APPLICATION OF GENETIC ALGORITHMS TO THE OPTIMIZATION OF AN INDUSTRIAL REACTOR OF PRODUCTION OF CYCLOHEXANOL

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Abstract

Genetic Algorithms (GAs) have gained great popularity in the last decades. The 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 to implement a GA in an industrial reactor of cyclohexanol (CHL) production for the optimization of operational parameters. The intention is to show that this technique is suitable for the maximization of cyclohexanol production obtaining good results with operational improvements (reduction of catalyst, and of process temperature). The results allow to conclude that better performance of the process was achieved. The developed procedure works very well in all considered conditions which cover the most usual operating range for the studied process.

Keywords

Global optimization, Genetic algorithms, Chemical process.

Introduction

Innumerable works have been developed aiming the optimization of diverse parameters involved in kinetic models of chemical processes, through genetic algorithm (Moros et al. (1996), Simant and Kalyanmoy (1997), Hongqing et al. (1999), Balland et al. (2000), Rajesh et al. (2001)). In this work, the objective is to find the best operating conditions of the CHL reactor, which involves the hydrogenation of phenol. The optimization of this unit was chosen for several reasons such as: CHL is a feedstock for several products of commercial interest, as nylon, the cyclohexanol reactor presents a complex behaviour and large energy consumption, associated with high levels of pressure and temperature reached in the operation of the process. As the reactor is a non linear distributed parameter system, leading to a set of differential equations, the optimization problem is a hard task and conventional optimization methods have show severe limitations, especially in terms of convergence. In this work, an optimization procedure based are Genetic Algorithms method is proposed.

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Genetic Algorithms (GAs)

These algorithms refer to a procedure of search and optimization motivated by the principles of natural selection (Holland (1992), Goldberg (1989), and Bäck et

al. (2000)). The GA is initiated with a population of represented random solutions in some series of structures. After this first stage, a series of procedures (operators) are applied repeatedly, up to convergence is achieve. 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 accordance to the proposals for optimization of the problem. The optimization is carried out by the estimation of an objective function that can 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.

Coding

The stage of coding is a crucial step to be developed in the solution of the optimization problem (Michalewicz (1996) and Bäck et al (2000)). The target is to create a representation of a parameter which allows its modification through the division in some position, being these parts separated sequences in conditions to be matched with others. A codified parameter seems to be a chromosome in genetics, in other words a modifiable sequence of information. For most of GA procedures, the coding method is based on representations of binary series number, however other forms of coding can be used as representations in real numbers and whole numbers. In this paper, the binary approach is adopted.

Population Size

Wehrens and Buydens (1998) mentioned that for each case, population size ranges 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 CHL optimization problem, the population size is 20 and about 500 generations.

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 Kalyanmoy (1991) and Michalewicz (1996)). The main idea is to select individuals that possess values above of the average of a current population. The most traditional methods of selection are the proportional selection, roulette wheel and those 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. Taking into account the characteristic of the optimization problem, the selection method considered in this work is tournament selection.

Crossover

Crossover is applied from mating pool, after the reproduction stage. In the same way that the reproduction operator, the idea is to find some operators of crossover applied in GA (Spears and De Jong (1991) and Syswerda (1989)). In the most of the operators, two series (individuals) are chosen randomly from the mating pool, and after this stage, a recombination of the construction tablets (parts of the series of the relatives) that correspond to the favorable sub-solution is made. The uniform crossover was used with crossover probability of 0.8.

Mutation

The main target of this genetic operator is to promote new solutions (individuals) that cannot be generated from another form. The mutation introduces an element of the random research (sometimes called exploration). The intentions of such procedure is to focus in promising regions of the research space (exploitation). The occurrence of this operator is determined by the user that can justify it with a mutation probability. This value is around 0.01 and is found inside a recommended range by a trial and error procedure (Bäck et al (2000)). 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 searches.

Description of the Process

The process is a multiphase catalytic reactor, where hydrogenation reactions take place. 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 eight tubes, which are immersed in a boiler. In fact, they consist of four concentrical tubes. The reactants flow through the tubular as well as through the external annular region, while the thermal fluid flows inside the other regions. The deterministic mathematical model used to describe the reactor is based on Santana (1999) and on Toledo et al. (2002). The reactor model is a set of differential equations as fllowing:

Mass Balance

$$\frac{dC}{dz} = f\left(C, T, P, T_{r_n}, \ldots\right) \quad (1)$$

Energy Balance

$$\frac{dT}{dz} = f\left(C, T, P, T_{r_n}, \ldots\right) \quad (2)$$

where C is concentration, T is temperature, P is pressure and T_{r_n} is the refrigerant temperature in the n-tubular module. 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 module for both regions, namely, the tubular and annular. Since the reactor is essentially a tubular one, axial dispersion is considered. Thus, the 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. The mathematical modeling was validated with industrial data.

Strategies of Optimization

The optimization using the mathematical model takes into account the real operating conditions of the reactor. The chosen parameters to implement the optimization are those more sensitivity in the production process. The objective is to maximize the production of CHL (Q_{CHL}), using as main variables the 6 outflows of cooling fluid (Q_{ri}), the feed reactants temperature (T_0) and the outflow of catalyst (Q_{cat}), in a total of eight variables. Table 1 shows the valid parameters values to be optimized. All the outflows are in the unit Kg/h and, the temperature is in ºC. The objective function is defined as:

$$f(T) = \sum_{i=1}^{np} \left(T_{Exp\ i} - T_{Sim\ i}\right)^2 \qquad (3)$$

In equation (3), T represents the temperature, np is the number of points (temperatures) of the problem, T_{Expi} is the experimental temperature and T_{Simi} is the simulated one obtained by optimization of the analysed parameters. The operational data set for each level and the genetic algorithms control parameters is supplied in Tables 1 and 2.

Table 1. Operating conditions for Three production levels (1, 2 and 3)

Parameters	Level 1 (99 t/d)	Level 2 (143 t/d)	Level 3 (144 t/d)
Q_{r1}	2520	360	390
Q_{r2}	2590	380	0
Q_{r3}	2760	2740	850
Q_{r4}	360	660	3490
Q_{r5}	520	1190	1190
Q_{r6}	290	1400	500
T_0	158	173	173
Q_{cat}	217	376	414
Q_{CHL}	4670	7125	6856

Table 2. Control parameters of genetic algorithms utilized in the optimization

Size Population	Parameters	Crossover Rate	Mutate Rate	Generations
20	8	80%	1%	500

Results and Conclusions

Table 3 presents the analysis of the performance of the CHL production before and after the optimization for the production levels 1, 2 and 3. The analyzed parameters are the outflows of cooling fluid (Q_{ri}), input temperature of the reagents (T_0) and outflow of catalyst (Q_{cat}). It may be verified that in the production levels 2 and 3 CHL production increased and the catalyst mass flows decreased, increasing the amount of cooling fluid used in the process. Figures 3 and 4 (level 2), 5 and 6 (level 3) indicate improvements in the product quality. Taking into consideration level 1, there was no increase of the CHL production with an almost constant value for the catalyst flow. Figures 1 and 2 (level 1) shows the reactant and cyclohexanol profiles with such operating conditions. The GA procedure revealed to be very efficient and robust for all the considered situations. Several testes with different population size, crossover and mutation values allow to conclude that the optimization by GA works well without be so dependent of its design values. Optimization of the same problem by conventional methods (as SQP) was not possible to be obtained in all the cases considered in this work.

Table 3. Results of Optimization

Results of Optimization						
Param.	Level 1		Level 2		Level 3	
	Before	After	Before	After	Before	After
Q_{r1}	2520	2575	360	409	390	390
Q_{r2}	2590	2594	380	409	0	0
Q_{r3}	2760	2575	2740	2574	850	718
Q_{r4}	360	410	660	641	3490	3503
Q_{r5}	520	525	1190	1182	1190	1183
Q_{r6}	290	293	1400	1337	500	719
T_0	158	170	173	171	173	175
Q_{cat}	217	216	376	300	414	300
Q_{CHL}	4670	4659	7125	7186	6856	6938
Total Q_{ri}	9040	8972	6730	6552	6420	6813

LEVEL 1

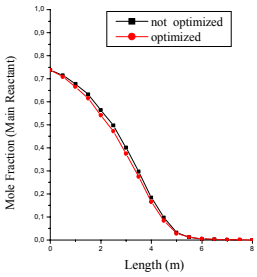

Figure 1. Main reactant mole fraction profiles along the reactor

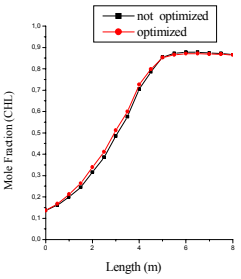

Figure 2. Cyclohexanol mole fraction profiles along the reactor

LEVEL 2

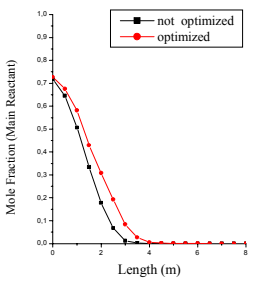

Figure 3. Main reactant mole fraction profiles along the reactor

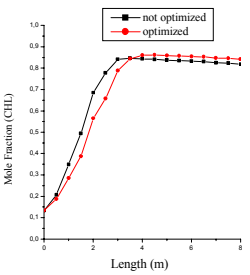

Figure 4. Cyclohexanol mole fraction profiles along the reactor

LEVEL 3

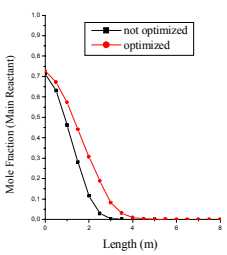

Figure 5. Main reactant mole fraction profile along the reactor

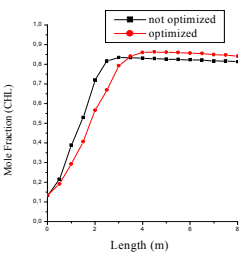

Figure 6. Cyclohexanol mole fraction profiles along the reactor

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