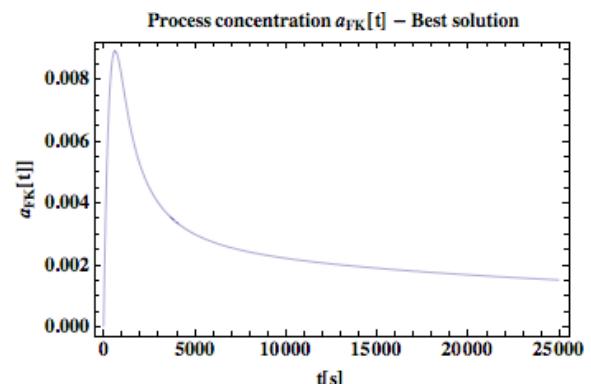


Figure 18: The best solution for aFK (SOMA)

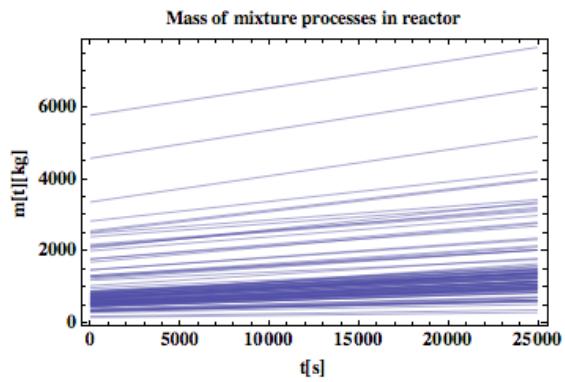


Figure 15: 100 simulations for m (SOMA)

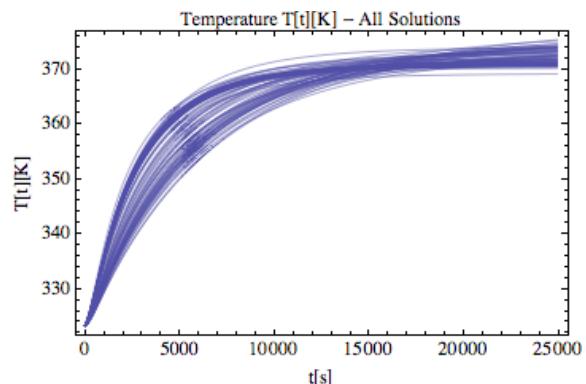


Figure 19: 100 simulations for T (SOMA)

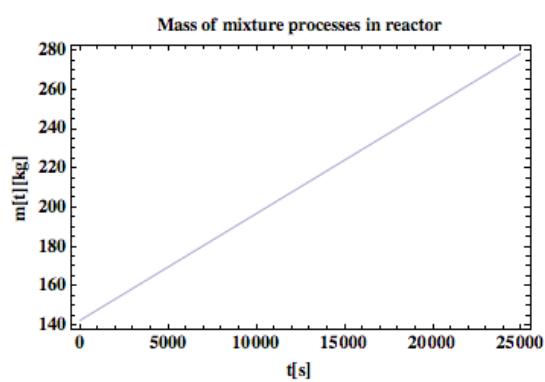


Figure 16: The best solution for m (SOMA)

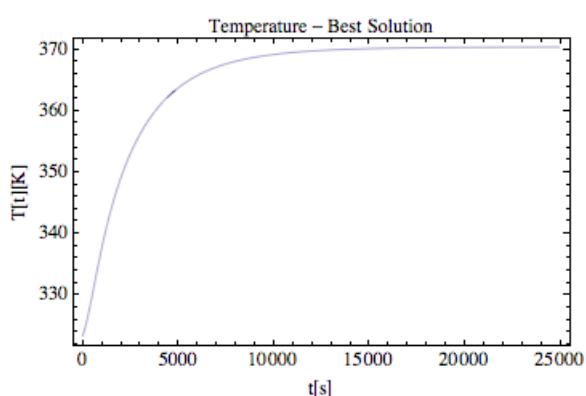


Figure 20: The best solution for T (SOMA)

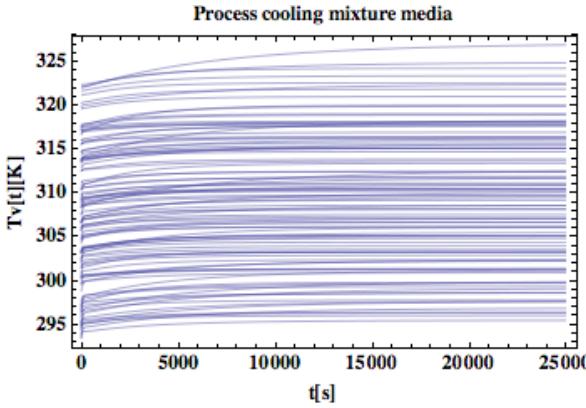


Figure 21: 100 simulations for TV (SOMA)

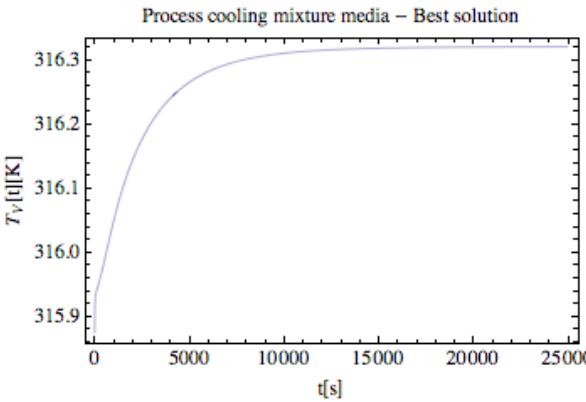


Figure 22: The best solution for TV (SOMA)

CONCLUSION

This paper has presented a systematic procedure to derive a solution model for operation of a dynamic chemical reactor process. The results produced by the optimizations depend not only on the problem being solved but also on the way how to define a given function.

The differences between both methods SOMA and DE are best seen in Tab.3 and tab.4. The first part shows the parameters of batch reactor designed by an expert, and the second part shows the parameters obtained through static optimization.

Calculation was 100 times repeated and the best, worst and average result (individual) was recorded from the last population in each simulation. All one hundred triplets (best, worst, average) were used to create Figure. 3 to Figure.6.

Both algorithms (SOMA, DE) have been applied 100 times in order to find the optimum of process parameters and the reactor geometry. The primary aim of this comparative study is not to show which algorithm is better or worse, but to show from the outputs of all simulations are depicted in Figure. 7-22 show that evolution SOMA represents the best solution from actual simulation more than DE. Based on data from all simulations, two comparison can be done. From parameter variation of view, the estimated

parameters depicted in Figure.3–Fig.6 show that both algorithms are comparable in performance (with small deviations).

From the graphs, it is evident that the courses of SOMA algorithm are more densities in a thin specter and not far from the start of mass axis. Only few values drifting out of the specter. The results of the DE algorithm are speedier in the weight specter. From these results we may conclude, that SOMA has much better convergence then DE algorithm (see Figure.7 & Figure.15).

Basic optimizations presented here were based on a relatively simple functional. Unless the experimenter is limited by technical issues when searching for optimal geometry parameters, there is no problem in defining more complex functional including as subcriterium 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. Future work objective is to formalize this process in order support the control system design to the best extent possible. According to all results obtained during time it is planned, the main activities would be focused expanding of this comparative study for genetic algorithms and simulated annealing. Furthermore, for the successful stabilization is to analyse more cost function CF.

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