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Control Strategies Evaluation for a Three-Phase Hydrogenation Catalytic Reactor

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Abstract: Hydrogenation reactions are widely applied industrially, and reactors have been designed for this purpose. It is a highly non-linear process, multivariable, with exothermic reaction. The model formulation was made focusing on the hydrogenation reaction of o-cresol to obtain the 2-methil-cyclohexanol, in the presence of a Ni/SiO_2 catalyst. A competitive advantage in such kind of system (a commodity with large production scale) is to operate an optimal level of performance under control. The present work introduces an optimization problem and control in a simulation study of the reactor. The model allowed to reproduce the main characteristics of its dynamic, as well as the evaluation of the performance of different control strategies (Feedback, Feedforward or both strategies). The analysed controller was the linear model predictive (QDMC), and extensive analysis allow to identify which control strategy was more suitable to operate the reactor in an efficient and safe way. These informations are important for the real time integration implementation procedure.

Keywords: hydrogenation, dynamic modelling, simulation, optimization, advanced controller.

1. INTRODUCTION

The control of many chemical processes like tubular reactors, with or without catalytic bed, is complicated by problems associated with the on-line measurements of desired control objectives, especially those concerned with concentrations. For the tubular reactors, the primary control objective is usually the regulation of the outlet concentration at optimum levels, while attention is paid to a safe operation and reactor temperatures that do not exceed some pre-specified maximum value. The outlet concentration cannot be easily measured on-line, so it must be inferred (estimated) from the available temperature measurements along the reactor.

Therefore, for the establishment of the control strategy of a chemical reactor, it is necessary to define its operational objective as well as to develop a model that predicts the main characteristics of the dynamic behaviour of this reactor. In this work, the priority of the control is not directly related to the outlet concentration, but the problem is seen as the thermal control of the reactor, making indirectly the control of the concentration. Therefore, the controllers were evaluated in order to absorb disturbances, which alter the thermal profile of the reactor. This is not a trivial task, and in fact, it is one of the most difficult and dangerous operations in the chemical industry, especially when large scale industrial reactors are considered. Another important objective, in the implementation of the control loop, is to know the physical and operational limitations of the manipulated and controlled variables of the reactor. This information is essential to have a suitable and feasible control strategy.

2. CONTROL

The system used as case of study is a multiphase reactor, where the hydrogenation reactor of o-cresol takes place. The deterministic model takes into account the heterogeneous dynamic behaviour of the system, and the model basically consists of mass and energy balance equations for the reactants as well as for the catalyst particles. The kinetic law considers the hydrogenation reaction of o-cresol to obtain the 2-methil-cyclo-hexanol, in the presence of the catalyst Ni/SiO_2. The utilized scheme to represent the reactor is shown in Figure 1 (Vasco de Toledo et al., 2001).

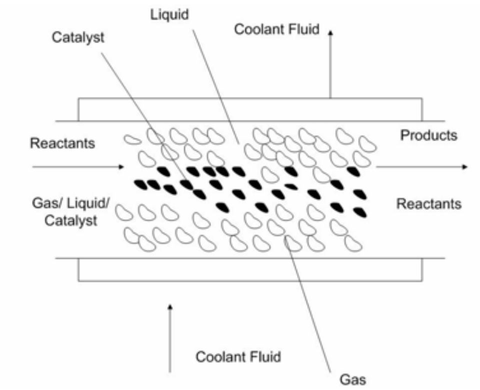

Figure 1 - Three-phase reactor.

The following hypothesis were adopted for the model development (Vasco de Toledo et al., 2001, Vasco de Toledo and Maciel Filho, 2004): a) negligible pressure variations; b) reaction of the type: A (g) + νB (l) $\rightarrow$ νC (l), occurring at the catalyst and with a kinetic that is dependent on the concentrations of A and B; c) no phase exchange in the system. The operational parameters of the reactor, mass and energy balance coefficients, and physical properties have been considered as constant. Some of these parameters were generated by empirical correlations (Mariano et al., 2004).

Very Few attentions have been paid for the control of this type of reactors, Resende et al., 2004 investigated the DMC performance on the control of the multi-phase reactor but only a superficial analysis was considered out.In this work, it was carried out the performance analysis of different control strategies (feedback, feedforward or both strategies), as it can be seen in the diagram represented in the figure 2. The feedforward strategy design frequently suffers from several inherent difficulties: it requires the identification of the disturbance, and a very good model of the process, something quite difficult for many systems in the chemical industry and the changes in the process parameters cannot be compensated unless a reliable estimation procedure is incorporated.

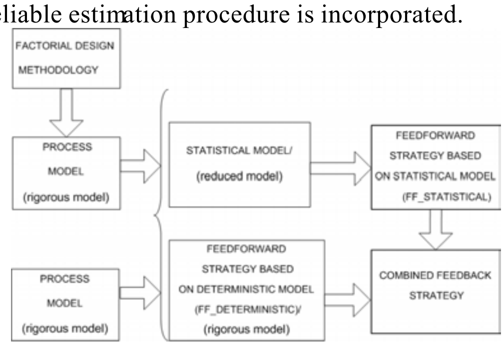

Figure 2- Schematic diagram of the strategies control

The objective of a feedforward controller is basically to generate anticipated corrective actions to compensate measured input disturbances. The control action of the feedforward strategy was generated by a deterministic model and a parametric model of the controlled and manipulated variables, which was developed by the application of the full factorial design method. The application of the factorial design to generate a working model for control purposes is a new procedure introduced in this work and seems to be powerful procedure due to its simplicity and predictions capabilities.

The performance of advanced controller and different control strategies for the thermal control of the reactor were extensively carried out and analysed. The control evaluation consists on problems of set point changes (servo control) and disturbance in the operational parameters of the reactor (regulatory control). These strategies and controller make use of advanced numerical techniques that allow an effective control of the process, due mainly to the several parameters adjustments procedure implemented.

2.1. Feedback Strategy

In the context of feedback strategy, it was used the predictive QDMC (*Quadratic Dynamic Matrix Control*), that is a model predictive controls (MPC) with constraints through the implementation of a optimization routine based on the method of Successive Quadratic Programming (SQP), Garcia and Morshedi, 1986; Zafiriou and Marchal, 1991; and Vasco de Toledo et al., 2004. Among the digital controllers, the QDMC was chosen by its robustness and flexibility to tune due to the presence of several parameters.

The QDMC algorithm predicts the performance of the controlled variables over a prediction horizon, by solving an optimization problem using a quadratic programming (QP) approach to find out the controller actions to a control horizon (smaller or equal to the prediction horizon) (Mayne et al., 2000). The predicted behaviour is calculated using a process model (convolution models). The projected errors, between the desired trajectory and the predicted response, are used to determine future control actions. Only the first control action is implemented. At the next sampling instance, the real plant measurement is used to correct for any plant/model mismatch and the optimization is repeated to find out the next optimal control solution.

When criteria of high level complexity are proposed to obtain the control action, considering restrictions in the controlled and manipulated variables it is necessary to use optimisation algorithms, because, in this case, there is no possibility of analytical solutions. In this work, the performance criterion, optimised via the SQP algorithm, is expressed as:

$$
\begin{aligned}
& J = \min_{\Delta u} \phi = \frac{1}{2} \Delta u^T H \, \Delta u + c^T \Delta u \\
& \text{where :} \\
& H = A^T W^T W A \\
& c^T = -E^{'T} W^T W A \\
& \text{subjected to the following operational constraints :} \\
& y_{min} \le y \le y_{max} \\
& u_{min} \le u \le u_{max}, \; \Delta u_{min} \le \Delta u \le \Delta u_{max}
\end{aligned}
\qquad (1)
$$

In these equations W is the weighting factor matrix (adjustable parameters that allow to penalize the control actions); A is the dynamic matrix of the system; $E^{'}$ is the array that stores the differences between past predictions and reference values; Δu is the array with the incremental of the manipulated variables and y is the controlled variable, u is the manipulated variable with maximum and minimum values, y_{max}, , y_{min} , u_{max} and u_{min}, respectively.

Although this controller, associated to optimisation algorithm, is able to consider more sophisticated control problems, the benefits obtained in this approach must justify the inherent increase of complexity (computational efforts for instance) when it is compared to analytical methods of solution.

2.2. Feedforward Strategy

The feedforward strategy was developed using two methodologies. In the first one, the deterministic model is used in an optimization problem in which the manipulated variable T_{fo} is used as optimization parameter, seeking to minimize the objective function specified by equation (2). The function may be written as:

$$
\begin{aligned}
& \min_{Tfo} \left((T - Tset\,point)^2 \right) \\
& \text{s.t. } Tfo_{min} \le Tfo \le Tfo_{max} \\
& \text{or} \\
& \min_{Tr} \left((T - Tsetpoint)^2 \right) \\
& \text{s.t. } Tr_{min} \le Tr \le Tr_{max}
\end{aligned}
\qquad (2)
$$

The objective was to minimize the difference of the square between the temperature of exit of the reactor and the calculated temperature of the new set point starting from the disturbances for T_{fo} and T_r. T is the exit temperature of the reactor.

Through the Levenberg-Marquardt algorithm was possible to implement this methodology, which allows to find out the value of the manipulated variable, knowing the desired set point and the disturbances of the process.

In the second methodology, the feedforward strategy was developed using a reduced model (statistical model) obtained through the full factorial design method**.** The factorial design was carried out in order to study the effects of some variables of the mathematical model in significant responses and with such information to develop the statistical model for exit temperature of the reactor. The runs were planned to obtain a model, with temperature as response. The central points provide additional degrees of freedom for pure error estimating, but in this case is not possible to calculate it because the responses were determined by simulation. The distance of the axial points was ±2.38, calculated from Eq. (3) (Khuri and Cornell, 1987), where a is the distance of the axial points and n is the number of independent variables. These independent variables and their levels are presented in Table 1. The software Statistical (Statsoft, v. 7) was used to analyse the results.

$$\alpha = \left(2^n\right)^{1/4} \qquad \textbf{(3)}$$

The estimated effects of variables, as well the interactions between them, on each response were determined for a 95% confidence level. To confirm the significance and influence of the studied factors were used statistical parameters. For example, $p < 0.05$, suggests significance at the 0.05 level (Box et al., 1978).

In estimated effects the variables that present statistically significant main effects in the temperature are the o-cresol and hydrogen concentrations in the liquid phase, and the both temperatures (T_{fo} and T_r). For the responses, the most significant variables are the temperatures (T_{fo} and T_r). However, it should be observed that the feed reactant temperature was disturbed in ±5% and the refrigerant one, as well as the other independent variables, in ±10%. Thus, when the main effects were analysed, initially the refrigerant temperature is presumed as the variable that has larger impact on the conversion as well as on the reactor exit temperature. In fact, the variable of larger impact is the feed reactant temperature due to its smaller disturbance. Therefore, as it will be seen later, this variable (T_{fo}) introduces great potential to be used as manipulated variable in the control layer, when compared to the refrigerant temperature (T_r). At this point it is worthwhile mentioning that for practical implementation changes in the refrigerant temperature are difficult to be used since usually thermal fluids have as characteristic present high heat capacity. This means that a large effort, in terms of heat exchanger designs and operation have to be made to change the temperature of large amount of fluid in a reasonable time interval.

The R-square value provided a measure of how much of the variability in the observed response values could be explained by the factors and their interactions. A good model (values above 0.9 are considered good) explains most of the variation in the model response. In fact, a way to obtain a reduced model using such approach to an existing process may be to carry out perturbation in the real plant (what is not always possible), otherwise, to develop a mathematical (deterministic) model, do a proper validation and then use such model in the proposed procedure. Based on the *F*-test, the model is predictive, since its calculated *F*-value is higher than the critical *F* value and the regression coefficient is close to unity, for the temperature. The developed statistical model for the temperature exit was used to solve the control problem.
The statistical analysis was used to obtain the empirical equation that describes the feed reactant temperature (T_{fo}) and the cooling temperature (T_r) as manipulated variables. The empirical equations are presented as a function of the exit reactor temperature (*Tset point*), the feed reactant temperature (when the manipulated variable is T_r), the cooling temperature (when the manipulated variable is T_{fo}), the o-cresol (B_{lfo}) and the hydrogen (A_{gfo} and A_{lfo}, gas and liquid phase, respectively) feed concentration. The linear empirical equations are given by equations (4) and (5), which were obtained from of the full factorial design. The statistical models are:

-feedforward strategy when T_{fo} as manipulated variable:

$$\begin{aligned} \mathrm{Tfo} = {} & \mathrm{Tset\ point} - (-62.50498252 + \\ & + 355.6215012 * \mathrm{Agfo} + 3.836649024 * \mathrm{Alfo} \\ & + 143.4758567 * \mathrm{Blfo} + 0.428379079 * \mathrm{Tr}) / 0.67691109 \end{aligned} \quad (4)$$

-feedforward strategy when T_r as manipulated variable:

$$\begin{aligned} \mathrm{Tr} = {} & \mathrm{Tset\ point} - (-62.50498252 + 355.6215012 * \mathrm{Agfo} + \\ & + 3.836649024 * \mathrm{Alfo} + 143.4758567 * \mathrm{Blfo} + \\ & 0.67691109 * \mathrm{Tfo}) / 0.428379079 \end{aligned} \quad (5)$$

Table 1 – Variables and levels for central composite design.

	-2.38*	-1	0	+1	+2.38*
A_{gfo} (± 10%)	1.14E-02	1.35E-02	1.50E-02	1.65E-02	1.86E-02
A_{lfo} (± 10%)	8.38E-03	9.90E-03	1.10E-02	1.21E-02	1.36E-02
B_{lfo} (± 10%)	1.83E-01	2.16E-01	2.40E-01	2.64E-01	2.97E-01
T_{fo} (± 5%)	476.00	513.00	540.00	567.00	604.00
T_r (± 10%)	381.00	450.00	500.00	550.00	619.00

$\pm 2.38^* = (2^5)^{1/4}$ (star point)

2.3. *Feedforward-Feedback Strategy*

The basic concept of this strategy is to couple both feedback and feedforward approaches aiming to take advantage of each one of the strategies simultaneously.

The feedforward strategy makes possible an increase in the velocity of the three-phase reactor control, and when it is associated to the feedback control, the result is a powerful plan of control, represented by equation (6), which was, among the control strategies studied, the most efficient, as it will be seen later.

$$\begin{aligned} & \mathrm{u\_(feedback + feedforward)} = \beta\, \mathrm{u\_feedforward} + \\ & + (1-\beta)\, \mathrm{u\_feedback} \qquad \text{where } 0 \le \beta \le 1 \end{aligned} \quad (6)$$

Therefore, the performance of five different strategies were analysed, to know: feedback strategy (FB), feedforward strategy based on deterministic model (FF_deterministic) and on statistical model (FF_statistical), combined feedback strategy and feedforward strategy based on deterministic model (FF_deterministic +FB) and combined feedback strategy and feedforward strategy based on statistical model (FF_statistical + FB).

3. RESULTS AND DISCUSSIONS

The open-loop dynamic behaviour of multiphase reactor was observed by Vasco de Toledo et al. (2001).The comparison of the performance for the studied strategies (feedback, feedforward and mixed feedforward and feedback) is shown in Figures 3 to 7.

In order to evaluate the feedforward-feedback strategy (FF and FB), with both types of model (deterministic and statistical), tests were performed for values of β (eq.6) equal to 0.1, 0.3, 0.5, 0.7 and 0.9. The best profiles for both cases (FF_deterministic + FB and FF_statistical + FB) were found when β =0.7, which is the value used in this work.

As expected, the feedforward strategy, using the deterministic model as well as the statistical model was more efficient to reach the desired set-points.

Care has to be taken for the variation of the manipulated variables which was in most of the cases, the abrupt and this may cause difficulties to the practical implementation of this strategy. The performance analysis of the feedback strategy for the controllers QDMC was considered for typical operating conditions. The SISO regulatory control with T_{f0} as manipulated variable (Figures 3, 4 (for example, the Figure 4 making indirectly the control of the concentration of the o-cresol) and 5) and the SISO servo control with T_r as manipulated variable (Figures 6 and 7) are depicted with a good controller performance.

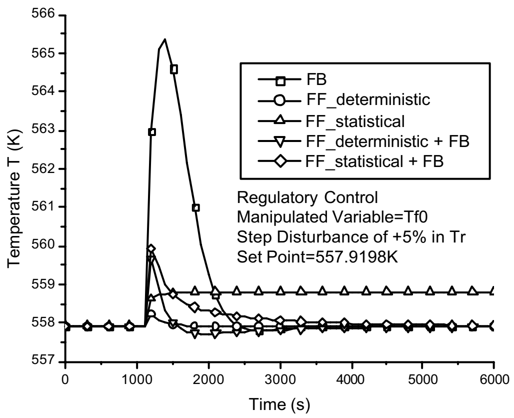

Figure 3. Regulatory SISO control of the reactor – controlled variable

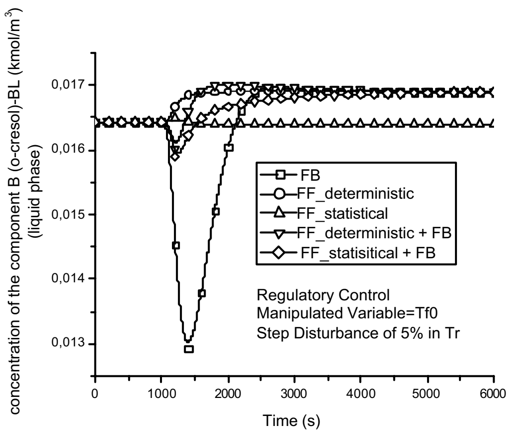

Figure 4. Regulatory SISO control of the reactor – controlled variable

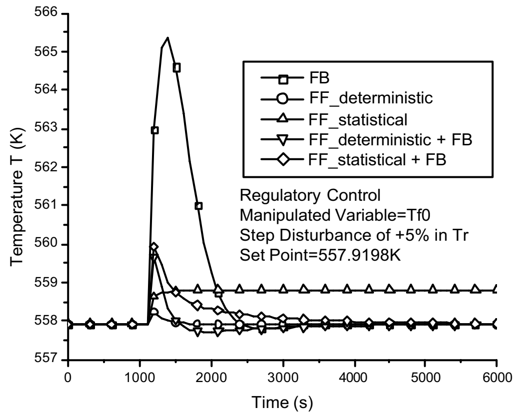

Figure 5. Regulatory SISO control of the reactor - manipulated variable.

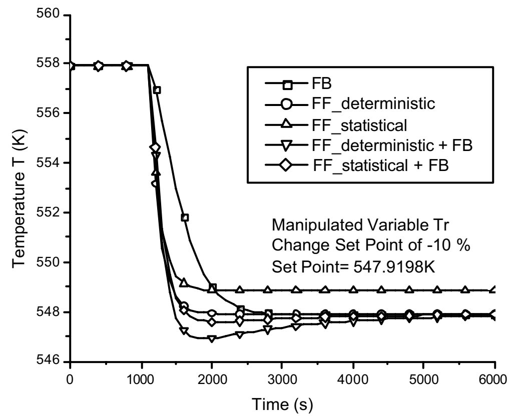

Figure 6. Servo SISO control of the reactor – controlled variable.

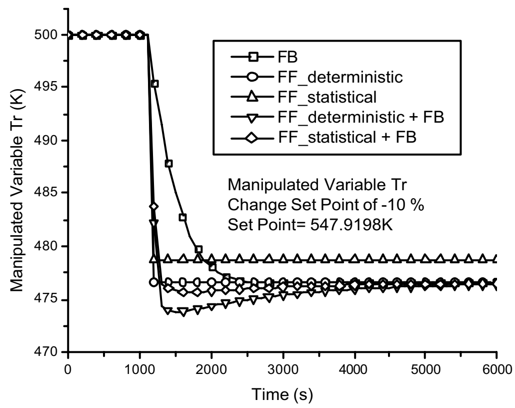

Figure 7. Servo SISO control of the reactor – manipulated variable

The feedforward strategy based on statistical model presented significant off-sets due, mainly, to its sensitivity and inherent errors, which do not allow to represent the dynamic behaviour of the process for the whole operating conditions. The use of statistical based model is a good approach to speed up the calculations but care has to be taken to the model representativity for all possible operation range.

The mixed strategy (Feedforward and feedback) using feedforward based on the statistical model did not present off set as in the case for the conventional feedforward, because the feedback strategy eliminates the off sets. This strategy has good performance and the mixed strategy (FF_deterministic + FB) is even better due to the prediction capabilities of the deterministic model when compared to statistical one.

Nevertheless, the feedforward with statistical model (FF_statistical) and the mixed configuration (FF_statistical + FB), presents advantage since its solution is more rapid, although for the case of the control feedforward (FF_statistical), it was generated off set in comparison with the control feedforward (FF_deterministic). Therefore, depending upon the objectives and operational constraints of the system, some particular strategy can be the most appropriate. For the case of this work, the mixed strategy feedforward-feedback was that presented the better performance.

Finally, the mixed configuration (feedforward + feedback) was able to conciliate quickness to reach the desired set-points with smooth changes in the manipulated variable, which is desired characteristic for an industrial implementation.

4. CONCLUSIONS

The results showed that was possible to evaluate different control strategies for the solution of the multiphase reactor control. This understanding made possible the elaboration of an efficient and safe control strategy with desirable characteristics for an industrial implementation, mixed configuration (feedforward + feedback).

This control strategy should conciliate quickness to reach the desired objectives (set-points) and generate smooth changes in the manipulated variable.

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