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Analysis of Genetic Algorithm Operators in the Productivity of a Large Scale Process

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This work aims to describe the results of the application of Genetic Algorithms (GAs) to optimize the productivity of a large scale process. Several optimization classic techniques have been used with this intention, but many of these techniques are not efficient, mainly when the problem is complex, with a high number of variables, described by nonlinear models with many possible solutions, and subject to constraints. As an alternative, a class of algorithms denominated Genetic Algorithms present good potential to be used as a tool for optimization of complex and large scale systems. The process considered here is a multiphase catalytic reactor, where hydrogenations reactions take place. This study is related to optimization of a specific cyclic alcohol (CA) production through adjustment of some important operational parameters. The present study is made through analysis of genetic operators' sensitivity (binary coding) and its influence on the cyclic alcohol productivity. The results show an increase in the CA productivity and a very robust and efficient optimization procedure.

1. Introduction

Hydrogenation reactions are widely applied in industry, usually for large scale commodities production. The reaction considered in this work occurs in catalytic three-phase reactors. Modeling this type of reactor is a difficult task because it involves many aspects like hydrodynamics, gas–liquid and liquid–solid mass/heat transfer, pore diffusion, and reaction and deactivation kinetics. In such conditions, very small process amendments may lead to a significant profit improvement. The success in the modeling of a three-phase reactor is intrinsically linked to the suitable treatment of heat and mass transfer phenomena, together with the kinetics involved (Vasco de Toledo *et al.*, 2001). The three-phase reactors mathematical modeling studies are concentrated mainly in three types most widely used in industrial processes, which are: slurry reactors, trickle bed reactors and slurry bubble column reactors (Vasco de Toledo *et al.*, 2001 and Victorino *et al.*, 2007).
Usually for large scale systems, the reactor is constituted by a series of tubes, cooled by a coolant flowing in a jacket around the tubes in order to maximize heat transfer from

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the tube-side to the coolant. In this work the objective is to find out the best operational conditions of the cyclic alcohol (CA) reactor, where the hydrogenation of a specific benzylic alcohol (main reactant – BA) takes place.
Genetic Algorithms (GAs) are optimization procedures (under evolutionary algorithms category), which are general-purpose search techniques based on the principles of natural selection (Goldberg, 1989 and Holland, 1992). Several studies are found in the literature involving optimization with genetic algorithms applied to different areas of engineering. Applications to the specific chemical engineering area with are found: Rajesh *et al.* (2001), Souza *et al.* (2003), Weifang *et al.* (2003), Anjana *et al.* (2003), Costa and Maciel Filho (2005), Bhutani *et al.* (2006), Victorino *et al.* (2007), Morais *et al.* (2007), among others.

2. Process Description

The process consists in a set of six concentric tubular reactors modules, where the flow of reactants and products begins at the innermost tube going for the following module up to the last tubular reactor. Figure 1 shows a single tubular module.
Since hydrogenation reactions are highly exothermic, a cooling system is coupled to the reactor to remove the reaction heat. In order to achieve a suitable reaction control is important to manipulate the coolant flow (Q_{r1}, …, Q_{r6}). The coolant flow is co-current. In the last two modules there are not coolant fluids.
The reactor model is a set of differential equations, considering two regions for each tube: tubular (tube-side) and annular (coolant side). 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 (Domingues, 1992).

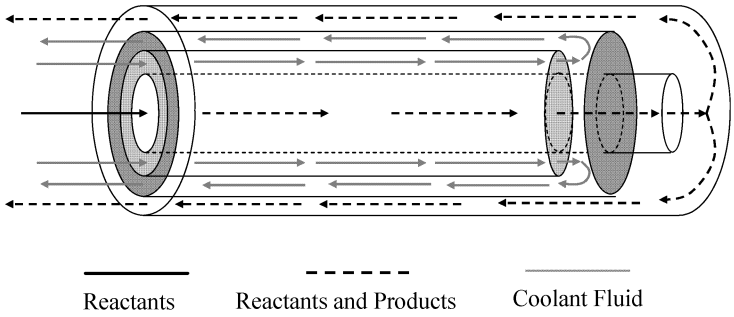

Figure 1 Schematics of a tubular reactor module

The following assumptions were adopted in developing the model used to represent the dynamic behavior of the reactor (Vasco de Toledo *et al.*, 2000a, 2000b, Victorino, 2005, and Victorino *et al.*, 2007): steady-state; plug-flow for the reactants and coolant fluid; homogeneous suspension (liquid+solid) considered as a pseudo-fluid; pressure variations negligible; there is phase change in the coolant fluid; pseudo-steady state for

solid phase; reaction following $A(g)+BA(l)\rightarrow CA(l)+C(l)$, occurring at the catalyst surface with a kinetics depending on A and B concentrations; heat and mass transfer resistance not considered within the catalyst particle; negligible axial and radial dispersion. The mathematical expressions of the reactant (BA) and the main product (CA) are found in the work by Victorino *et al.* (2007). The main reaction considered is the hydrogenation of BA to CA. The equations are written to each part of the reactor (tubular and annular region) as well as for each phase of the system.
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, components physical properties are obtained by prediction models (Victorino *et al.*, 2007). This model does not consider some intermediate stages such as CEX (cycloalkene) formation. The formation of alcohols is explained assuming a mechanism of adsorption in individual small sites of the catalyst.

3. Optimization Strategies

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 (operational parameters). The GA code used is the version 1.7a of a FORTRAN software by David Carroll (Carroll, 1996a, 1996b), with some modifications in order to deal with inequality constraints and adapted to the model considered herein. In this work the objective function is devoted to increase to the productivity of the main product (cyclic alcohol) and considers the following constraints presented in Table 1. The constraints are related to the product of interest (CA), the main reactant (BA) and secondary product (C).

Table 1 Production to be optimized considering the respective constraints

Flows	Constraints
Q_{CA}	$Q_{CA} - 0.9340 \geq 0.0$
Q_{BA}	$0.0140 - Q_{BA} \geq 0.0$
Q_C	$0.4640 - Q_C \geq 0.0$
Q_{CA}, Q_{BA} and Q_C are dimensionless	

3.1 Genetic Algorithms Parameters

Table 2 shows the selected genetic algorithms parameters for the process. These parameters are: crossover forms: Uniform (Un) and Single-Point (SP) and the crossover rates equal to 20, 40, 60 and 80% using population size (npop) equal to 20.

Table 2 Control parameters of genetic algorithms utilized in the optimization

Genetic Parameters	Values
Population Size (npop)	20
Model Parameters	8
Crossover (Un) and (SP) Probability	20, 40, 60, 80%
Jump Mutation Rate (JM)	Calculated (Carroll, 1996a and 1996b)
Creep Mutation (CM)	Calculated (Carroll, 1996a and 1996b)
Niche	Yes (using)
Generations	250

4. Results And Conclusions

In the sequence, they are presented in Figures 2 and 3 the results obtained by the optimization procedure. Table 3 shows the CA productivity results considering the best run from all. Table 3 presents the best result using uniform crossover (npop=20, with crossover probability pcross=0.60) compared with the non optimized real case. There is an increase of CA productivity and reduction of spent catalyst. The increase in the coolant flow is small. The CA non optimized productivity in the real case is 0.934 (dimensionless values).

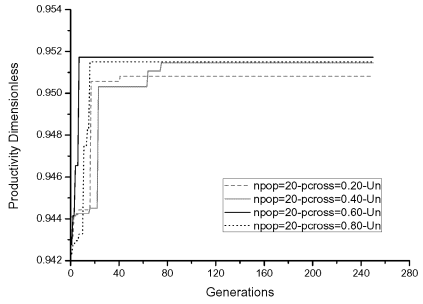

Figure 2 CA Productivity profile using npop=20, uniform crossover (Un) and probability variations adopted.

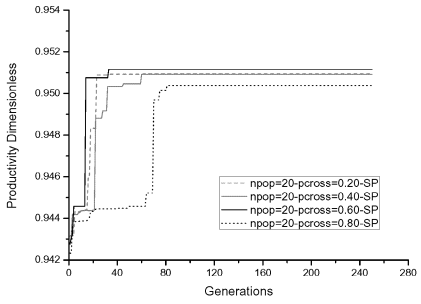

Figure 3 CA Productivity profile using npop=20, sigle-point crossover (SP) and probability variations adopted.

For SP crossover, similar results are found with crossover probability pcross=0.60 with the same population size (npop=20). The Un crossover presents slightly better results when compared to SP crossover form.

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 concluding that the optimization by GA works well without being so dependent on process design values as well as its initial values. The optimization of the same problem by conventional methods (as SQP-Successive Quadratic Programming) presents to

many convergence problems that it is almost impossible to obtain practical results in all the cases considered in this work. When SQP methods were used, the results were dependent upon the initial values (results not shown). This is not the case for the GA. The GA code coupled to the reactor model showed to be a very efficient technique for reactor optimization.

Table 3 Optimization results utilizing npop=20, pcross=0.60, uniform crossover (Un)

Parameters	Non Optimized Real Operational Values	Optimized Operational Values
Q_{r1}	0.50400	0.50467
Q_{r2}	0.51800	0.49934
Q_{r3}	0.55200	0.58429
Q_{r4}	0.07200	0.08042
Q_{r5}	0.10400	0.09452
Q_{r6}	0.05800	0.05104
T_0	0.63200	0.77143
Q_{cat}	0.72333	0.42484
Q_{CA}	0.93400	0.95173
Q_{BA}	0.01316	0.00921
Q_C	0.46320	0.35083
Q_{ri}'s Total	1.80800	1.81428

5. Acknowledgements

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