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Optimization for large scale process based on evolutionary algorithms: Genetic algorithms

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Abstract

This work has as objective the development of an optimization methodology, using Genetic Algorithms (GAs), as evolutionary procedure coupled with the concepts of evolutionary. As case study a large scale multiphase catalytic reactor is considered. The reactor is tubular in shape and is built-up with concentric tubes using the same concept of the auto-thermal reactors, with coolant fluid flow in the external annular. The mathematical equations of the deterministic model are based on conservation principles (mass, energy and momentum) for the reactants and for the coolant fluid and validated with real operational data. The model represents the steady-state with the plug-flow assumption which is quite reasonable due to the large flow rates usually found in industrial reactors. The desired product is a specific cyclical alcohol (CA), and the minimization of the by-products is required for economical and environmental reasons. For that it is necessary to optimize some important operational parameters. This problem is of difficult solution since the reactor is a large scale system with complex behavior and conventional optimization tools as Successive Quadratic Programming tends to fail in such situation since local minima may be achieved.

In this work is shown that the Genetic Algorithms technique can be useful to CA production maximization, obtaining good results with operational improvements (reduction in the catalyst rate, as well as in the undesired product rate—cycloalkane (C)). The GA parameters used for the process optimization are population size, crossover types with variation of crossover rates. The used coding was the binary form.

The results are quite good, showing high performance in the CA productivity (considerable increase CA production) with changes in the operational parameters analyzed and showing that this optimization procedure is very robust and efficient. The results point out that this technique is very promising to deal with large scale system with complex behavior due to non-linearity and variable interactions.

Keywords: Global optimization; Genetic algorithms; Three phase catalytic reactor

1. Introduction

Multiphase catalytic reactors, where hydrogenation reactions take place are important systems usually working at very high throughput. In such conditions very small process improvements will cause a significant financial earn. A typical process of industrial interest is the hydrogenation of *ortho*-cresol [1]. The deterministic mathematical model used to describe the reactor is based on the work by Victorino [2], and Santana [3]. A series of parallel and consecutive reactions may happen, so that the reactor has to be operated in a suitable way to achieve high conversion as well as high selectivity.

Usually for large scale system, the reactor is constituted of a series of tubes, cooled by coolant flowing in a jacket around the tubes.

In this work the objective is to find the best operating conditions of a Cyclic Alcohol (CA) reactor, which involves the hydrogenation of a specific benzylic alcohol (main reactant—BA). This system presents a complex behavior and existence of a great energy expense associated to the pressures and temperatures variations in the operation of the process. As the reactor is a non-linear multivariable distributed parameter system leading to a system of differential equations, the optimization problem is a hard task and conventional optimization methods have shown severe limitations, especially in terms of convergence. Bearing this in mind in this work is proposed an optimization procedure based on Genetic Algorithms method.

Abbreviations: GA, genetic algorithm; GAs, genetic algorithms; CA, cyclic alcohol; BA, benzylic alcohol; CEX, cycloalkene; C, cycloalkane; Not Opt., not optimized

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Nomenclature

b_1, b_2, b_3 kinetic parameters (constants or dependent temperature)
C_1 represents the benzylic alcohol mole fraction in the liquid phase
C_2, C_3 cyclic alcohol and water mole fraction, respectively (%)
C_{cat} catalyst concentration
C_{pi} calorific capacity (component *i*), (kJ/kg K)
D diameter of tubes (m)
F molar flow (kmol/h)
F_i catalyst activity factor
h heat transfer coefficient (kJ/m^2 s K)
ΔH_1, ΔH_2 main and secondary reaction enthalpies, respectively
ΔH_R heat of reaction (kJ/kmol)
k_1, k_2, k_3 kinetic constant (represented Arrhenius function) (kmol/kg cat s)
k constant of superficial reaction rate
L reactor length (m)
Q mass flow (kg/h)
Q_{cat} flow mass catalyst (kg/h)
Q_{ri}'s flow mass coolant fluid (kg/h)
r reaction rate
r_i rate reaction of catalytic process (associated with the catalyst concentration) (mol *i*/min m^3)
R_A reaction rate express (mol BA/min g catalyst)
R_{ei} reaction effective rate
R_i reaction rate without catalyst
t time of reaction (h)
T temperature in the expressions of the kinetic constant (K)
T_0 feed reactant temperature (°C)
T_r Coolant temperature (°C)
T_{R0} Fed coolant fluid temperature (K)
T_S Boiler saturation temperature (K)
U_1, U_2, U_3 global coefficients of heat transfer tube-cooling, anule-cooling and anule-boiler fluid, respectively, (kJ/m^2 s K)
X_{BA}, X_{CA} main reactant (BA) and cyclic alcohol (CA) conversion, respectively (%)
z dimensionless reactor axial position

Subscripts
0 referring to initial conditions
1i, 1e inner and outside diameters of tube 1
2i, 2e inner and outside diameters of tube 2
3i, 3e inner and outside diameters of tube 3
4i, 4e inner and outside diameters of tube 4
BA component BA
C component C
CA component CA
e effective value
g gas phase
l liquid phase
r coolant fluid
R referring to cooling fluid

Superscript
s catalyst surface

The literature supplies innumerable genetic codes that can be adapted and be used in diverse applications. In this study the Carroll's genetic code (1996) was adopted, since it is relatively easy to be adapted for the problem and very good results have been achieved for several interesting application.

2. Genetic algorithms (GAs)

These algorithms are an optimization procedure developed based on the principles of natural selection (Holland [4]; Goldberg [5]). The GA initiates with a population of represented random solutions in some series of structures. After this first stage, a series of operators, are applied repeatedly, up to convergence is achieved. In fact the optimization procedure based in such approach can be considered as a global optimization method with the advantage to do no be dependent upon the initial value to achieve the convergence. Most probably the more significant disadvantages are the computer time and burden required. The operators are: coding, reproduction, crossover and mutation. These two last operators are used to create new and better populations. This procedure continues until a termination criterion defined according to the need to achieve the goal in the optimization problem is reached. The determination of the parameters is made through the development of an objective function that represents the problem in a suitable way. The application of the GA follows some steps as: coding, determination of the population size, selection (reproduction), crossover and mutation.

In the binary codification, the following parameters have to be analyzed in order to achieve a good optimization algorithm performance: population sizes, chosen to be analyzed between 10 and 40; crossover operator, in two forms to know, uniform and of single-point; the selection form adopted is the tournament one. The elitism and the mutation (Jump and Creep mutation) are fixed values. Fig. 1 shows a flowchart of the reactor optimization problem.

3. Process description

The hydrogenation plant is composed by storage tanks of catalyst and reactants, a heat exchanger system to lead the feed streams at desired temperature conditions, the reactor, and a splitting system which has as objective to separate the liquid phase from the solid catalyst (slurry of catalyst, reactants and formed products). As the reaction is highly exothermic a cooling system is coupled to the reactor to remove the reaction heat. To attend the high production demand a set of tubular modules are usually used with a cooling system that can be individual to each module of tubes which, in principle may have different

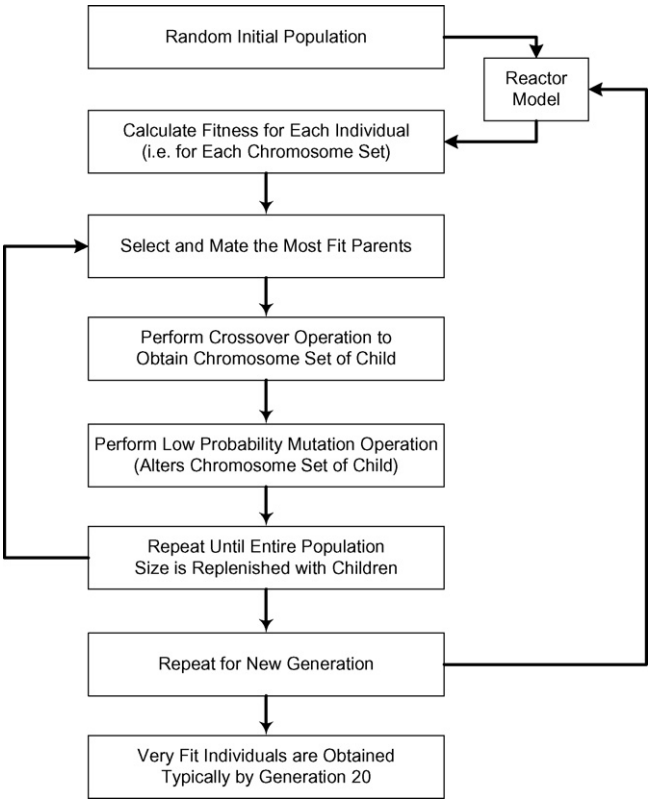

Fig. 1. Flowchart of Genetic Algorithm optimization reactor, based in Victorino [2] and Carroll [8].

temperatures T_r and coolant flow (Q_{r1}, Q_{r2}, ...). The sum of the lengths of each of these tubular modules where the reaction take place, from the first to the last module, is defined as Axial Reactor Length. The cooling system applied to each module of tubes will provide more operational flexibility although it is an expensive arrangement especially for different temperatures. Thus, in order to have a more realistic view of the system the same coolant temperature is adopted but different coolant flow rates can be used.

The reaction of hydrogenation of BA is exothermic, and depending on the operating temperature of the reactor as well as of catalyst flow, some products can be formed, such as ketones, or alicyclic alcohols, aromatic and alicyclic hydrocarbons. The reactions that occur in the system are described in Eqs. (1)–(3):

$$\text{Benzylic alcohol (BA)} + H_2 \xrightarrow{\text{catalyst}} \text{Cyclic alcohol (CA)} \quad (1)$$

$$\text{Cyclicalcohol (CA)} \rightarrow \text{Cycloalkene (CEX)} + H_2O \quad (2)$$

$$\text{Cycloalkene (CEX)} \rightarrow \text{Cycloalkane (C)} + H_2O \quad (3)$$

where CA is the desired product, and C is the undesired product.

The reactor model is a set of differential equations, considering two regions of each reactional module: tubular and annular. In the sequence the mass and energy balances for the BA and CA, respectively, are presented. In this work the reactor was considered at steady-state regimen.

The reactor design is such that different flow rates of coolant may be used in each zone of the reactor, since this increases the operational flexibility as shown for a fixed bed catalytic reactor.

3.1. Model equations

The equations are customized to the situation of the CA-reactor from the general mass and energy balance equations by Froment and Bischoff [6].

Mass balance for benzylic (4) and cyclic (5) alcohols—tubular region:

$$\frac{dX_{BA}}{dz} = \frac{\pi D_{1i}^2}{4}\frac{1}{F_{BA_0}} R_{eBA} \quad (4)$$

$$\frac{dX_{CA}}{dz} = \frac{\pi D_{1i}^2}{4}\frac{1}{F_{CA_0}} R_{eCA} \quad (5)$$

Mass balance for benzylic (6) and cyclic (7) alcohols—annular region:

$$\frac{dX_{BA}}{dz} = \frac{\pi (D_{4i}^2 - D_{3e}^2)}{4}\frac{1}{F_{BA_0}} R_{eBA} \quad (6)$$

$$\frac{dX_{CA}}{dz} = \frac{\pi (D_{4i}^2 - D_{3e}^2)}{4}\frac{1}{F_{CA_0}} R_{eCA} \quad (7)$$

Energy balance for reactants and products—tubular (8) and annular (9) regions:

$$\frac{dT}{dz} = \frac{1}{\sum F_i C_{pi}}\left[(-\Delta H_1)\frac{\pi D_{1i}^2}{4} R_{eBA} + (-\Delta H_2)\frac{\pi D_{1i}^2}{4} R_{eCA}\right] \quad (8)$$

$$\frac{dT}{dz} = \frac{1}{\sum F_i C_{pi}}\left[U_3 \pi D_{4i}(T_S - T) + (-\Delta H_1)\frac{\pi (D_{4i}^2 - D_{1e}^2)}{4} R_{eBA} + (-\Delta H_2)\frac{\pi (D_{4i}^2 - D_{1e}^2)}{4} R_{eCA}\right] \quad (9)$$

Energy balance for the coolant: annular regions—I (10) and II (11):

$$\frac{dT_R}{dz} = -\frac{U_1 \pi D_{1i}}{Q_R C_{pR}}(T_R - T) \quad (10)$$

$$\frac{dT_R}{dz} = -\frac{U_2 \pi D_{3e}}{Q_R C_{pR}}(T_R - T) \quad (11)$$

In the previous equations there are three global coefficients of heat transference, which corresponds to the diverse circuits of the reaction medium mixture, U1, U2 and U3 (coefficients tube-coolant, annular-coolant and annular-heating system, respectively). The main reaction considered is the hydrogenation of benzylic alcohol to CA.

These equations are written to each part of the reactor (tubular and annular region) as well as for each phase of the system, since

the reactor is a multiphase one. Moreover, equations for predicting the heat coefficients must be present as well as a way to describe evaporation that may occur, depending upon the operating conditions. Each of these equations must be applied to each tube for both regions, namely, the tubular and annular. Since the reactor is essentially a tubular one usually operating at high flow rates, axial dispersion is neglected. Thus, steady-state process model presents a set of ordinary differential equations if radial dispersions is neglected, which is, together with the hypothesis that the solid–liquid phase is a single pseudo-homogenized fluid, a reasonable simplification that can be made in order to reduce the complexity of the process model.

3.2. Kinetic equations

The kinetic model considered by Coussemant and Jungers [7] was applied in this work and all the data and calculations related to the global coefficient of heat exchange, pressures, physical properties of the components are obtained by prediction models [3]. This model does not consider some intermediate stages. The intermediate stages with CEX (cycloalkene) formation are not considered in the model. The formation of alcohols is explained by admitting a mechanism of adsorption in individual small sites of the catalyst. The main reaction considered is the hydrogenation of benzylic alcohol to CA. The kinetic model considered follows the work of Coussemant and Jungers [7], when nickel is used as catalyst of the type autoclave reactor. It was found evidence of formation in intermediate stages of cyclohexanone, and that to a high enough pressure the reaction possesses order zero in relation to hydrogen. The global benzylic alcohol conversion (R_{BA}) to CA is described by the following relation:

$$R_{BA} = -\frac{dC_1}{dt} = k_1 \frac{b_1 C_1}{b_3 + (b_1 - b_3)C_1 + (b_2 - b_3)/(K-1)(C_1 - C_1^K)} \quad (12)$$

The rate of reaction R_{BA} is expressed in mol BA/mim g catalyst, and the temperature T, in the expressions of the kinetic constants must be in K.

The secondary reaction considered is the dehydration of the CA with water formation and cycloalkene, which is immediately hydrogenated with consequent formation of cycloalkane (undesirable product, C). The rate of formation of C (R_{CA}) from dehydration of CA is described in relation (13), as follows:

$$R_{CA} = k_3 \frac{\sqrt{C_2}}{\sqrt{C_2} + bC_3} \quad (13)$$

The parameters $b, b_1, b_2, b_3, k_1, K, C_1, C_2$ and C_3 are described in Coussemat and Jungers (1950). The rate of reaction of a catalytic process is directly associated with the catalyst concentration, being expressed by Eq. (14):

$$r_i = C_{cat} R_i \quad (14)$$

where r_i must be expressed in mol-i/min m^3, whereas the catalyst used in the hydrogenation processes is considered as highly active. It has a certain level of activity related to presence of the metal on the catalyst. Thus, in the formulation of the expressions for the rates of the considered reactions, a F_i factor that attempts to quantify the effectiveness of the catalyst for the two reactions was introduced so that each one of the reaction effective rates is expressed in the form of Eq. (15):

$$R_{ei} = F_i r_i \quad (15)$$

The factor F_i can vary in a range of (0 and 1), where the null value represents activity absence (absence of the reaction) and unitary value meaning the maximum of the catalytic activity (full activity). Intermediate values can characterize different states of the activity of the catalyst.

4. Optimization strategies

The optimization using the mathematical model takes into account large scale operational conditions of the reactor. The chosen parameters to implement the optimization are those with more sensitivity in the production process. The objective is to maximize the production of CA (Q_{CA}), using as main variables the outflows of coolant fluid (Q_{ri}'s), the feed reactants temperature (T_0) and the outflow of catalyst (Q_{cat}), in a total of eight variables. All other variables were maintained in their nominal value. In this way, the objective function applied to the optimization is the cyclic alcohol (CA) production. Table 1 shows the valid parameter limits to be optimized. These parameters are dimensionless, and were generated according to Eq. (16):

$$P = \frac{P_{opt-proc}}{P_{ref-val}} \quad (16)$$

where $P_{opt\ proc}$ is the current value for the parameter in the optimization, and $P_{ref\ val}$ is the reference value for the same parameter. The reference value is based in a real plant value, and the publication of these values was not authorized. The genetic code developed by Carroll [8] was coupled with the reactor model. The genetic code possesses the following characteristics: binary code; uses the elitism; search in niches and selection by tournament. In the reactor all the flows are measured in kg/h (Q_{CA}, Q_{BA}, Q_C, Q_{cat} and Q_{ri}'s, respectively) and the temperature is in Celsius degrees.

Operational values above and below of the lower and upper limits range lead to discontinuity in the model solution, and hence were not used.

Table 1
Limits of validity of the operational parameters to be optimized (dimensionless values)

Parameters	Lower limits of variable	Upper limits of variable
Q_{r1}	0.05	2.50
Q_{r2}	0.05	2.50
Q_{r3}	0.05	2.50
Q_{r4}	0.05	2.50
Q_{r5}	0.05	2.50
Q_{r6}	0.05	2.50
T_0	0.75	1.05
Q_{cat}	0.00	0.60

Table 2
Production to be optimized considering the respective constraints (dimensionless values)

Flows	Constraints
Q_{CA}	$Q_{CA} - 2.33 \geq 0$
Q_{BA}	$3.50 \times 10^{-5} - Q_{BA} \geq 0$
Q_C	$0.12 - Q_C \geq 0$

4.1. Objective function

The optimization is performed through the development of an objective function. In this work the objective function is related to the productivity of the main product (cyclic alcohol) and considers the following restrictions presented in Table 2. The constraints are related to the product of interest (CA), the main reactant (BA) and secondary product (C) without interest, as can be observed in Table 2, and the limits of the operational parameters to be optimized, described in Table 1.

The CA production considered is shown in Table 3 (large scale operational values).

4.2. Parameters of control of the genetic algorithms

Table 4 shows the selected genetic algorithms control parameters for the process. The parameters to be optimized were codified in the binary form, as great part of published works. In this work it was analyzed three genetic parameters of the code and their influence in the reactor productivity. These parameters are: the population size, crossover forms (uniform and single-point) and the crossover rates (10–80%).

Table 3
Operational conditions for large scale production (dimensionless values)

Parameters	Large scale operational values
Q_{r1}	1.26
Q_{r2}	1.30
Q_{r3}	1.38
Q_{r4}	0.18
Q_{r5}	0.26
Q_{r6}	0.15
T_0	0.79
Q_{cat}	0.43
Q_{CA}	2.34
Q_{BA}	3.50E−05
Q_C	0.12

Table 4
Control parameters of genetic algorithms utilized in the optimization

Genetic parameters	Values
Size population	10–40
Parameters	8
Crossover (U) and (SP)	10–80%
Mutation rate (JM)	1%
Creep mutation (CM)	2%
Generations	500

U is uniform crossover and SP is single-point crossover. JM is jump mutation and CM is creep mutation.

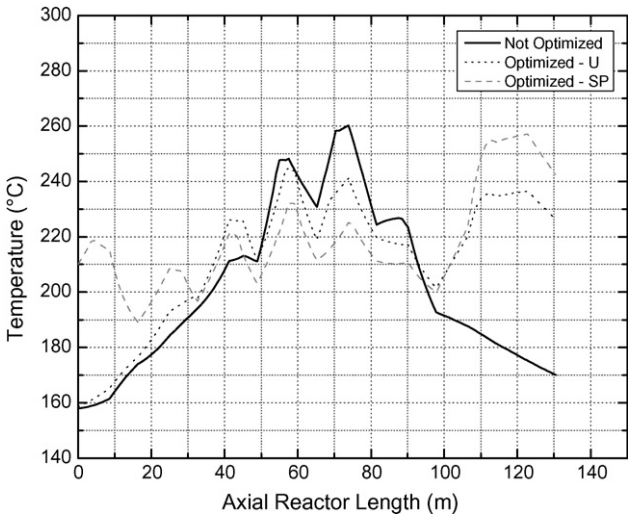

Fig. 2. Temperature profiles to the long the reactor length, considering the two crossover forms (uniform (U) and single-point (SP)) and comparing with the real model without optimization.

The parameters to be optimized were codified with the binary form, based and adapted of many published literature works (Carroll [8]; Deb [9]; Back et. al [10]; Goldberg [5]). The control parameters of the genetic algorithms can be varied and tested in the same way. In this work it was decided to use these values only to verify the application of the optimization method.

5. Results and conclusions

In the sequence, it is presented in Tables 5–7 and Figs. 2–7 the results obtained by optimization. Tables 5 and 6 show the CA productivity results considering the population sizes and rates crossover variations. Table 5 shows results for uniform crossover (U) and Table 6 presents the case using single-point (SP) crossover. It may be verified that there was an increase in the CA production, and reduction of catalyst mass flows,

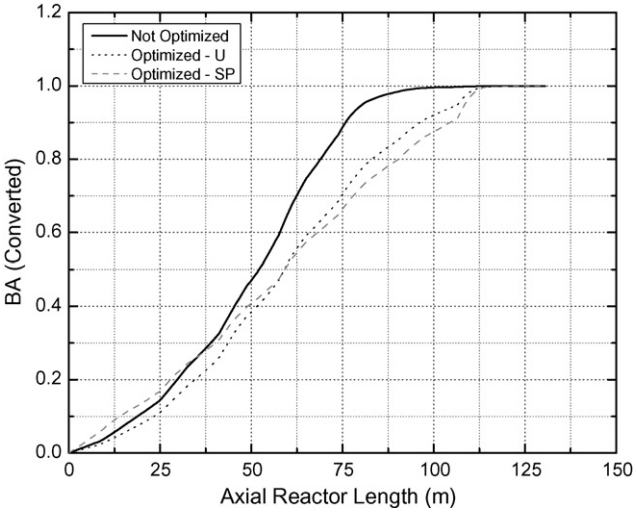

Fig. 3. BA converted profile (main reactant) to the long the reactor length, considering the two crossover forms (uniform (U) and single-point (SP)) and comparing with the real model without optimization (not optimized).

Table 5
Optimization results utilizing uniform crossover (U) with crossover rates 10–80% and population size (npz) between 10 and 40, respectively (dimensionless values)

Not opt.	npz	Crossover rates (%) – Uniform crossover (U)							
		10	20	30	40	50	60	70	80
2.3350	10	2.3717	2.3724	2.3719	2.3716	2.3708	2.3720	2.3722	2.3719
	20	2.3726	2.3721	2.3721	2.3694	2.3700	2.3702	2.3704	2.3710
	30	2.3727	2.3704	2.3711	2.3685	2.3700	2.3706	2.3712	2.3720
	40	2.3709	2.3696	2.3686	2.3685	2.3695	2.3700	2.3704	2.3710

Table 6
Optimization results utilizing single-point crossover (SP) with crossover rates 10–80% and population size (npz) between 10 and 40, respectively (dimensionless values)

Not opt.	npz	Crossover rates (%) – single-point crossover (SP)							
		10	20	30	40	50	60	70	80
2.3350	10	2.3729	2.3716	2.3709	2.3705	2.3721	2.3715	2.3730	2.3715
	20	2.3733	2.3734	2.3732	2.3717	2.3722	2.3723	2.3713	2.3706
	30	2.3727	2.3712	2.3712	2.3705	2.3703	2.3710	2.3713	2.3689
	40	2.3711	2.3716	2.3700	2.3703	2.3705	2.3706	2.3697	2.3703

amount of coolant fluid used in the process and BA and C flows. Figs. 2–6 indicate the temperature, BA and CA converted and molar fraction profiles compared with the not optimized situation. It can be depicted from these figures, that the parameters used in the optimization had changed the profiles of the conversions and molar fractions through the length of the reactor. In Fig. 2, it can be observed that the optimized values resulted in an increase in the temperature at the end of the axial length of the reactor. In Figs. 3–6, the optimized values leaded to a small conversion through of CA to C (desired situation) the length of the reactor, reducing the mass flow of the undesirable product (C), maximizing the mass flow of the desired product (CA) and shows high consumption of main reactant (BA). Fig. 7 presents the optimization evolution in the simulation. For the case with uniform crossover, the population size of 30 (crossover rate 10%) supplied better result (2.3727) as can be verified in Table 5 and when the single-point crossover was used (Table 6), the better result (2.3734) occur with population size of 20 (crossover rate 20%) the productivity increase oscillated around 0.03% above of the previous case (worthless difference). In Table 7 are presented the best cases (optimized operational parameters) obtained involving the two crossover forms (Uniform and Single-Point Crossover) compared with the large scale operational case.

The optimization promoted a CA productivity to increase around 1.6%, when compared with the nominal situation. Although appears to be a modest increase, it is significant in production terms. The catalyst mass flow (Q_{cat}) was reduced and confirmed in Table 7 (reduction of costs), and reduction

Table 7
Optimization results considering: the best results using the uniform (U) and single-point (SP) crossover form

Parameters	Not optimized	Optimized	
	Real operational values	Operational values (U)	Operational values (SP)
Q_{r1}	1.2600	0.2071	0.0611
Q_{r2}	1.2950	0.2005	0.2002
Q_{r3}	1.3800	0.2328	0.2008
Q_{r4}	0.1800	0.2029	0.2127
Q_{r5}	0.2600	0.0500	0.6659
Q_{r6}	0.1450	1.7855	2.0310
T_0	0.7900	0.7930	1.0500
Q_{cat}	0.4340	0.3006	0.2806
Q_{CA}	2.3350	2.3726	2.3734
Q_{BA}	3.50E−05	3.30E−05	1.58E−05
Q_C	0.11550	0.0975	0.0969
Q_{ri}'s total	4.5200	2.6789	3.3715

Parameters optimized in both crossover forms (dimensionless values).

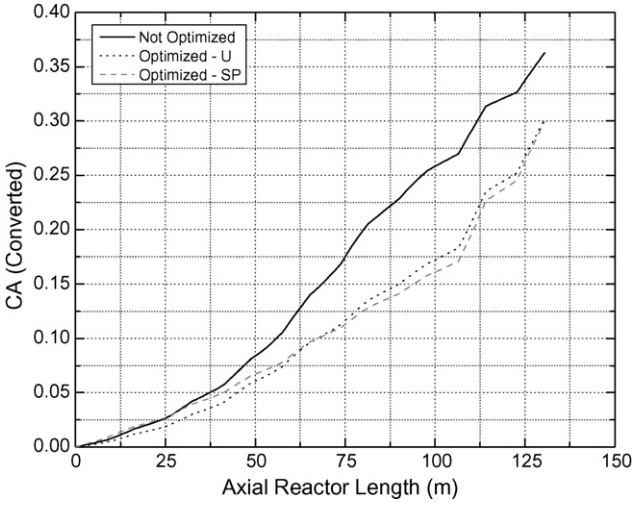

Fig. 4. CA converted profile (main product) to the long the reactor length, considering the two crossover forms (uniform (U) and single-point (SP)) and comparing with the real model without optimization (not optimized).

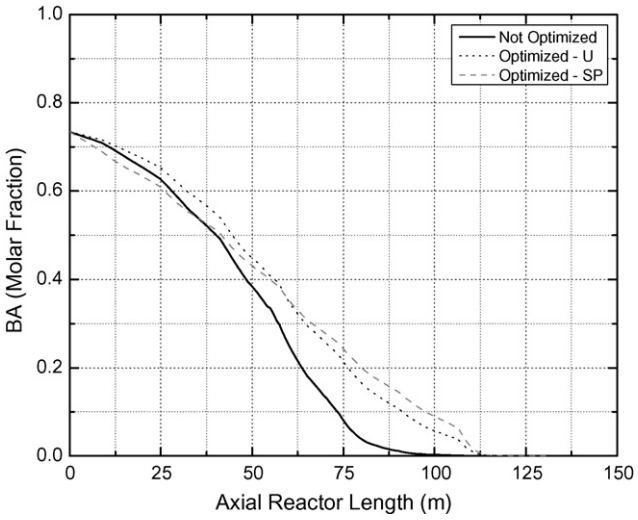

Fig. 5. Main reactant (BA) mole fraction to the long the reactor length, considering the two crossover forms (uniform (U) and single-point (SP)) and comparing with the real model without optimization (not optimized).

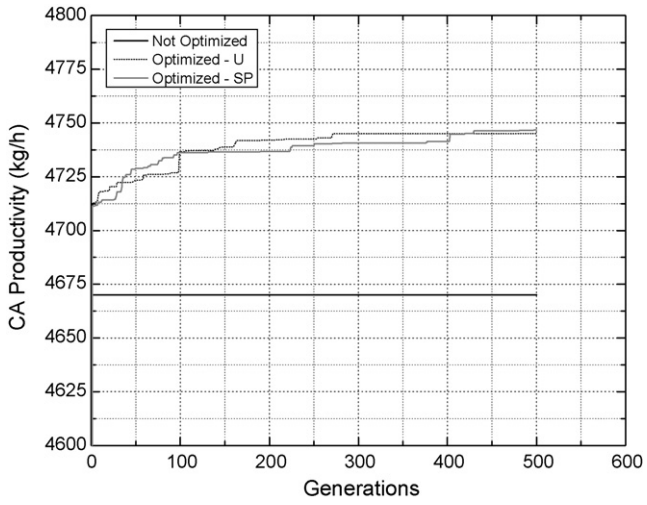

Fig. 7. CA rates profiles (CA productivity) with the optimization evolution, considering the two crossover forms (uniform (U) and single-point (SP)) and comparing with the real model without optimization (not optimized).

in both the cases of the total amount of coolant fluid (mass flow—Q_{ri}'s), not optimized (4.5200), Optimized—Uniform Crossover (2.6785) and Optimized—Single-Point Crossover (3.3715) (dimensionless values). The BA (Q_{BA}—main reactant) and C (Q_C—undesired product) mass flows also are reduced, indicating a better performance of the reaction process.

In the sequence the profiles of desired product (CA) and main reactant (BA) are shown from Figs. 2–6 for the case of the AG with 500 generation and the optimization evolution (Fig. 7).

The GA procedure revealed to be very efficient and robust for all the considered situations. Several tests with different population sizes and crossover values allow to conclude that the optimization by GA works well without to be so dependent of its design values as well as the initial value. Optimization of the same problem by conventional methods (as SQP) was not possible to be obtained in all the cases considered in this work.

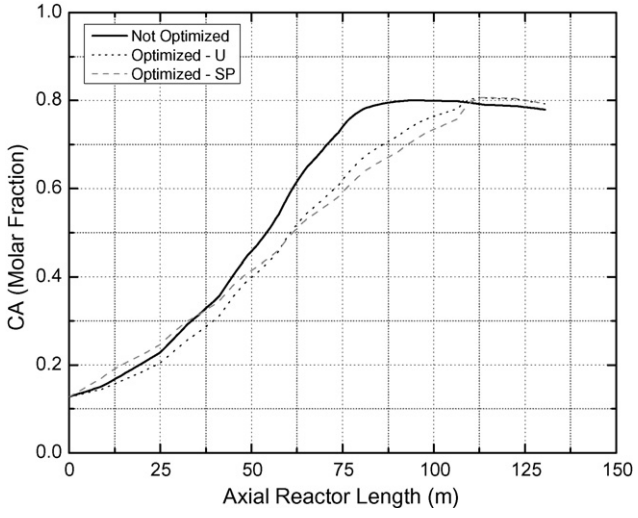

Fig. 6. Product (CA) mole fraction profile to the long the reactor length, considering the two crossover forms (uniform (U) and single-point (SP)) and comparing with the real model without optimization (not optimized).

When SQP method were used the results were dependent upon the initial values and a relatively high number of convergence difficulties are relatively common for large dimensional problem. This was not the case for the GA. In relation to the GA used in this study an attention has to be verified in some parameters this code. The population size used was of 10–40 and not of 50 or 100 as recommended (Carroll [8]) because of the high computational time and the performance is not so good (results not shown). The crossover rates of 10 and 20% are satisfactory to supply good results. There are not significant changes when the number of generations is increased, therefore a number around 500 generations is enough to achieve the optimization. The mutation rates did not follow the determined rules for the code. The values used for jump and creep mutation were: 0.01 and 0.02, respectively. The GA code coupled to the reactor model showed to be a very efficient technique for reactor optimization.

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