ADCHEM 2006

International Symposium on Advanced Control of Chemical Processes
Gramado, Brazil – April 2-5, 2006

APPLICATION OF GENETIC ALGORITHMS TO THE OPTIMIZATION OF AN INDUSTRIAL REACTOR

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Abstract: Genetic Algorithms (GAs) have shown great potential and ability to solve complex problems of optimization in diverse industrial fields, including chemical engineering process. In this paper, the main objective is to develop and implement a GA code in an industrial reactor of Cyclic Alcohol (CA) production for the optimization of operational parameters. The intention is to show that this technique is suitable for the maximization of Cyclic Alcohol production, obtaining good results with operational improvements (reduction of catalyst, reduction of the temperature of the process). The results show that the best performance of the process was achieved with the application of GAs. The developed procedure works very well in all the considered conditions which cover the most usual operating range for the considered process.

Keywords: Global optimization, Genetic algorithms, Chemical process.

1. INTRODUCTION

Several works have been carried out having as objective to optimize, through Genetic Algorithms (GAs), the diverse parameters involved in kinetic models of chemical processes (Moros, et al.,1996; Simant and Deb, 1997; Hongqing et al., 1999). 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 – MR or BA). The optimization of this unit was chosen for several factors among which: the reactor of Cyclic Alcohol presents a complex behaviour 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 show severe limitations, especially in terms of convergence. Bearing this in mind in this work is proposed an optimization procedure based on Genetic Algorithms method.

2. GENETIC ALGORITHMS (GAS)

These algorithms are a procedure of optimization developed based on the principles of natural selection (Holland, 1992; Goldberg, 1989). 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 achieve. In fact the optimization procedure based in such approach can be considered as an global optimization method with the advantage to do no be dependent upon the initial value to achieve the convergence. Most probably the more significant disadvantage is the computer time and burden required. These 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 in accord to the need to achieve the goal in the optimization problem. The determination of the parameters is made through the development of an objective function that represent 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.

2.1 Coding

The coding stage is very important for the success of the genetic code application in the solution of the optimization problem (Goldberg, 1989). The target is to create a parameter representation which allows to its modification through the division in some position. The formed parts are separated sequences in conditions to be matched with others. A codified parameter should be seen as a chromosome in genetics, in other words a modifiable carrier of information. In some GA algorithm, the coding method is based on the representations of binary series number; other forms of coding can be used as

representations in real numbers and whole numbers. In this paper the binary approach is adopted.

2.2 Population Size

Wehrens and Buyders, 1998 mentioned that for each case, population sizes range can vary, but for most of the cases is used between 20-500. In general, when many parameters are optimized larger populations are used. For the CA optimization problem the population size is considered to be about 20 and 500 generations.

2.3 Selection – Reproduction

The reproduction is normally the first procedure applied in the population, and it is a choice of good individuals (series) in order to form one mating pool. Some types of reproduction are found in literature (Goldberg and Deb, 1991). The main idea is to select individuals that possess values above of the average of a current population. The more traditional methods of selection are the proportional selection, roulette wheel and based in rank. The main feature in the stage of selection is the prevention of individuals (series) that promote values of the undesirable evaluation function (fitness) considering the objective of the problem. In this work was considered tournament selection form. This method is the most popular forms of selection in evolutionary algorithms (EAs). In its simplest form, a group of n individuals is chosen randomly from the current population, and the individual with the best fitness is selected (Bäck et al., 2000). This selection performs tournaments by first sampling individuals uniformly and randomly from the population and then selecting the best of the sample for some genetic operation. This sampling process needs to be repeated many times, creating a new generation.

2.4 Crossover

Crossover is applied in the series originated from mating pool (after the stage of reproduction). In the same way that the reproduction operator, the idea is to find some operators of crossover applied in GA (Syswerda, 1989). In the majority of the operators two series (individuals) are chosen randomly from the mating pool. After this stage it is made a recombination of the construction tablets (parts of the series of the relatives) that correspond to the favorable sub-solution. The uniform crossover was used with crossover probability 0.8.

2.5 Mutation

The main target of this genetic operator is to promote new solutions (individuals) that cannot be generated for another form. The mutation introduces an element of the random research (sometimes called exploration). The intention of such procedure is to focus in promising regions of the search space (exploitation). The occurrence of this operator is determined by the researcher through a mutation probability. This value is around 0.01 and it is inside a recommended range by a tray and error procedure (Goldberg, 1989). Usually, this value is smaller than the adopted one for the crossover and the criterion for a good value is to prevent too much random search.

3. DESCRIPTION OF THE PROCESS

The process is a multiphase catalytic reactor, where hydrogenation reactions take place. A typical process of industrial interest is the hydrogenation of ortho-cresol (Vasco de Toledo et al., 2001). 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.

The reactor is constituted of a series of tubes, cooled by pressured water which flows in a jacked around the tubes. The reactants flow inside the tubes, while the thermal fluid flows through the annular regions. The deterministic mathematical model used to describe the reactor is based on the work by Santana, 1995 and Vasco de Toledo et al., 2001. 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. For the other components of the reactional system, the equations are similar and can be found in the studies of Santana, 1995.

3.1 Model Equations

The equations are customized to the situation of the reactor-CA from the general expressions for the modelling of described mass and energy by Froment and Bischoff, 1990.

Mass Balance for Benzylic Alcohol - Tubular Region:

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

Mass Balance for Benzylic Alcohol – Annular Region:

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

Mass Balance for Cyclic Alcohol - Tubular Region:

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

Mass Balance for Cyclic Alcohol – Annular Region:

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

Energy Balance – Reactants and Products - Tubular Region:

$$\frac{dT}{dz} = \frac{1}{\sum F_i C_{pi}} \begin{bmatrix} U_2 \pi D_{3e}(T_R - T) + U_3 \pi D_{4i}(T_S - T) + \\ (-\Delta H_1)\frac{\pi(D_{4i}^2 - D_{3e}^2)}{4} R_{eBA} + \\ (-\Delta H_2)\frac{\pi(D_{4i}^2 - D_{3e}^2)}{4} R_{eCA} \end{bmatrix} \quad (5)$$

Energy Balance – Reactants and Products – Annular Region:

$$\frac{dT}{dz} = \frac{1}{\sum F_i C_{pi}} \begin{bmatrix} U_2 \pi D_{3e}(T_R - T) + U_3 \pi D_{4i}(T_S - T) + \\ (-\Delta H_1)\frac{\pi(D_{4i}^2 - D_{3e}^2)}{4} R_{eBA} + \\ (-\Delta H_2)\frac{\pi(D_{4i}^2 - D_{3e}^2)}{4} R_{eCA} \end{bmatrix} \quad (6)$$

Energy balance for the coolant:

Annular Region – I

$$\frac{dT_R}{dz} = -\frac{U_1 \pi D_{1i}}{Q_R C_{pR}}(T_R - T) \quad (7)$$

Annular Region – II

$$\frac{dT_R}{dz} = -\frac{U_2 \pi D_{3e}}{Q_R C_{pR}}(T_R - T) \quad (8)$$

In the previous equations there appear three global coefficients of heat transference, correspondent to the diverse circuits of the reaction medium mixture, U_1, U_2 and U_3 (coefficients tube-coolant, annular-coolant and annular-heating system respectively).

The considered main reaction is the hydrogenation of Benzylic Alcohol to CA. The kinetic model considered by Coussemant and Jungers, 1950 was applied in this work and all the data and calculations related to the global coefficient of heat exchange, pressures, physical properties prediction of the components are described with details by Santana, 1995.

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 work developed by Coussemant and Jungers, 1950 does not consider some stages and is represented in accord to with the main equations that occur in the process, described below:

$$BA + 2H_2 \xrightarrow{Ra/Ni} CA + H_2 \xrightarrow{Rb/Ni} C + H_2O$$

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.

3.3 Kinetics of the Main Reaction

The considered main reaction is the hydrogenation of Benzylic Alcohol to CA. The kinetic model considered by Coussemant and Jungers, 1950 is used they studied this nickel process using a catalytic reactor of the type autoclave. It was found evidence of formation in intermediate stages of Cyclohexanone, and that to a pressure raised enough the reaction possesses order zero in relation to hydrogen. The global Benzylic Alcohol conversion (R_{BA}) to CA is described by the following relation:

$$R_{BA} = -\frac{dC_1}{dt} = k_1 \frac{b_1 C_1}{b_3 + (b_1 - b_3)C_1 + \frac{b_2 - b_3}{K - 1}(C_1 - C_1^K)} \quad (9)$$

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

3.4 Kinetic of Secondary Reaction

The considered secondary reaction is the dehydration of the CA with water formation and Cycloalkene, which is immediately hydrogenated, with consequent formation of C (Cycloalkane - undesirable product). The rate of formation of C (R_{CA}) from dehydration of CA is described in relation (10), as follows:

$$R_{CA} = k_3 \frac{\sqrt{C_2}}{\sqrt{C_2} + bC_3} \quad (10)$$

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.

3.5 Effective Rates of Reaction

The rate of reaction of a catalytic process is directly associated with the catalyst concentration, being expressed by the equation (11):

$$r_i = C_{cat} R_i \quad (11)$$

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 formularization 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 (hydrogenation of BA and dehydration of the Cycloalkene), was introduced so

that each one of the reaction effective rates is expressed in the form of equation (12):

$$R_{ei} = F_i r_i \quad (12)$$

the factor F_i can be seen as a numerical constant whose value 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 wheels is function of the reactor severity (operation temperature).

Other details of components physical properties and other considerations are described in Santana, 1995.

4. OPTIMIZATION STRATEGIES

The optimization using the mathematical model takes into account the real 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. Table 1 shows the valid parameter limits to be optimized. The genetic code developed by Carroll, 1996 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. The presented values in the tables are in the normalized form. In the industrial reactor all the flows are measured in kg/h (Q_{CA}, Q_{MR}, Q_C, Q_{cat} and Q_{ri}'s respectively) and the temperature is in Celsius degrees.

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

Parameters	Lower limits of variable	Upper limits of variable
Q_{r1}	0.01	1.00
Q_{r2}	0.01	1.00
Q_{r3}	0.01	1.00
Q_{r4}	0.01	1.00
Q_{r5}	0.01	1.00
Q_{r6}	0.01	1.00
T_0	y*	0.84
Q_{cat}	0.0000	x*

The value of y^* is related to the inferior limit of the initial temperature of the reactants mixture and products in the entrance of the reactor (normalized values), being 0.60 for the Level 1 of production and 0.68 for the two other production Levels (2 and 3 respectively). In the Levels 2 and 3, smaller values than 0.68 supply discontinuous values for solution of the reactor model. This is not appropriate to be used in the optimization.

The value of x^* refers to the maximum catalyst flow (Q_{cat} normalized) (upper limits) that also depends of the operational level of production that is analyzed. For the Level 1 the maximum value is 0.6000, the Level 2 the value is 0.8000 and last (Level 3) assumes the value of 1.0000. Values above the upper limits of each level also lead to discontinuity in the model solution, and hence were not used.

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 the following restrictions presented in Table 2. The restrictions are related to the product of interest (CA), the main reactant (MR) and secondary product (C) without interest, as can be observed in Table 2.

Table 2 Production Levels to be optimized considering the respective restrictions (normalized values)

Level 1	Level 2	Level 3
$0.0100 \le Q_{ri} \le 1.0000$	$0.0100 \le Q_{ri} \le 1.0000$	$0.0100 \le Q_{ri} \le 1.0000$
$0.60 \le T_0 \le 0.84$	$0.68 \le T_0 \le 0.84$	$0.68 \le T_0 \le 0.84$
$0.0000 \le Q_{cat} \le 0.6000$	$0.0000 \le Q_{cat} \le 0.8000$	$0.0000 \le Q_{cat} \le 1.0000$
$Q_{CA} - 0.6554 \ge 0$	$Q_{CA} - 1.0000 \ge 0$	$Q_{CA} - 0.9621 \ge 0$
$0.1833 - Q_{MR} \ge 0$	$1.0000 - Q_{MR} \ge 0$	$0.2111 - Q_{MR} \ge 0$
$0.4851 - Q_C \ge 0$	$0.7551 - Q_C \ge 0$	$1.0000 - Q_C \ge 0$
i = 1, 2, 3....6		

The three levels of CA production are considered, as shown in the Table 3 (industrial operational values).

Table 3 Operating conditions for three industrial production levels (Levels 1, 2 and 3) (normalized values)

Parameters	Level 1	Level 2	Level 3
Q_{r1}	0.2520	0.0360	0.0390
Q_{r2}	0.2590	0.0380	0.0000
Q_{r3}	0.2760	0.2740	0.0850
Q_{r4}	0.0360	0.0660	0.3490
Q_{r5}	0.0520	0.1190	0.1190
Q_{r6}	0.0290	0.1400	0.0500
T_0	0.6320	0.6920	0.6920
Q_{cat}	0.4340	0.7520	0.8280
Q_{CA}	0.6554	1.0000	0.9622

4.2 Parameters of Control of the Genetic Algorithms

In accordance to Table 4 were selected the control parameters of the genetic algorithms in the process optimization. The parameters to be optimized were codified in the binary form, as great part of published works.

Table 4 Control parameters of genetic algorithms utilized in the optimization

Size Population	Parameters	Crossover (UC)	Mutation Rate (JM)	Generations
20	8	80%	1%	500
UC is Uniform Crossover				JM is Jump Mutation

The parameters to be optimized were codified with the binary form, based and adapted of many published literature works (Carroll, 1996; Deb, 1998; Goldberg, 1989).

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. In future works these parameters will be modified, besides the coding form.

5. RESULTS AND CONCLUSIONS

In the sequence it is presented in the Table 5 (results optimized) and Figures 1 to 3 (evolution of optimization in 500 generations) the results obtained by optimization.

Table 5 shows the results of the parameters before and after the optimization. It may be verified that in the production Levels 1, 2 and 3 there were increase of the CA production and reduction of mass flows of catalyst with an increase of the amount of coolant fluid used in the process. Figures 1 (Level 1), 2 (Level 2) and 3 (Level 3) indicate improvements in the productivity. The results had been presented of normalized form. Taking into consideration the operation Levels 1, 2 and 3 there were increase of the CA production (increase of 0.0078 – Level 1, 0.0140 – Level 2 and 0.0179 – Level 3 – all values are normalized) with an reduction in the value for the catalyst flow (reduction of 0.1252 – Level 1, 0.1884 – Level 2 and 0.2585 – Level 3).

Table 5 Analysis of the performance of the CA production before and after the optimization for the production Levels 1, 2 and 3 (normalized values)

Parameters	Level 1		Level 2		Level 3	
	Before	After	Before	After	Before	After
Q_{r1}	0.2520	0.1158	0.0360	0.7895	0.0390	0.8430
Q_{r2}	0.2590	0.2524	0.0380	0.4920	0.0000	0.2744
Q_{r3}	0.2760	0.0124	0.2740	0.2434	0.0850	0.9258
Q_{r4}	0.0360	0.7095	0.0660	0.0516	0.3490	0.1193
Q_{r5}	0.0520	0.7036	0.1190	0.1550	0.1190	0.4813
Q_{r6}	0.0290	0.3337	0.1400	0.0700	0.0500	0.6179
T_0	0.0158	0.0176	0.0173	0.0171	0.0173	0.0184
Q_{cat}	0.0217	0.0154	0.0376	0.0282	0.0414	0.0285
Total Q_{CA}	0.6554	0.6632	10,000	10,140	0.9622	0.9801
Total Q_n's (Coolant)	0.9040	2.1273	0.6730	1.8016	0.6420	3.2617

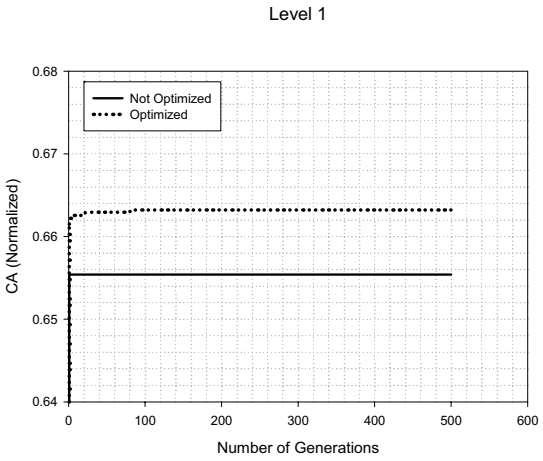

Fig. 1. Profile CA productivity (mass rate normalized) for production Level 1 with the optimization evolution.

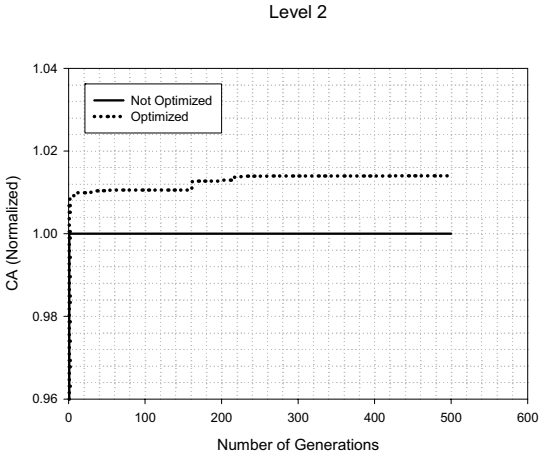

Fig. 2. Profile CA productivity (mass rate normalized) for production Level 2 with the optimization evolution.

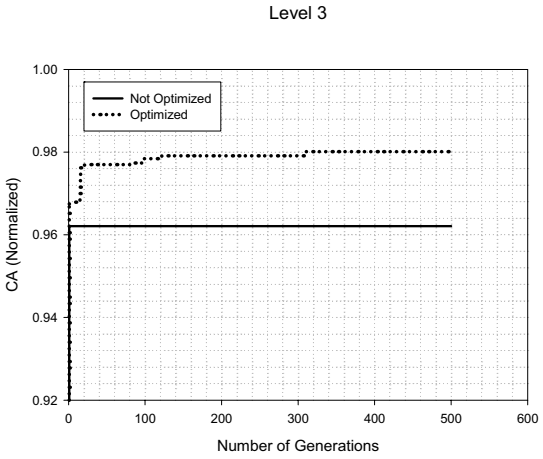

Fig. 3. Profile CA productivity (mass rate normalized) for production Level 3 with the optimization evolution.

The GA procedure revealed to be very efficient and robust for all the considered situations. Several testes with different population sizes, crossover and mutation values allow to conclude that the optimization by GA works well without 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.

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 20 and not of 50 or 100 as recommended (Carroll, 1996) because the computational time is very high. The crossover rate of 80% is 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 didn't follow the determined rules for the code. The values used for jump and creep mutation were: 0.01 and 0.02 respectively. These values allowed good efficiency, unlike what was usually recommended (Carroll, 1996). The GA code coupled to the reactor model showed to be a very efficient technique for reactor optimization. Similar problems or other systems can be studied for verification of his efficiency.

ACKNOWLEDGEMENTS

The authors are grateful to the Fundação de Amparo à Pesquisa do Estado de São Paulo - FAPESP and to the Conselho Nacional de Desenvolvimento Científico e Tecnológico - CNPq for their financial support.

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