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Maximum principle vs genetic algorithms in optimization of a plug flow chemical reactor

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Abstract. There are presented two methods for optimization of a plug flow tubular chemical reactor for o-xylene catalytic oxidation to phthalic anhydride: maximum principle and a genetic algorithm. Mathematically, this reactor described by differential equations is a system with distributed parameters. The objective consists in the maximization of effluent concentration of phthalic anhydride by a suitable temperature policy along the reactor. Despite the fact that genetic algoriths were very seldom applied to optimization of systems with distributed parameters, in the present case all the four solutions obtained by the genetic algorithm are better than the solution obtained with maximum principle (up to 7.2 %). Unfortunately, these solutions have mainly theoretical significance, the practical implementation being momentanly problematic.

Keywords. Optimal control, chemical reactor, maximum principle, genetic algorithms

1. Introduction

The plug flow chemical reactors are systems with distributed parameteres described by models containing differential equations. Usually, in these reactors take place several reactions, especially in organic chemical industry. In the total production price of a chemical product the cost of raw materials has a weight of around 80 % [1]. In this circumstance, a very important optimization problem, with a strong economic implications, consists in establish the best control policy which maximize the selectivity in the desired product. To solve this kind of problems is not easy. Here are presented two methods for optimization of a plug

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flow tubular chemical reactor for o-xylene catalytic oxidation to phthalic anhydride: maximum principle [2–4] and genetic algorithms [5–7]. Also, an useful comparison of the performances of these methods is exposed.

2. Plug flow reactor for o-xylene catalytic oxidation to phthalic anhydride

Phthalic anhydride is an important industrial chemical, especially for the large-scale production of plasticizers for plastics [8]. The main industrial process for obtaining of phthalic anhydride consists in o-xylene oxidation catalyzed by vanadium pentoxide (V_2O_5). In commercial processes, o-xylene is generally oxidized in the gas phase with an excess of air over a fixed bed catalysts arranged in multitube reactors with up to 10000 tubes [9]. In the intertubular space are flowing molten salts as cooling agent. This is recycled through a steam generator in order to increase the energy efficiency.

As a numerical application is considered that the oxidation of o-xylene to phthalic anhydride take place in a tubular catalytic reactor with 2500 tubes, each having the internal diameter of 0.025 m and the length of 3 m [10, 11]. The heat of reaction is removed in the intertubular space by molten salts. The total feed flowrate of the reactor is 4684 Nm^3/h. The feed mole fraction of o-xylene is 0.0093, and of oxygen 0.208. The average pressure in the reactor is 1.75 at and the bulk density of the catalyst (V_2O_5 on α-Al_2O_3) is 1300 kg/m^3. It will be used the next kinetic model of o-xylene oxidation [12]:

$$C_8H_{10} + 3\,O_2 \xrightarrow{k_1} C_8H_4O_3 + 3\,H_2O$$

$$C_8H_4O_3 + O_2 \xrightarrow{k_2} 8\,CO_2 + 2\,H_2O$$

$$C_8H_{10} + 21/2\,O_2 \xrightarrow{k_3} 8\,CO_2 + 5\,H_2O$$

The corresponding reaction rates (expressed in $kmol/m^3h$) are:

$$v_{R1} = k_1\, p_A\, p_O\, \rho_c = k_1\, P^2\, y_A\, y_O\, \rho_c \tag{1}$$

$$v_{R2} = k_2\, p_B\, p_O\, \rho_c = k_2\, P^2\, y_B\, y_O\, \rho_c \tag{2}$$

$$v_{R3} = k_3\, p_A\, p_O\, \rho_c = k_3\, P^2\, y_A\, y_O\, \rho_c \tag{3}$$

where the indices A, B, O indicate o-xylene, phthalic anhydride, and oxygen, p and y are the corresponding partial pressures and mole fractions, ρ_c is the bulk density of the catalyst, and P is the average total pressure expressed in at.

The constants of reaction rates are the following expressions:

$$k_1 = 4.12 \cdot 10^8 \exp(-13500 / T) \tag{4}$$

$$k_2 = 1.15 \cdot 10^9 \exp(-15500 / T) \tag{5}$$

$$k_3 = 1.73 \cdot 10^8 \exp(-14300 / T) \tag{6}$$

the temperature T being expressed in absolute degrees.

Taking into account the relation of transformation of molar fractions into molar concentrations:

$$y_i = c_i\, R\, T / P \tag{7}$$

where the constant of the ideal gas R has the value 0.082 $at{\cdot}m^3/kmol{\cdot}K$, the expressions of the reaction rates can be rewritten as:

$$v_{R1} = \beta\, k_1\, T\, c_A \tag{8}$$

$$v_{R2} = \beta\, k_2\, T\, c_B \tag{9}$$

$$v_{R3} = \beta\, k_3\, T\, c_A \tag{10}$$

were β is the group of constants:

$$\beta = P\, R\, \rho_c\, y_O \tag{11}$$

(oxygen being in excess, the corresponding concentration y_O can be considered constant).

The conservation equations of o-xylene and phthalic anhydride for an infinitesimal element of length dl of the plug flow reactor are:

$$u\frac{dc_A}{dl} = -v_{R1} - v_{R3} \tag{12}$$

$$u\frac{dc_B}{dl} = v_{R1} - v_{R2} \tag{13}$$

where u is the gas velocity inside the reactor.

Defining the dimensionless length $z = l\,/\,L$ where L is the total length of the tube reactor, and replacing the expressions of reaction rates from eqs (8) – (10) into eqs (12) – (13), it obtained:

$$\frac{dc_A}{dz} = -C\,T\,(k_1 + k_3)\,c_A \tag{14}$$

$$\frac{dc_B}{dz} = C\,T\,(k_1 c_A - k_2 c_B) \tag{15}$$

were C is the group of constants $\beta\, L\,/\,u$.

The velocity u is the ratio between volumetric flow rate and the total cross section:

$$u = \frac{G_v}{\frac{\pi d^2}{4} N_t} \tag{16}$$

where d is the internal diameter of the tube, and N_t is the total number of tubes. Replacing with numerical values in the group of constants C gives:

$$C = \frac{\pi\, d^2\, N_t\, P\, R\, \rho_c\, y_O\, L}{4 G_v} = 0.0305 \tag{17}$$

This value will be substitutes in eqs (14) – (15). According with the relation (7) between molar fractions and molar concentrations, the initial conditions for the first order differential equations (14) and (15) are:

$$\text{At } z = 0 \;:\; c_{A0} = 3.26 \cdot 10^{-4} \;\text{ and }\; c_{B0} = 0 \tag{18}$$

In the system of the two differential equations (14) and (15) with the initial conditions (18) there are three distributed variables: $c_A(z)$, $c_B(z)$, and $T(z)$ (the last by the constants of reaction rates $k_1 - k_3$, defined in eqs (4) – (6)). Therefore, is one degree of freedom. To obtain a solution of this system is necessary to impose values for T(z). An optimization problem consists in the establish of the values for $T(z)$ which gives the maximum of c_B at the outlet of the reactor, respectively at z = 1. This problem will be solved by two quite different methods: maximum principle (MP) and a genetic algorithm (GA).

3. Maximum principle

Pontryagin's maximum (or minimum) principle is used in optimal control theory to find the best possible control for taking a dynamical system from one state to another, especially in the presence of constraints for the state or input controls. It was formulated in 1956 by the Russian mathematician Lev Pontryagin and his students [2]. It has as a special case the Euler–Lagrange equation of the calculus of variations.The principle states, informally, that the control Hamiltonian must take an extreme value over controls in the set of all permissible controls. Whether the extreme value is maximum or minimum depends both on the problem and on the sign convention used for defining the Hamiltonian. The normal convention, which is the one used in Hamiltonian, leads to a maximum hence maximum principle. The initial application of this principle was to the maximization of the terminal speed of a rocket.

The general formulation of a problem that can be solved by MP is:

- it must be established the optimum value of the functional f:

$$Opt\ f = \int_{z_0}^{z_F} F[\mathbf{x}(z), \mathbf{D}(z)]dz \qquad (19)$$

- subject to the local restrictions:

$$\frac{d\,x_i}{dz} = h_i\,[\mathbf{x}(z), \mathbf{D}(z)] \qquad i = 1, 2 \ldots n \qquad (20)$$

- with initial conditions:

$$x_i = x_{i0} \quad \text{at} \quad z = z_0 \qquad (21)$$

A necessary, but not sufficient condition for functional f to be maximum (or minimum) consists in selecting of functions $\mathbf{D}(z)$ so as to maximize (or minimize) the Hamiltonian H:

$$H = F + \sum_{i=1}^{n} \lambda_i\,(z)\,h_i\,[\mathbf{x}(z), \mathbf{D}(z)] \qquad (22)$$

where $\lambda_i\,(z)$ are Lagrange multipliers.

An usual procedure [11] to solve this problem consists in the use of the gradient of Hamiltonian following the next steps:

1. For the control functions $\mathbf{D}(z)$ are given values over the entire domain [z_0 - z_F];
2. It is solved (usual numerical) the system of the local restrictions (20) in which $\mathbf{D}(z)$ has the anterior values, and are obtained the values of $\mathbf{x}(z)$.
3. The Lagrange multipliers $\lambda(z)$ are obtained by integration (usual numerical) of the differential equations system:

$$\frac{d\lambda_i}{dz} = -\sum_{j=1}^{n} \frac{\partial h_j}{\partial x_i} \lambda_j - \frac{\partial F}{\partial x_i} \qquad i = 1, 2 \ldots n \qquad (23)$$

- with the boundary conditions:

$$\lambda_j = 0 \quad \text{at} \quad z = z_F \qquad (24)$$

4. The assumptions made at the step 1 are improved using the gradient of Hamiltonian:

$$\mathbf{D}^{(k+1)}(z) = \mathbf{D}^{(k)}(z) + p\frac{\partial H^{(k)}}{\partial \mathbf{D}} \tag{25}$$

where *k* is the iteration count, and *p* is the step on gradient direction.

5. If $\frac{\partial H^{(k)}}{\partial \mathbf{D}} \neq 0$ the procedure is resumed from step 2.

For optimization of the tubular reactor for o-xylene catalytic oxidation to phthalic anhydride using MP the maximization of the effluent concentration of phthalic anhydride correspond to maximization of the the functional:

$$\max f = \max \int_0^1 \frac{dc_B}{dz}\, dz \tag{26}$$

If *F* is the primal of the functional *f*, it can be observed that this is identical with right hand term h_2 of the local restriction (15):

$$F = \frac{dc_B}{dz} = h_2 \tag{27}$$

Using the notation h_1 and h_2 for the right hand terms of the local restrictions (14) – (15) , the applied expressions of eqs (23) are:

$$\frac{\partial \lambda_1}{\partial z} = -\frac{\partial h_1}{\partial c_A}\lambda_1 - \frac{\partial h_2}{\partial c_A}\lambda_2 - \frac{\partial F}{\partial c_A} \tag{28}$$

$$\frac{\partial \lambda_2}{\partial z} = -\frac{\partial h_1}{\partial c_B}\lambda_1 - \frac{\partial h_2}{\partial c_B}\lambda_2 - \frac{\partial F}{\partial c_B} \tag{29}$$

After substitutions of derivatives in the previous equations and the substitution:

$$\overline{\lambda}_2 = \lambda_2 + 1 \tag{30}$$

the eqs (28) –(29) became:

$$\frac{\partial \lambda_1}{\partial z} = CT\left[(k_1 + k_3)\lambda_1 - k_1\overline{\lambda}_2\right] \tag{31}$$

$$\frac{\partial \overline{\lambda}_2}{\partial z} = CT\,k_2\,\overline{\lambda}_2 \tag{32}$$

- with the boundary conditions:

$$\text{At } z = z_F, \quad \lambda_1 = 0; \quad \overline{\lambda}_2 = 1 \tag{33}$$

The expression of Hamiltonian is:

$$H = F + \lambda_1 h_1 + \lambda_2 h_2 = \lambda_1 h_1 + \overline{\lambda}_2 h_2 \tag{34}$$

and the corresponding gradient is:

$$\frac{\partial H}{\partial T} = \lambda_1 \frac{\partial h_1}{\partial T} + \bar{\lambda}_2 \frac{\partial h_2}{\partial T} \tag{35}$$

The procedure of maximizing the Hamiltonian using its gradient has started with assuming an integration step $\Delta z = 0.1$, and an initial temperature (control variable) of 633 K (isothermal regime) for all the length steps. At the second step were integrated the local restrictions (14) – (15) with corresponding initial conditions (18). The integration was made by Runge-Kutta fourth order method with constant step (Matlab function *ode45* [13]). At the third step were computed the Lagrange multipliers by integration of eqs (31) – (32) with the boundary conditions (33). It was used the same numerical method, starting at the end of integration domain, and using a negative integration step. The initial assumed temperatures were improved using recursive relation (25), where the gradient of Hamiltonian was given by eq (35). The value of the step on gradient direction p was 10 for the first 10 iterations, and 1 for the next iterations.

The optimal solution, corresponding with the vanish of the gradient of Hamiltonian was obtained after 27 iterations. The first iteration (isothermal regime) and the optimum solution are given in Table 1. The optimal solution is also represented in Figs. 3 and 4, in confrontation with the solutions obtained by GA. It can be observed that the increase of effluent concentration of phthalic anhydride is realized by temperature decreasing along the reactor which favorize the selectivity in the desired product. In this way is prevented phthalic anhydride subsequent oxidation to carbon dioxide and water. In the isothermal regime the concentration of phthalic anhydride attains a maximum value of $2.233 \cdot 10^{-4}$ mol/L at the middle length of reactor, and next decreases due to oxidation reaction.

Table 1. Temperatures (K) and concentrations profiles (mol/L) for isothermal and optimal regime

	Isothermal regime			Optimal regime		
z	T	$c_A \cdot 10^{-4}$	$c_B \cdot 10^{-4}$	T	$c_A \cdot 10^{-4}$	$c_B \cdot 10^{-4}$
0	633	3.260	0	626.43	3.260	0
0.1	633	2.004	1.092	620.20	2.274	0.866
0.2	63	1.232	1.709	616.97	1.691	1.356
0.3	633	0.757	2.036	614.96	1.296	1.671
0.4	633	0.465	2.187	613.60	1.011	1.884
0.5	633	0.286	2.233	612.62	0.798	2.030
0.6	633	0.176	2.217	611.90	0.634	2.131
0.7	633	0.108	2.164	611.36	0.507	2.199
0.8	633	0.066	2.092	610.95	0.408	2.243
0.9	633	0.041	2.009	610.62	0.328	2.268
1	633	0.025	1.929	610.37	0.265	2.278

It can be observed that in optimal regime the conversion of o-xylene is lower than in isothermal regime (the outlet concentration of o-xylene for optimal regime is more than 10 times greater than in isothermal regime). Therefore, the increase of effluent concentration of phthalic anhydride with 18% comparing with isothermal regime is exclusively due to the increasing of selectivity, and not due to the increse of the reference reactant conversion.

4. Genetic Algorithms

Appeared and developed in 1970s, GA were recognized as a valuable optimization tool after more than a decade, because the progress in computational capacities of modern computers. Inspired from the process of natural selection of biological organisms which the evolution theory of Darwin has condensed into the words ”survival of the fittest”, GA have several features [5,7] which differentiate them from other general optimization algorithms and search procedures:

-the representation of parameters on chromosome-like structure; the parameters are either binary encoded or directly stored, for a fast retrieval and processing;

- the optimal value is searched for a within group of possible solutions, seen as a population of points, as opposed to searching on a sequential one-by-one points;
- the result of the objective function is used to compute a fitness value which is assigned to each individual; there is no need to employ derivatives or other additional information to the problem;
- several probabilistic instead of deterministic rules are used to generate new solutions; these are expressed as genetic operators which are applied in order to create new offspring from the best fitted individuals.

There are tens of variants of GA [5-7], but all of them have common the principles of probabilistic selection of the individuals from a population based of their fitness and the generation of new offspring with several genetic operators.

The GA used here consists in the next steps:

[1] The codification and generation of initial population: this consists in 40 chromosomes, each of them having 11 genes (Fig.1). Each gene represent a value of temperature thus: the first gene correspond to the temperature in the first reactor length step (z = 0 to 0.1), the next gene correspond to the temperature in the second reactor length step (z = 0.1 to 0.2), and so on, up to the last eleven reactor length step (z = 0.9 to 1).

Fig. 1. Genetic structure of each chromosome.

The generation of the genes values for each chromosome in the domain [T_{min} - T_{max}] was made with the relation:

$$T_i = T_{min} + r\,(T_{max} - T_{min}) \qquad i = 1,2...11 \qquad (36)$$

where r is a pseudo-random number generated by computer in the range [0 - 1].

[2] Evaluation of the chromosomes finess: this is the objective function, respectively the effluent concentration of phthalic anhydride c_B at $z = 1$. This was made in the user fitness function (named *roc* in Matlab) which involves the numerical integration of differential eqs (14) – (15) by Runge-Kutta fourth order method with constant step (Matlab function *ode45* [13]). There was used the same integration method with the procedure in MP, in order to make a fair comparison.

[3] Probabilistic selection of chromosomes for offsprings generation: this selection is not deterministic, the probability of selection is proportionally with the fitness values. A frequent method used is so called ’roulette wheel’[6].

[4] Application of genetic operators: the most frequently operators used are crossover and mutation. In crossover two selected chromosomes generates two or more offsprings. A crossover with two parents and two offsprings (childs) with one cutting point is represented in Fig. 2.

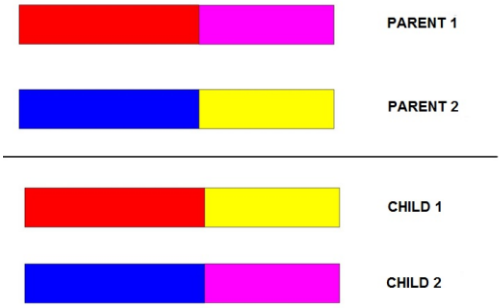

Fig. 2. A crossover with two parents and two offsprings (childs) with one cutting point.

By crossover there are not generated new solutions as there were present in the initial population. The generation of new solutions are made by mutation: the values of some genes in some chromosomes are slightly perturbed to new values. The proportion of mutation must be low (usually up to 5%) in order not to perturbate the evolutionary character of GA.

[5] The generation of a new population: in function of fitness values some chromosomes are probabilistic retained in the new generation, others are replaced with the new offsprings.

There are different stopping criteria of the GA: a maximum number of generation, a maximum computer time, a minimum value of tolerance function (a lower bound on the change in the best value of fitness during one generation), etc.

Here are presented the results of four case studies of optimization of the tubular chemical reactor for o-xylene catalytic oxidation to phthalic anhydride using GA. It was used for GA the Matlab function *ga* [13] that calls the function *roc* for chromosomes fitness evaluation. In all four cases were used the same following main parameters of GA: size of initial population = 40; population type: double vector; crossover fraction = 0.8; selection function: stohastic uniform; mutation function: Gaussian distribution centered on zero; stopping criteria: function tolerance = 10^{-24}. The diferences between the four cases were the domain of the initial population presented in Table 2. In this table are also indicated the best solutions, the comparison with the optimum solution obtained by MP, and the total number of generations. It must be noted that because the probabilistic components of GA, the total number of generations can be different from each run of *ga*.

Table 2. The four solutions obtained by GA

Case	Domain of initial population T_{min} - T_{max}	Best solution c_B at z=1	Comparison with MP	Number of generations
GA1	600 - 630	$2.282 \cdot 10^{-4}$	+ 0.176%	679
GA2	600 - 650	$2.295 \cdot 10^{-4}$	+0.746%	965
GA3	600 - 700	$2.354 \cdot 10^{-4}$	+3.336%	972
GA4	550 - 700	$2.442 \cdot 10^{-4}$	+7.199%	1000

In the Table 3 and in Figs. 3 and 4 are presented for the four cases the corresponding profiles of temperatures and concentrations of phthalic anhydride.

Table 3. The profiles of temperatures and concentrations of phthalic anhydride for cases GA1-GA4

	GA1		GA2		GA3		GA4	
z	T	$c_B \cdot 10^{-4}$	T	$c_B \cdot 10^{-4}$	T	$c_B \cdot 10^{-4}$	T	$c_B \cdot 10^{-4}$
0	630	0	607.43	0	600	0	585.53	0
0.1	620.05	0.792	600	0.415	600	0.041	558.68	0.096
0.2	630	1.475	650	1.683	600	0.075	668.41	2.152
0.3	619.32	1.795	634.84	2.109	600	1.038	652.52	2.486
0.4	600	1.912	600	2.165	600	1.283	550.53	2.483
0.5	611.42	2.044	600	2.209	683.56	2.959	567.17	2.476
0.6	610.29	2.138	600	2.242	612.87	2.654	565.69	2.470
0.7	609.57	2.203	600	2.266	600	2.568	570.53	2.462
0.8	609.01	2.245	600	2.282	600	2.490	566.23	2.455
0.9	608.56	2.270	600	2.291	600	2.420	564.94	2.448
1	608.23	2.282	600	2.295	600	2.354	563.69	2.442

Despite the fact that all these solutions are superior with the solution obtained by MP, the value of these policies are theoretical, not practical. For GA2, GA3 and GA4 the temperature profiles correspond to bang-bang controls. Mathematically or within a computing context there may be no problems, but the physical realization of bang-bang control systems gives rise to several complications [14].

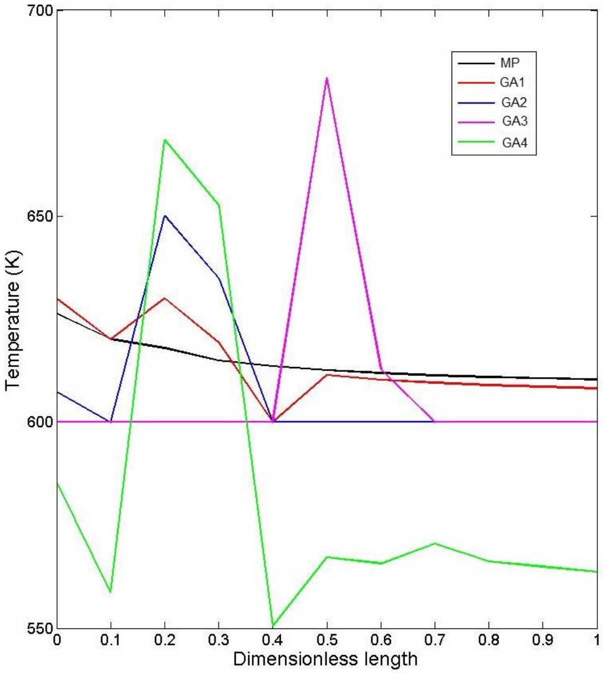

Fig. 3. The temperature profiles for the best solutions of MP and GA1-GA4.

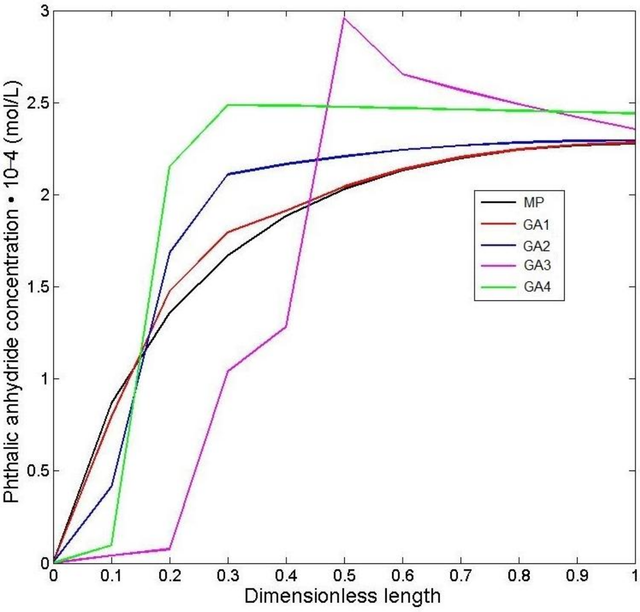

Fig. 4. The concentrations profiles of phthalic anhydride
for the best solutions of MP and GA1-GA4.

An exemplification of GA evolution (for the case GA3) is represented in Fig. 5. Because function *ga* is a minimization procedure, for fitness maximization was considered the negative value of c_B.

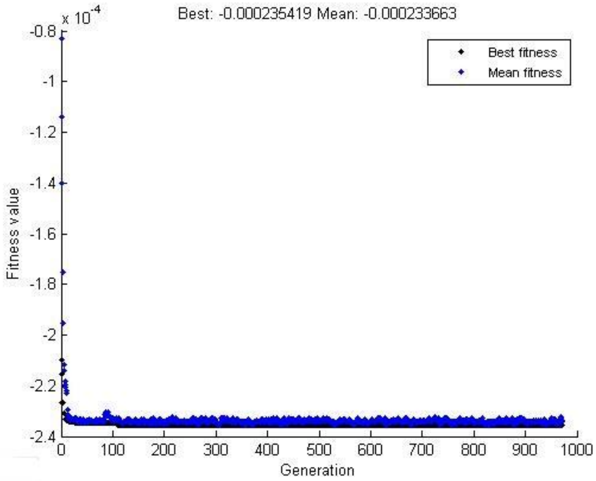

Fig. 5. Exemplification of GA evolution (case GA3).

Taking into account the above best temperature profiles (established by MP and GA), the heat of reaction, and heat transfer from the reactor, it can be obtained temperatures profiles at the external wall of the tubes. These profiles will be also variable along the tube length. It is very difficult, practical impossible, to realize these temperature profiles. The industrial reactor is cooled with molten salts which are flowing in the intertubular space, and in these conditions the temperature at the external wall of the tubes is, in fact, constant, the internal temperature profile having a maximum. This internal temperature profile is not favorable for the selectivity in the desired product. An avangard method will be to cool the reactor by evaporation (under pressure) a binary mixture with the vaporization curve close to the external tube optimal temperature profile.

5. Conclusions

It was demonstrated the ability of GA to solve optimal control problems for systems with distributed parameters described by models containing differential equations. Despite the fact that GA is nowadays a frequently used optimization technique, this method was very seldom applied in the field of systems with distributed parameters. For this kind of optimization problems was frequently used MP, an old and classical method. It is known that in optimal control there are present a lot of local optimum solution, much more than in scalar optimization problems. The advantage of GA is the fact that are finding a lot of local optimal solution, and sometimes in a fortunate case, the global optimum. Here, GA has found four solutions better than the optimum obtained with MP. These solutions were obtained by modification of the initial population domain. Other solutions can be obtained by modification of other GA parameters. A raffination of the solutions obtained both with MP and GA is possible by decreasing of integration step, but it was not the aim of these investigations to obtain raffinated solutions. As it was already mentioned, it is very difficult to apply optimal control to spatially distributed systems. Therefore, the solutions obtained here for optimization of the tubular cathalitic reactor for o-xylene catalytic oxidation to phthalic anhydride, a very important industrial and economic application, are useful mainly from theoretical point of view, than practical. But, in the future, due to technical evolution, practical application must not be excluded. For time distributed systems, such as temperature control in a well mixed batch reactor, the implementation of optimal policies do not lift up no problems. Due to the actual and future performances of control devices, this is also true for bang-bang control.

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