CHEMICAL ENGINEERING TRANSACTIONS Volume 17, 2009
Editor Sauro Pierucci
 ISBN 978-88-95608-01-3 ISSN 1974-9791
DOI: 10.3303/CET0917234

Large Scale Optimization Procedure by Genetic Algorithm: Application to Three Phase Slurry Catalytic Reactor

Victorino, I. R. S.; Morais, E. R.; Barbosa, A. G.; Maia, J. P.; Vasco de Toledo, E. C., and Maciel Filho, R.
Laboratory of Optimization, Design and Advanced Control.
Department of Chemical Processes. School of Chemical Engineering.
State University of Campinas (UNICAMP)
PO BOX 6066 - ZIP 13081-970 - Campinas, SP - Brazil.
e-mails: igor.rsv@gmail.com / maciel@feq.unicamp.br
FAX +55-19-3521-3965

This work has as objective the development of an optimization methodology, based on genetic algorithms (GAs) applied to deterministic mathematical models representing a catalytic three-phase reactor that is widely used in petroleum and petrochemical, chemical and pharmaceutical industries. These reactors also have a potential application in waste water treatment and in bio-chemical reactions. The GA optimization technique provides satisfactory results leading towards better control strategies, improved profitability and operational security. The reactor model used here describes the dynamic behavior during the hydrogenation of o-cresol on Ni/SiO_2 catalyst. This model allows the reproduction of the main characteristics of the reactor in face to several changes in the operational parameters and is fundamental for the development of an efficient optimization strategy, as well as for simulation studies and reactor design. The optimization strategy focuses on production maximization with the due required quality standards considering the available data. The influence of the GA's parameters (population size, generations and crossover rates) is evaluated. The results show that GA is a suitable optimization tool, allowing the reactor to operate in a high performance level.

Keywords: *global optimization, genetic algorithms, chemical process, slurry catalytic reactor, o-cresol*

1. Introduction

Catalytic multiphase reactors where hydrogenation reactions take place are important systems usually working at very high unstable situations. Three-phase reactors can be found in several important applications, including hydrogenation and oxidation processes. A three-phase catalytic reactor is a system in which a gaseous and a liquid phase are put into contact with a solid phase catalyst; thus, three phases are present.

Please cite this article as: Victorino I.R.D.S., Morais E.R., Agremis G.B., Maia J.P., Vasco De Toledo E. and Maciel Filho R., (2009), Large scale optimization procedure by genetic algorithm: application to three phase slurry catalytic reactor, Chemical Engineering Transactions, 17, 1401-1406 DOI: 10.3303/CET0917234

Modeling such type of reactors is a difficult task because it involves many aspects like hydrodynamics, gas–liquid and liquid–solid mass and heat transfer, pore diffusion, and reaction/deactivation kinetics. The three-phase reactor 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 (Victorino *et al.*, 2007). A typical process of industrial interest is the hydrogenation of ortho-cresol (Vasco de Toledo *et al.*, 2001). The deterministic mathematical model used to describe the reactor in this work is based on the work by Santana (1995).

Genetic Algorithms (GAs) are optimization procedures 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. Victorino (2005) and Victorino *et al.* (2007) studied the optimization of the same reactor under different genetic operators. Morais *et al.* (2007) considered the GA optimization for estimating the parameters of the Arrhenius equation for maleic anhydride synthesis, obtaining a noticeable success. In this study, David Carroll's genetic algorithm code, version 1.7a, coded in FORTRAN, (Carroll, 1996a, 1996b) is adopted, since it is relatively easy to be adapted for the problem considered in this work. Very good results have been achieved with this code for several interesting applications as found in many works: Souza *et al.* (2003), Costa and Maciel Filho (2005), Costa *et al.* (2005), Victorino (2005), Victorino *et al.* (2007), Morais *et al.* (2007), Rezende *et al.* (2008) and others.

2. Process Description and Model Equations

The three-phase reactor dynamic model formulated in this work is based on the work by Vasco de Toledo *et al.* (2001). The model consists of mass and energy balance equations for the catalyst particles as well as for the gas and liquid bulk phases and an equation for the coolant fluid. This model describes the dynamic behavior of the o-cresol hydrogenation on Ni/SiO_2 catalyst, (Hichri, Armand, & Andrieu, 1991). This non-isothermal heterogeneous model includes: the resistances to mass and heat transfers at the gas–liquid and liquid–solid interfaces, and at the catalyst particle; the heat exchange with the coolant fluid; the change of physicochemical properties and mass/heat-transfer phenomena. The developed model can easily be adapted to other reactions due to the generality of its development. This model reproduces the main dynamic characteristics of the reactor in face of several changes in the operational parameters. The scheme representing the reactor is shown in Figure 1.

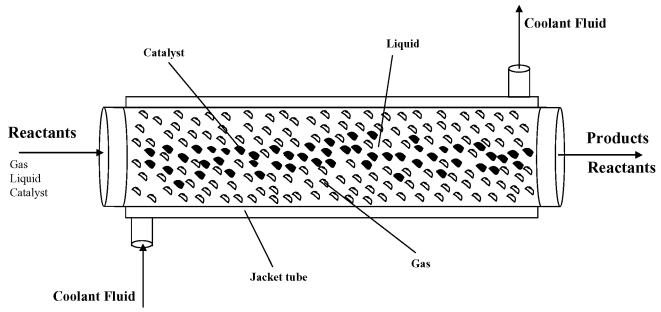

Figure 1 Three-phase o-cresol reactor

2.1 Model Equations

The following hypotheses were adopted: plug-flow for the reactant and thermal fluid; homogeneous suspension (liquid+solid), considered as a pseudo-fluid; pressure variations negligible; no phase change in the system. The radial dispersion has been neglected for the fluid phase; this is very common in multiphase reactor as normally found in literature (Vasco de Toledo *et al.*, 2001). The kinetic model describes the reaction of o-cresol hydrogenation on Ni/SiO_2, producing 2-methylcyclohexanol, which stoichiometry is represented by:

$$3\,H_2(g) + C_6H_4OHCH_3(l) \rightarrow C_6H_{10}OHCH_3(l)$$

The following expression has been obtained for the reaction rate (Hichri *et al.*, 1991) and more details are found in Santana (1995) and Vasco de Toledo *et al*. (2001).

$$R_A = k\frac{K_A K_B C_A C_B}{(1 + K_A C_A)(1 + K_B C_B)} \tag{1}$$

where A stands for hydrogen, B for o-cresol, and C for 2-methylcyclohexanol and the constant is a function of temperature according to an Arrhenius type law.

3. Optimization Strategies

The GA code developed by Carroll (1996a) was coupled with the reactor model. Table 1 shows the parameters of the GA code used in this work. The analysis considered two population sizes 10 and 20, crossover rates of 20, 40, 60 and 80%; and 50, 100 and 200 generations; all of them evaluated through the impact over the productivity of the product of interest (2-methylcyclohexanol). Table 2 shows the parameters used for optimization analysis.

Table 1 GA parameters of code used in the simulations

Genetic Algorithm Parameters		
Population Size (npop)	10 and 20	
Crossover	Uniform (Un)	Crossover Rates (%) 20, 40, 60 and 80
Mutation	Forms	Mutation Rates (%)
	Jump (JM)	1
	Creep (CM)	2
Niche Operator	Yes (used in simulations)	
Selection Types	Tournament and Elitism	
Generations	50, 100 and 200	

where T_{fo} is the reactor feed temperature (K); T_{ro} is the coolant fluid feed temperature (K); u_g is the gas phase linear velocity (m/s); u_l is the liquid phase linear velocity (m/s); u_r is the coolant fluid linear velocity (m/s); A_{lfo} is the feed concentration of the component A in the liquid phase (kmol/m^3); A_{gfo} is the feed concentration of the component A in the gas phase (kmol/m^3); B_{lfo} is the feed concentration of the component B in the liquid phase (kmol/m^3). These are the most sensitive parameters for the reactor (Vasco de Toledo *et al.*, 2001).

Table 2 Operational Parameters of o-cresol hydrogenation reactor

Parameters	Values	Lower Limit	Upper Limit	Range (%)
T_{fo}	540.0	486.0	594.0	± 10
T_{ro}	500.0	425.0	575.0	± 15
u_g	1.80	1.44	2.16	± 20
u_l	0.0080	0.0064	0.0096	± 20
u_r	0.0050	0.0040	0.0060	± 20
A_{lfo}	0.0015	0.0012	0.0018	± 20
A_{gfo}	0.0015	0.0012	0.0018	± 20
B_{lfo}	0.024	0.0192	0.0288	± 20

4. Results and Conclusions

The preliminary results present excellent performance and the desired productivity increase. The application of the genetic algorithm code was very important in the production improvement. Table 3 shows results related to the population size (npop) equal to 10 while Table 4 depicts results with population size of 20. It can be observed that the difference among the optimized cases are not significant, but in comparison to design conditions without optimization, the difference is expressive since the not optimized productivity stays around 0.44×10^{-4} kmol/(m^3.s) with a conversion of about 46%, and in the optimized situation the productivity is as high as 1.09×10^{-4} kmol/(m^3.s) (increase of 147%) and conversion of approximately 79% (increase of 71%). This means that the optimization procedure largely contributed for improving the reactor performance.

Table 3 Results using population size (npop = 10)

Uniform Crossover (Un) - Population Size (npop) = 10				
	Generations = 50			
Crossover Rates (%)	20	40	60	80
Productivity ($x10^{-4}$)	1.0427	1.0589	1.0767	1.0629
Converted	0.7887	0.7839	0.7817	0.7788
	Generations = 100			
Crossover Rates (%)	20	40	60	80
Productivity ($x10^{-4}$)	1.0819	1.0788	1.0863	1.0897
Converted	0.7915	0.7807	0.7858	0.7927
	Generations = 200			
Crossover Rates (%)	20	40	60	80
Productivity ($x10^{-4}$)	1.0950	1.0996	1.0960	1.0967
Converted	0.7924	0.7967	0.7932	0.7946

Several runs with different setups (population sizes, crossover rates, and generations) allow concluding that the GA optimization works well without being so dependent on design values as well as initial values like other conventional optimization methods, such as SQP (Successive Quadratic Programming) which show a relatively high number of convergence difficulties when dealing with a large scale problem. This is not the case for the GA optimization procedure. The only concern to be taken into account is the high computational time related to larger population sizes (above npop=200). There are few significant changes when the number of generations is increased; therefore a number around 200 generations is enough to achieve the optimum.

Table 4 Results using population size (npop) 20

Uniform Crossover (Un) - Population Size (npop) = 20				
	Generations = 50			
Crossover Rates (%)	20	40	60	80
Productivity ($x10^{-4}$)	1.0784	1.0540	1.0858	1.0900
Converted	0.7856	0.7860	0.7883	0.7928
	Generations = 100			
Crossover Rates (%)	20	40	60	80
Productivity ($x10^{-4}$)	1.0813	1.0813	1.0891	1.0926
Converted	0.7827	0.7863	0.7911	0.7945
	Generations = 200			
Crossover Rates (%)	20	40	60	80
Productivity ($x10^{-4}$)	1.0958	1.0954	1.0966	1.0952
Converted	0.7946	0.7943	0.7943	0.7946

5. 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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