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ALGORITHMS FOR REAL-TIME INTEGRATED OPTIMIZATION AND CONTROL: ONE LAYER APPROACH

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Abstract: In this work, control and optimization algorithms are presented in order to be used in real-time process integration. The process considers as case study the o-cresol hydrogenation to obtain 2-methyl-cyclohexanol which is carried out in a three phase catalytic reactor. The real-time integration problem is postulate in one layer approach basis. Dynamic Matrix Control (DMC) is the control algorithm to be used and the optimization problem is solved by Genetic Algorithms. These algorithms showed to be efficient and robust to find out the optimal conditions and they can be used simultaneously to solve the problem in an one layer fashion.

Keywords: Real-time; Three-phase reactor; Control; Optimization; Genetic algorithm.

1. INTRODUCTION

Real-time process integration is an important task to feasible operation at high levels of operational performance. Conventional operational procedures, which require to have platforms specified by heuristic procedures and the controllers, which are tuned in a non-hierarchical way in relation to the operational specification, tend to fail for non-linear and complex systems. In this situation, the solution of the optimization problem coupled with the design and the controller tuning (Process Integration) can be carried out dynamically and at periods of time constrained by the process time constant (in real-time), becoming a necessary solution to reach the desired performance level.

The integration of chemical process in real-time is an interesting operation mechanism, because of the benefits that such approach may bring to the process in terms of profit and safety. Besides, it requires the development and application of several tools which may lead to a better understanding the steps and mechanisms taking place in the process.

One of the elements of real-time process integration is the advanced control, whose main function is to maintain the process in the desired set point, defined by an optimization strategy in the context of the real time process integration, and at the same time to avoid that the process variables violate their constraints. The controller, normally, is a linear multivariable predictive controller. Other element is the optimization algorithm used to solve simultaneously a large amount of equations and to send the optimal values (the set points) to the advanced controller.

The real-time optimization is mainly concerned with steady-state economics and uses nonlinear models while, at the advanced process control level, the objective functions used are not directly related to economics and the models employed are linear (Kookos, 2005).

An important point in real-time optimization is the necessity of a robust algorithm to converge to the optimal conditions, taking into account the need to obtain the response at relatively short time and with a lower computer burden.

Diehl et al. (2002) describe a new real-time and Nonlinear Model Predictive Control (NMPC) schemes based on the direct multiple shooting method. This approach shows CPU times in the range of a few seconds per optimization problem.

The real time optimization can be carried out through an optimization in one or two layers (Rezende et al., 2004). In the two layers approach, the low layer is responsible for the dynamic control. The high layer determines the optimum steady state for the process variables, which are used in the low layer as set points of controlled and manipulated variables (Zanin, 2001). In the one layer optimization approach, the problems of the control and economic optimization are solved simultaneously in a single algorithm (Tvrzská de Gouvêa, 1997).

In this work, it is addressed the problem of real-time integration for the multiphase reactor that produces 2-methyl-cyclohexanol, considering the most relevant aspects necessary to postulate and to solve the problem in a one layer fashion. A simple to use and easy to implement control structure, using SISO approach, for the desired product concentration is proposed and analyzed. For the optimization problem, responsible to generate the set points for the controllers, an algorithm is used coupled with the reactor rigorous model.

2. CASE STUDY

In this paper the o-cresol hydrogenation to obtain 2-methyl-cyclohexanol, which is carried out in a three phase catalyst slurry reactor, is considered as the representative of many important industrial processes. The hydrogenation of o-cresol is represented by:

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

A scheme of a slurry reactor can be seen in Figure 1, for a co-current operating mode, in which the gas and liquid phase flow in the same direction of the solid catalyst slurry.

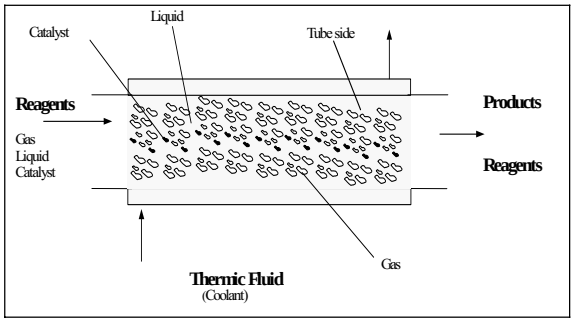

Fig. 1. A scheme of a three phase catalyst slurry reactor.

2.1 Mathematical Modeling.

The slurry type three phase system is represented by a non linear deterministic mathematical model developed by Vasco de Toledo and Maciel Filho (2004). This is a heterogeneous model constituted by material and energy balances for the three phases of the tube side, and the energy balance to the coolant fluid, with the following equations:

- Mass Balance for reactant A (hydrogen) in gas phase:

$$\varepsilon_g \frac{\partial A_g}{\partial t} = \frac{D_{eg}}{L^2}\frac{\partial^2 A_g}{\partial z^2} - \frac{u_g}{L}\frac{\partial A_g}{\partial z} - \left(K_{gl}\right)_A a_{gl}\,(A^* - A_l) \qquad (1)$$

Boundary Conditions:

$$\left.\frac{D_{eg}}{L}\frac{\partial A_g}{\partial z}\right|_{z=0} = u_g\left(A_g - A_{gf}\right) \qquad (2)$$

$$\left.\frac{\partial A_g}{\partial z}\right|_{z=1} = 0 \qquad (3)$$

- Mass Balance for reactant A (hydrogen) in liquid phase:

$$\varepsilon_l \frac{\partial A_l}{\partial t} = \frac{D_{el}}{L^2}\frac{\partial^2 A_l}{\partial z^2} - \frac{u_l}{L}\frac{\partial A_l}{\partial z} + \left(K_{gl}\right)_A a_{gl}\,(A^* - A_l) - \left(K_{ls}\right)_A a_{ls}\,(A_l - A_s^s) \qquad (4)$$

Boundary Conditions:

$$\left.\frac{D_{el}}{L}\frac{\partial A_l}{\partial z}\right|_{z=0} = u_l\left(A_l - A_{lf}\right) \qquad (5)$$

$$\left.\frac{\partial A_l}{\partial z}\right|_{z=1} = 0 \qquad (6)$$

- Mass Balance for reactant B (o-cresol) in liquid phase:

$$\varepsilon_l \frac{\partial B_l}{\partial t} = \frac{D_{el}}{L^2}\frac{\partial^2 B_l}{\partial z^2} - \frac{u_l}{L}\frac{\partial B_l}{\partial z} - \left(K_{ls}\right)_B a_{ls}\,(B_l - B_s^s) \qquad (7)$$

Boundary Conditions:

$$\left.\frac{D_{el}}{L}\frac{\partial B_l}{\partial z}\right|_{z=0} = u_l\left(B_l - B_{lf}\right) \qquad (8)$$

$$\left.\frac{\partial B_l}{\partial z}\right|_{z=1} = 0 \qquad (9)$$

- Energy Balance in the fluid phase:

$$\left(\varepsilon_g \rho_g Cp_g + \varepsilon_l \rho_l Cp_l\right)\frac{\partial T}{\partial t} = \frac{\left(\varepsilon_g \lambda_g + \varepsilon_l \lambda_l\right)}{L^2}\frac{\partial^2 T}{\partial z^2} - \frac{\left(\varepsilon_g \rho_g Cp_g u_g + \varepsilon_l \rho_l Cp_l u_l\right)}{L}\frac{\partial T}{\partial z} + h_s a_{ls}(T_s^s - T) - \frac{4U}{D_t}(T - T_r) \qquad (10)$$

Boundary Conditions:

$$\left.\frac{\left(\varepsilon_g \lambda_g + \varepsilon_l \lambda_l\right)}{L}\frac{\partial T}{\partial z}\right|_{z=0} = \left(\varepsilon_g \rho_g Cp_g u_g + \varepsilon_l \rho_l Cp_l u_l\right)\left(T - T_f\right) \qquad (11)$$

$$\left.\frac{\partial T}{\partial z}\right|_{z=1} = 0 \qquad (12)$$

- Energy Balance for the coolant:

$$\rho_r \, Cp_r \frac{\partial T_r}{\partial t} = - \frac{\rho_r \, Cp_r \, u_r}{L} \frac{\partial T_r}{\partial z} + \frac{4U}{D_t} (T - T_r) \qquad (13)$$

Boundary Conditions:

$$T_r = T_{rf}, \qquad z = 0 \qquad (14)$$

- Mass Balance for reactant A (hydrogen) in solid phase:

$$(1-\varepsilon)\varepsilon_s \frac{\partial A_s}{\partial t} = (K_{ls})_A \, a_{ls} (A_l - A_s) - \frac{(1-\varepsilon)\rho_s}{A_{ref}} R_W(A_s, B_s, T_s) \qquad (15)$$

- Mass Balance for reactant B (o-cresol) in solid phase:

$$(1-\varepsilon)\varepsilon_s \frac{\partial B_s}{\partial t} = (K_{ls})_B \, a_{ls} (B_l - B_s) - \frac{\nu(1-\varepsilon)\rho_s}{B_{ref}} R_W(A_s, B_s, T_s) \qquad (16)$$

- Energy Balance in solid phase:

$$(1-\varepsilon)\rho_s \, Cp_s \frac{\partial T_s}{\partial t} = h_s \, a_{ls} (T_s - T) + \frac{(1-\varepsilon)\rho_s (-\Delta H_R)}{T_{ref}} R_W(A_s, B_s, T_s) \qquad (17)$$

where

a	surface area, m^{-1}
A	concentration of hydrogen, $kmol/m^3$
*A**	solubility of the component A, $kmol/m^3$
B	concentration of o-cresol, $kmol/m^3$
De	effective diffusivity, m^2/s
D_t	reactor diameter, m
h	heat transfer coefficient, kJ/m^2 s
K	mass transfer coefficient between the phases, cm/s
L	reactor length, m
Rp	radius particle, m
R_w	reaction rate, kmol/kg catalysts.s
T	absolute temperature
u	linear velocity, m/s
U	global heat transfer coefficient, kJ/m^2 s
ΔH_R	heat of reaction, kJ/kmol
ε	porosity
λ	heat conductivity, kJ/m s K
ρ	density, kg/m^3
ν	stoichiometric coefficient

Subscripts:

A	component A (hydrogen)
B	component B (o-cresol)
f	feed
g	gas phase
gl	gas-liquid
l	liquid phase
ls	liquid-solid
p	particle
r	coolant fluid
ref	reference value used to turn the equations dimensionless
s	solid

Superscripts:

s	catalyst surface

The model equations lead to a system of partial differential equations that are converted into a system of ordinary differential equations through discretization by orthogonal collocation. The resulting equations were integrated using DASSL software which is suitable for stiff systems.

3. ALGORITHMS FOR REAL-TIME INTEGRATED OPTIMIZATION AND CONTROL

3.1 Optimization procedure.

The real time optimization causes a lower profit when a local optimizer is used. This problem can be averted by using a global optimizer in the real time optimization procedure (Lacks, 2003). In this work, a global optimizer, based on the Genetic Algorithms, is chosen and proposed to be used in a posterior Real Time Integration.

The aim of the optimization is to find out an optimal steady state of the three phase reactor that produces 2-methyl-cyclohexanol using a rigorous model of this process. The optimal condition is the new set point in which, the reactor should be operated to have higher performance.

The objective function considered was the productivity of 2-methyl-cyclohexanol subjected to the conversion of o-cresol in the liquid phase, which is usually required for practical implementations:

$$\text{Productivity} = \frac{(B_{lf} - B_l) * u_l}{L} \qquad (18)$$

As constraint, it was considered the operation of the unit under limits of o-cresol conversion larger than 90%, since the environment constraints require such levels of conversion.

$$\text{Conversion} = \frac{B_{lf} - B_l}{B_{lf}} > 0.90 \qquad (19)$$

In order to proceed with the reactor optimization, the mathematical model (Eqs. (1-17)) is incorporated to the Genetic Algorithm code and the objective function is defined. The optimization is carried out in steady state so that the reactor is represented by equations 1 to 17 setting the derivatives in respect to time to zero.
The optimization problem can be written as:

Maximize: Productivity
Subject to: Model equations (Eqs. (1-17))
Conversion > 90%
$0.004195 \le u_l \le 0.011805$
$0.000608 \le A_{gf} \le 0.002392$
$0.009732 \le B_{lf} \le 0.038268$
$459.0 \le T_f \le 621$
$425.0 \le T_{rf} \le 575.0$
$1.08 \le u_g \le 252.0$
$0.003 \le u_r \le 0.007$
$0.00075 \le A_{gf} \le 0.00225$

In this work, the GA code used is the Fortran Genetic Algorithm Driver by David Carroll, version 1.7a (Carroll, 2004), with some modifications. This is a binary code that starts with a random population of chromosomes that are a set of solutions to the optimization problem. Each solution is evaluated by the fitness function that associates a value to the solution, determining the best ones. In this point, the genetic operators, that are the kernels of Genetic Algorithms, responsible to promote the evolution of the solutions are applied (Wang, 2005). This procedure is repeated along the iterations, also called generations, until a termination criterion is satisfied.

In this work the termination criterion is given by the number of generations, since the solutions are better along the generations. During the optimization, it was set the population size, the crossover and mutation probabilities, the maximum number of generations and number of children per pair of parents. In this code is possible to set elitism, niching and micro-GA techniques. The details of the tools can be found in Deb (1999). As genetic operators are used tournament selection, single-point crossover and jump and creep mutation. It was set elitism, two children per pair of parents and niching. In order to handle the constraint present at the reactor optimization problem, the constraint handling method proposed by Deb (2000) is incorporated to the Carroll's code. This method exploits the feature of the GAs algorithm of pairwise comparison in tournament selection (Deb, 2000; Costa and Maciel Filho, 2005).

Extensive simulations lead to the convergence to the optimal conditions. The results obtained with the optimization by GA are the productivity of 2-methyl-cyclohexanol of 1.64×10^{-4} Kmol/m^{3}s and the conversion of o-cresol of 90.18%. It shows an improvement of three times the productivity of 2-methyl-cyclohexanol and twice the conversion, compared to the steady state at previous work using the same model (Rezende et al., 2004).
Bearing in mind the high dimensionality and non linearity of the model, the genetic algorithm showed to be robust to converge to the optimal conditions.
before a main or secondary heading.

3.2 Control Procedure

For the layer of the control, a predictive controller based on the Dynamic Matrix Control (DMC), is implemented. The DMC algorithm development for monovariables systems (SISO) can be found at Rezende et al. (2004).
DMC makes use of a linear model, the convolution model, which is obtained through step disturbances in the input variables. In this work is presented the DMC algorithm developed to monovariable systems SISO, since a reliable control strategy was defined.
The DMC algorithm is based on the calculation of NC (Control Horizon) future values of the manipulated variables from a minimization of NP (Prediction Horizon) future values of the square of the difference between set point and output predicted by a convolution model with NM (Model Horizon) output values obtained from the step response to the manipulated variable.
The model horizon (NM), the prediction horizon (NP), the control horizon (NC) and the suppression factor (f) are parameters to be tunned in order to obtain a good performance of the controller.
In order to verify the controller performance, several sets of controller parameters were tested for load disturbances. The objective of the controller is to reach a suitable control for the o-cresol concentration at the reactor exit, able to work in a relatively wide range of operation conditions specified by the optimization algorithm.

Control of the o-cresol concentration at the reactor exit. The simulations to study the o-cresol concentration control at the reactor exit considered disturbances of ± 5% in the manipulated variable, step disturbance of ± 5% and alteration of the ± 5% in the set point. The set of operating variables is: ul = 0.0096 m/s, Agf = 0.001875 Kmol/m^3, Blf = 0.0300 Kmol/m^3, Tf = 648 K e Trf = 600 K. The required set point of the output reactor o-cresol concentration in the liquid phase is 0.00258 Kmol/m^3. A different set of parameters was tested in order to find out a set of parameters that allows for a good performance of the controller. This set of parameters is: NM = 4, NP = 3, NC = 1, and f = 0.0001. On-line concentration measurement can be obtained by near-infrared measurement with a good and robust performance in industrial environment. A sampling time of 100 s is used in this work, as this is the value normally found in industrial practice.
The controlled and manipulated variables profiles, observed in the Figures 2 and 3, show that the performance of the controller is satisfactory to this set of operating variables.
Figure 2 shows that the controlled variable reaches the set point around 1500s and remains on it along the period; the overshoot is small and oscillations were not observed.

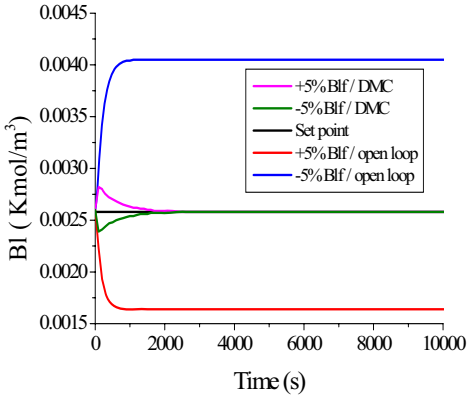

Fig. 2. Open and closed loop concentration response for disturbances of ± 5% in Blf.

Figure 3 shows that the manipulated variable reaches a steady state in approximately 2000s and does not present oscillations along the period. These results show the very good performance and robustness of the proposed control structure, for a relative large range of operational conditions.

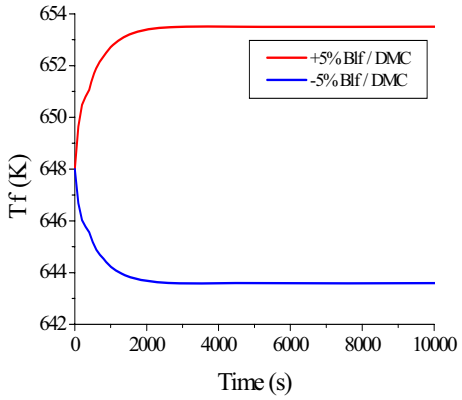

Fig. 3. Profile of manipulated variable (Feed temperature).

4. REAL TIME INTEGRATED OPTIMIZATION AND CONTROL

In order to proceed with the real-time integration, a robust and efficient algorithm to find out the optimal conditions in a relatively short time is required. This is essential especially for the one layer approach since the controller action depends on the convergence of the whole optimization/control problem. Figure 4 shows a scheme of the one layer approach.

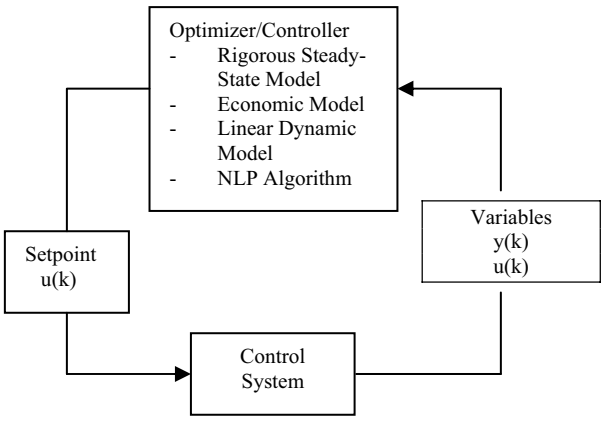

Fig. 4. Schematic diagram for the one layer approach.

The mathematical formulation of the control/optimization problem is described bellow (Zanin, 2001):

$$\min_{x_s,u_s,\Delta u(jT_a);j=1,...NC} \sum_{i=1}^{NP} \left\| W_1\left(y_p(iT_a)-y_{sp}\right)\right\|_2^2 + \sum_{j=1}^{NC} \left\| W_2\Delta u(jT_a)\right\|_2^2 + W_3 f_{eco} \quad (20)$$

Subject to the following constraints:

$$h_p(x_s,u_s,d_s)=0 \quad (21)$$

$$h_e(f_{eco},x_s,u_s,d_s)=0 \quad (22)$$

$$u_s^{inf} \le u_s \le u_s^{sup} \quad (23)$$

$$x_s^{inf} \le x_s \le x_s^{sup} \quad (24)$$

$$-\Delta u^{max}(jT_a) \le \Delta u(jT_a) \le \Delta u^{max}(jT_a) \quad j=1,...,NC \quad (25)$$

$$u^{inf}(jT_a) \le u_{at} + \sum_{i=1}^{j} \Delta u(iT_a) \le u^{sup}(jT_a) \quad j=1,...,NC-1 \quad (26)$$

$$u_s = u_{at} + \sum_{j=1}^{NC} \Delta u(jT_a) \quad (27)$$

$$y_p(iT_a) = y_{pf}(iT_a) + \sum_{j=1}^{\min(NP,NC)} a_{dmc}((i-j+1)T_a)\Delta u(jT_a) \quad j=1,...,NP \quad (28)$$

where:

a_{dmc}	matrix of the coefficients of the process linear model
ds	vector of the perturbations at the steady-state
f	weighting factor in the DMC algorithm
f_{eco}	economic objective function
h_e	economic model constraints
h_p	nonlinear model constraints
NC, NP	control horizon and prediction horizon
NM	model horizon
T_a	sampling period
u	vector of the manipulated variables
u_{at}	vector of the manipulated variables at the current time
u_s	vector of the manipulated variables at steady-state
x_s	vector of the nonlinear model variables in the steady-state
W_1	diagonal matrix of the weight of the dinamically controlled variables
W_2	diagonal matrix of the supression factor of the manipulated variables
W_3	weight of the economic parcel in the objective function
y_p	vector of the linear prediction of the dynamically controlled variables
y_{pf}	vector of the linear predicition of the dynamically controlled variables, based on passed control actions
y_{sp}	vector of the set points of the dynamically controlled variables
Δu	vector of the amplitude of the control actions

The challenge in the implementation of the optimizer is to be able to work with an integrated optimization and control procedure in a real time basis.

The process considered in this work is characterized by high dimensionality and non linearity of the model. Because of this, the solution of the optimization problem may bring difficulties related to the convergence. Optimization algorithms based on

the GA principles are robust and care has to be taken in the required computer time (Costa and Maciel Filho, 2005). For this particular problem the GA presented quite good performance with a reasonable computer time, around ten minutes in a Pentium 4, 2.8GHz, 512 MB RAM. It is an important aspect in real time applications of the GA optimization technique coupled with the high nonlinear and multivariable model, making this approach to be a good candidate to real time process integration.

5. CONCLUSION

This work presents the steps necessary to carry out the real-time process integration for the multiphase reactor that produces 2-methyl-cyclohexanol, through a one layer approach. The objective function of the control/optimization problem is composed of parcels from the dynamic control and the economic optimization. As controller of the process, it was used the DMC that showed to be efficient to control the reactor. The optimization problem was solved by Genetic Algorithm that revealed to be robust enough to lead to the convergence to the optimal conditions with a short computational effort. The results showed that the both techniques can be used simultaneously to deal with one layer real time integration.

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