OPTIMIZATION AND CONTROL OF A DYNAMICAL PROCESS BY GENETIC ALGORITHM

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ABSTRACT

In this paper, the modeling of a dynamic chemical engineering process is presented in a highly understandable way using a unique combination of the simplified fundamental theory and direct hands-on computer simulation. The main aim is to use them for analysis, optimise and adaptive control of behavior of dynamical system, especially of a given chemical reactor. A non-linear mathematical model is required to describe the dynamic behaviour of a continuous stirred tank reactor (CSTR). Evolutionary algorithm from the field of artificial intelligent - Genetic algorithm (GA) is used in this investigation.

The optimizations and control of a chemical reactor processes have been performed in several ways, each one for a different set of reactor parameters or different cost function. The optimized and adaptive control chemical reactor processes were used in simulations with optimization by genetic algorithm and the results are presented in graphs. Finally, experimental results are reported, followed by conclusion.

INTRODUCTION

Continuous stirred tank reactors (CSTRs) belong to a class of nonlinear systems where both steady-state and dynamic behaviour are nonlinear. Their models are derived and described in e.g. (Ogunnaike and Ray, 1994), (Schmidt, 2005) and (Corriou, 2004). verification can be found in (Stericker and Sinha, 1993).

Chemical process control requires intelligent monitoring due to the dynamic nature of the chemical reactions and the non-linear functional relationship between he input and output variables involved. CSTR is one of the major processing unit in many chemical, pharmaceutical and petroleum industries as well as in environmental and waste management engineering. In spite of continuing advances in optimal solution techniques for optimization and control problems, many of such problems remain too complex to be solved by the known techniques (Emuoyibofarhe O.Justice, Reju A Sunday, 2008).

In chemical engineering, evolutionary optimization has been applied by the author and others to system identification (Pham and Coulter, 1995); 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).

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).

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).

Designing optimal reactor parameters including control constitutes is 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.

In this work, the methods of artificial intelligence by evolutionary algorithm GA is presented for optimizing chemical engineering processes, particularly those in which the genetic algorithm is used for static optimization and adaptive control of a chemical CSTR reactor.

MATHEMATICAL PROBLEMS

Consider a CSTR with the first order consecutive exothermic reaction according to the scheme $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ and with a perfectly mixed cooling jacket. Using the usual simplifications, the model of the CSTR is described by four nonlinear differential equations (see Dostál, P., Gazdoš, F., Bobál, V., Vojtěšek, J., 2007).

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$$\frac{dc_A}{dt} = -\left(\frac{Q_r}{V_r} + k_1\right)c_A + \frac{Q_r}{V_r}c_{Ai} \quad (1)$$

$$\frac{dc_B}{dt} = -\left(\frac{Q_r}{V_r} + k_2\right)c_B + k_1 c_A + \frac{Q_r}{V_r}c_{Bi} \quad (2)$$

$$\frac{dT_r}{dt} = \frac{h_r}{(\rho c_p)_r} + \frac{Q_r}{V_r}(T_{ri} - T_r) + \frac{A_h U}{V_r(\rho c_p)_r}(T_c - T_r) \quad (3)$$

$$\frac{dT_c}{dt} = \frac{Q_c}{V_c}(T_{ci} - T_c) + \frac{A_h U}{V_c(\rho c_p)_c}(T_r - T_c) \quad (4)$$

with initial conditions $c_A(0) = c_A^s$, $c_B(0) = c_B^s$, $T_r(0) = T_r^s$ and $T_c(0) = T_c^s$. Here, t is the time, c are concentrations, T are temperatures, V are volumes, ρ are densities, c_p are specific heat capacities, Q are volumetric flow rates, A_h is the heat exchange surface area and U is the heat transfer coefficient. The subscripts are denoted $(\cdot)_r$ for the reactant mixture, $(\cdot)_c$ for the coolant, $(\cdot)_i$ for feed (inlet) values and the superscript $(\cdot)^s$ for steady-state values. The reaction rates and the reaction heat are expressed as

$$k_j = k_{0j}\exp\left(\frac{-E_j}{RT_r}\right), j = 1,2 \quad (5)$$

$$h_r = h_1 k_1 c_A + h_2 k_2 c_B \quad (6)$$

where k_0 are pre-exponential factors, E are activation energies and h are reaction entalpies. The values of all parameters, feed values and steady-state values are given in Tab 1. (Dostál, P., Gazdoš, F., Bobál, V., Vojtěšek, J., 2007).

Tab 1. Parameters, inlet values and initial conditions.

$V_r = 1.2$ m^3	$Q_r = 0.08$ m^{3}min^{-1}
$V_c = 0.64$ m^3	$Q_c^s = 0.03$ m^{3}min^{-1}
$\rho_r = 985$ kg m^{-3}	$c_{pr} = 4.05$ kJ kg^{-1}K^{-1}
$\rho_c = 998$ kg m^{-3}	$c_{pc} = 4.18$ kJ kg^{-1}K^{-1}
$A = 5.5$ m^2	$U = 43.5$ kJ m^{-2}min^{-1}K^{-1}
$k_{10} = 5.616 \cdot 10^{16}$ min^{-1}	$E_1/R = 13477$ K
$k_{20} = 1.128 \cdot 10^{18}$ min^{-1}	$E_2/R = 15290$ K
$h_1 = 4.8 \cdot 10^4$ kJ kmol^{-1}	$h_2 = 2.2 \cdot 10^4$ kJ kmol^{-1}
$c_{Ai} = 2.85$ kmol m^{-3}	$c_{Bi} = 0$ kmol m^{-3}
$T_i = 323$ K	$T_{ci} = 293$ K
$c_A^s = 0.1649$ kmol m^{-3}	$c_b^s = 0.9435$ kmol m^{-3}
$T_r^s = 350.19$ K	$T_c^s = 330.55$ K

STATIC OPTIMIZATION REACTOR

In this model of CSTR the parameters were optimized: the parameters of volumetric flow rates of the reactant mixture and the coolant Q_r, Q_c, the parameter of concentration for feed values c_{Ai} and temperature reactant mixture and colant T_{ri}, T_{ci}.(see Tab. 2)

Tab 2. Parameters of reactor, "highlight color" were optimized

$V_r \rightarrow \text{Meter}^3$	$V_c \rightarrow \text{Meter}^3$
$A_r \rightarrow \text{Meter}^2$	$Q_r \rightarrow \frac{\text{Meter}^3}{\text{min}}$
$c_{pc} \rightarrow \frac{\text{KiloJoule}}{\text{KilogramKelvin}}$	$U \rightarrow \frac{\text{KiloJoule}}{\text{Meter}^2\ \text{min Kelvin}}$
$h_1 \rightarrow \frac{\text{KiloJoule}}{\text{KiloMole}}$	$h_2 \rightarrow \frac{\text{KiloJoule}}{\text{KiloMole}}$
$c_{Ai} \rightarrow \frac{\text{KiloMole}}{\text{Meter}^3}$	$c_{Bi} \rightarrow \frac{\text{KiloMole}}{\text{Meter}^3}$
$\rho_r \rightarrow \frac{\text{Kilogram}}{\text{Meter}^3}$	$\rho_c \rightarrow \frac{\text{Kilogram}}{\text{Meter}^3}$
$Q_c \rightarrow \frac{\text{Meter}^3}{\text{min}}$	$c_{pr} \rightarrow \frac{\text{KiloJoule}}{\text{KilogramKelvin}}$
$\frac{E_1}{R} \rightarrow \text{Kelvin}$	$\frac{E_2}{R} \rightarrow \text{Kelvin}$
$k_{10} \rightarrow \frac{1}{\text{min}}$	$k_{20} \rightarrow \frac{1}{\text{min}}$
$T_{ri} \rightarrow \text{Kelvin}$	$T_{ci} \rightarrow \text{Kelvin}$
$T_r^s \rightarrow \text{Kelvin}$	$T_c^s \rightarrow \text{Kelvin}$

The Cost Function (CF)

In this research, the objective used to minimize the area arising as a difference of the process between the observed and real selected time interval, which was the duration of a CSTRs cycle. With the inlet concentration $c_{Bi} = 0$ kmol m^{-3}, the cost function, that was minimized is given in (7). In the cost function, we multiplied by (-1) in order to transfer from maximization into minimization.

$$f_{\cos t} = (-1) * \sum_{t=0}^{t} |c_B[t]| \quad (7)$$

Genetic Algorithm

Genetic Algorithms (GA) imitate the evolutionary processes with emphasis on genotype based operators (genotype/phenotype dualism). The GA works on a population of artificial chromosomes, referred to as individuals. Each individual is represented by a string of L bits. Each segment of this string corresponds to a variable of the optimizing problem in a binary encoded form.

The population is evolved in the optimization process mainly by crossover operations. This operation recombines the bit strings of individuals in the population with a certain probability *Pc*. Mutation is secondarily in most applications of a GA. It is responsible to ensure that some bits are changed, thus allowing the GA to explore the complete search space

even if necessary alleles are temporarily lost due to convergence.

The following pseudocode describes the general principle of a genetic algorithm (see JCell Documentation of A. Zell, http://www.ra.cs.uni-tuebingen.de/software/JCell/tutorial/tutorial.html):

```
t = 0;
initialize(P(t=0));
evaluate(P(t=0));
while is NotTerminated() do
P_p (t) = P(t).selectParent();
P_c(t) = reproduction(P_p);
mutace(P_c(t));
evaluate(P_c(t));
P(t+1) = buildNextGenerationForm(P_c(t), P(t));
t=t+1;
end
```

Figure 1. Pseudocode of GA

Parameter Setting

The control parameter settings have been found empirically and are given in Tab. 3. 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). Number of optimized reactor parameters and their range inside represents in Tab. 4.

Tab. 3 GA parameter setting

	A
PopSize	20
MutationCostant	0.2
Generations	200
Individual Length	6
CF Evaluations	4000

Tab. 4 Optimized reactor parameters and their range inside which has been optimization done

Parameter	Range
Q_c [m^3min^{-1}]	0.015 – 0.1
Q_r [m^3min^{-1}]	0.05 – 0.012
c_{Ai} [kmol m^{-3}]	2 – 3.5
T_{ri} [K]	303 – 333
T_{ci} [K]	288-303

EXPERIMENTAL RESULTS OF STATIC OPTIMIZATION REACTOR

Evolutionary algorithms (in this work using genetic algorithm) are partly of stochastic nature, a large set of simulations has to be done in order to get data for statistical data processing. The algorithms GA have been applied 100 times in order to find the optimum of process parameters and. All important data has been visualized directly or/and processed for graphs demonstrating performance of this algorithms. Estimated parameters and their diversity (minimum, maximum and average) are depicted (see Tab. 5). From Fig. 2 it is visible that results from GA algorithm are showed detail "optimal points". For the demonstration are graphically the solutions shown in Fig. 3- 6.

Tab. 5 Estimated parameters for GA

Parameter	Min	Avg	Max
Q_c [m^3min^{-1}]	0.0152769	0.0706135	0.0994583
Q_r [m^3min^{-1}]	0.105348	0.115416	0.119818
c_{Ai} [kmol m^{-3}]	2.00811	2.69678	3.49589
T_{ri} [K]	314.177	320.645	324.491
T_{ci} [K]	290.091	299.845	302.908
Q_c [m^3min^{-1}]	0.0152769	0.0706135	0.0994583

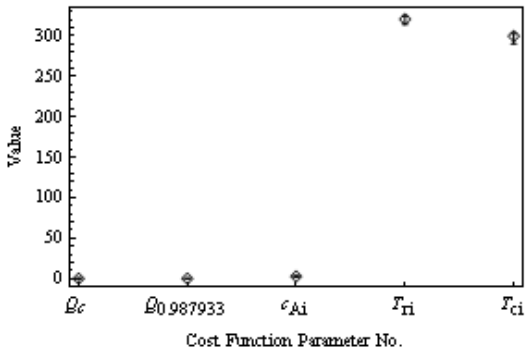

Figure 2. Parameter variation

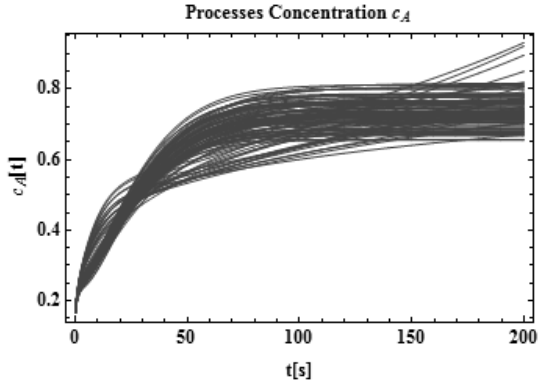

Figure 3. 100 simulations for c_A

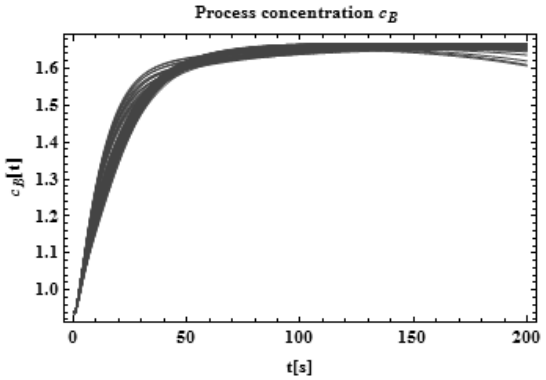

Figure 4. 100 simulations for c_B

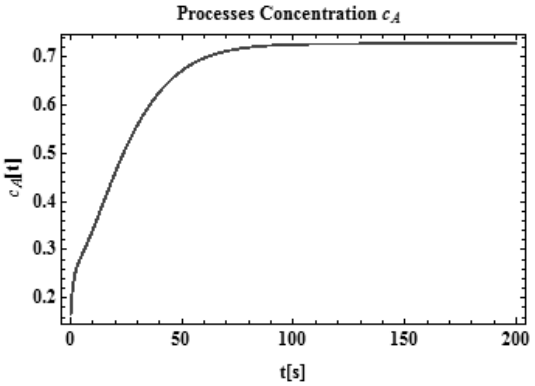

Figure 7. Best solution for c_A

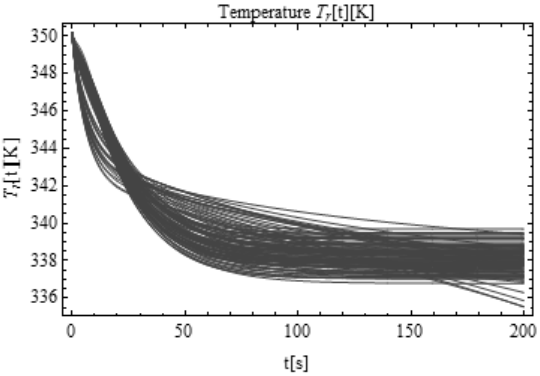

Figure 5. 100 simulations for T_r

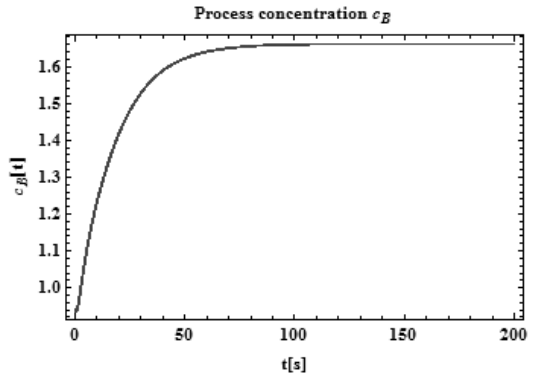

Figure 8. Best solution *for* c_B

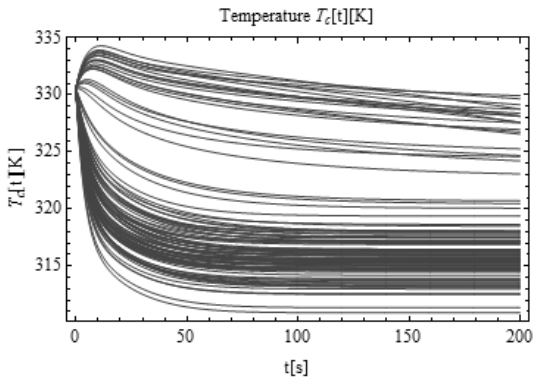

Figure 6. 100 simulations for T_c

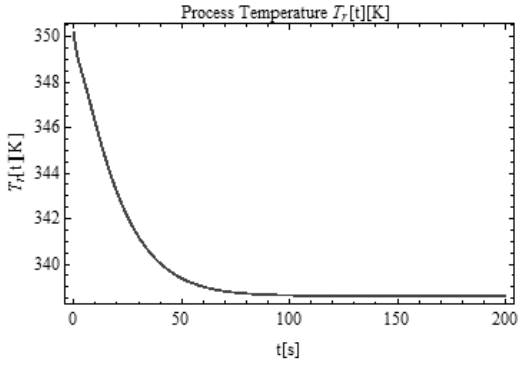

Figure 9. Best solution for T_r

From investigation on optimization of process parameter of CSTR we can see, that evolutionary algorithm GA has presented diversity of parameters (100 lines in diagram are processes of 100 simulation repeated). On optimization of GA, it is evident that the courses of algorithm are densities in a thin. Alongside it, sometime few values drift out of the actual solution. But by the repetition of simulation was recorded the best result. On Fig. 7 – Fig. 10, the processes of parameters by GA algorithm obtained best solutions for the optimization.

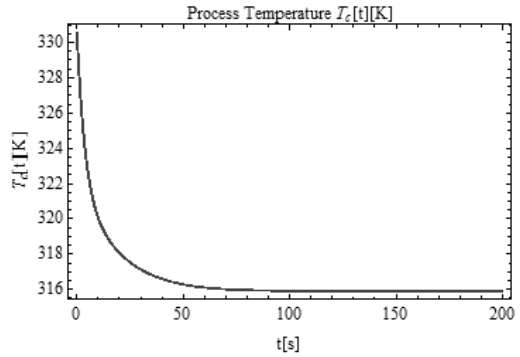

Figure 10. Best solution for T_c

OPTIMIZATION REACTOR WITH ADAPTIVE CONTROL

Adaptive control by mean evolutionary algorithms is very robust method, particular in system with many disturbing effects and failures. It's also a powerful tool in the search for optimal solutions to very complex problem in the field of control process. The basic idea is to find a set of action that lead to the principle optimization with required value. The block of adaptive control is shown in Fig. 11. (Tran, T.D., 2009).

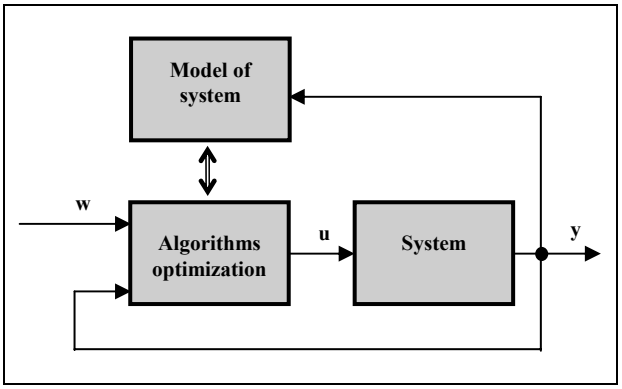

Figure 11. Principle of adaptive control by evolutionary algorithm

In block „Algorithms optimization“ are evolutionary algorithm (here is genetic algorithm), the adaptive control is selected by minimising the commonly cost function *J*:

$$J(N_1,N_2,N_u)=\sum_{j=N_1}^{N_2}[y(k+j)-w(k+j)]^2 + \sum_{j=1}^{N_u}\lambda(j)[\Delta u(k+j-1)]^2 \quad (8)$$

Here *y* is the output of system, *u* is actuating signal, *w* is the controlled value, Δu is the control value change, *k* is the control step, N_1 is the lower and N_2 is the upper output prediction horizon, *Nu* is control horizon and λ is a weight sequence control of action.

Block "system" is a control process and block "model system" is used to adaptive its behaviour, it often represented in the appropriate algorithms of artificial intelligent, commonly artificial neural network.

Adaptive control proceed when change of required value running optimization algorithms in conjunction with model of system and minimising cost function (8) is found optimal action, which is for chosen system.

This optimization was minimized 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 CSTR cycle. The cost function was minimized is given in (9) for T_c temperature and (10) for T_r.

$$f_{\cos t}=\sum_{t=0}^{t}\left|w_1-T_c[t]\right| \quad (9)$$

$$f_{\cos t}=\sum_{t=0}^{t}\left|w_2-T_r[t]\right| \quad (10)$$

Where w_1, w_2…are required values (control point)

For static optimization of CSTR reactor with adaptive control, we have added required value for simulation of temperature T_r and T_c belong following below Tab. 6. The range inside of temperature T_r and T_c for adaptive control is <273.;380> [K] (see Tab. 7).

Tab. 6 Range inside for adaptive control of CSTR

Parameter	Range
T_r [K]	273 – 380
T_c [K]	273 – 380

Tab.7 Parameters setting for adaptive control

Time simulation[s]	**Required value *for* T_r [K]**	**Required value *for* T_c [K]**
0 - 80	360	340
80 - 150	340	320
150 - 200	320	300
200 - 300	370	370

Simulation

Simulations were conducted so, that the first minimising cost function using the adaptive horizon is found within the optimal action and intervention that was held for the control horizon. After that, it was calculated new intervention and has been applied during control horizon etc. till to do filling of reactor. For the CSTR reactor, required values were selected: N_1 = 1, N_2 =300 a N_u = till to change.

EXPERIMENTAL RESULTS OF OPTIMIZATION REACTOR WITH ADAPTIVE CONTROL

On investigation of adaptive control chemical reactor CSTR, at the same principle setting parameter of GA and the algorithm have been applied 100 times. The evolutionary processes of temperature that control by GA algorithm show in follow graphs from Fig. 12-13.

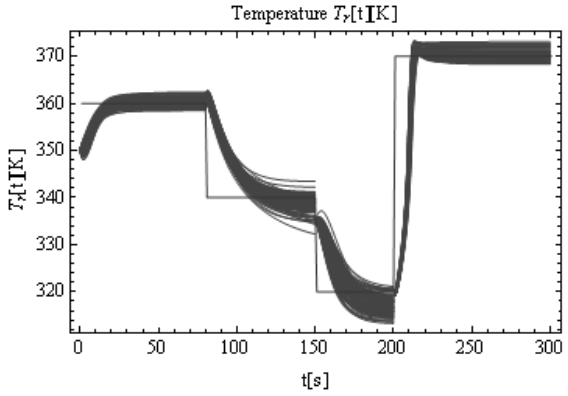

Figure 12. Evolutionary process for T_r

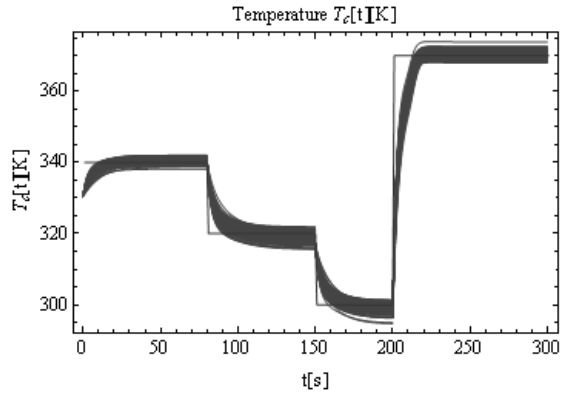

Figure 13. Evolutionary process for T_c

CONCLUSION

This work was performed static optimization and adaptive control on non-linear system using genetic algorithms. Based on these results it can be stated as follows:

- Genetic algorithm is used successfully to static optimise and adaptive control of a chemical reactor process.
- 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 Tab. 5.
- From the graphs, we have chosen the best solution of process parameters. Alongside it, sometime few values drift out of the actual solution. From Fig. 3 - Fig. 6 we have defined the cost function by concentration c_B and it obtained optimal value for the optimization of process parameters CSTR. On the pictures of Fig. 12 and Fig. 13 shown the evolutionary processes of temperatures T_r and T_c of reactor by definition of the cost function in (9) & (10).
- The optimizations and control chemical reactor have been performed in several ways, each one for a different set of reactor parameters or different cost function. From the obtained results, it is possible to say that all simulations give satisfactory results and thus genetic algorithm is capable of solving this class of difficult problems and the quality of results does not depend only on the problem being solved but they are extremely sensitive on the proper definition of the cost function, selection of parameters setting of algorithm.

From this work GA have shown good potential and ability to solve complex problems of optimization, not only at the filed of chemical engineering process but also in diverse industrial fields.

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