Advanced Control of a
Three-Phase Slurry Catalytic Reactor
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Abstract
This work deals with advanced control of a three-phase slurry catalytic reactor represented by a non-isothermal heterogeneous dynamic model to describe the system behaviour. 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) as well as of several control algorithms. The analyzed controllers were the classic PI; linear model predictive and adaptive controls with restrictions using optimization routines. The results allowed a larger understanding of the nature and the main characteristics of the reactor in close loop, moreover to identify which control strategy and algorithm controller were more suitable to operate the reactor in a efficient and safe way.

Keywords: Predictive Control, Adaptive Control, Three-Phase, Slurry Reactor.

1. Introduction
The control of many chemical processes like tubular reactors, with or without catalytic beds, is complicated by problems associated with the on-line measurements of desired control objectives. For the tubular reactor the primary control objective is the regulation of the outlet concentration at optimum levels, while at the same time attention is paid to the maintenance of a safe operation, by requiring that the temperatures in the reactor 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 length of the reactor. Therefore, for the establishment of the control strategy of a chemical reactor it is necessary to define its operational objective. Both, the control and operational objectives are strictly related. In this context, in the case of this work, the priority of the control was not directly the outlet concentration, but the problem is seen as the thermal control of the reactor, making the control of the concentration indirectly. For this, the controllers developed and tested were appraised in the sense of absorbing disturbances that alter the thermal profile of the reactor. This is not a trivial task, and in fact it is one of the most difficult operations in the chemical industry especially when large scale industrial reactors are considered, due to non-linearities and interactions among chemical reactions and heat

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transfer. Another subject also important 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.

In this work were analysed the controllers, classic PI, the predictives Quadratic Dynamics Matrix Control (QDMC) and Quadratic Generic Predictive Control (QGPC), the adaptive predictives Self Tuning Quadratic Dynamics Matrix Control (STQDMC) and Self Tuning Quadratic Generic Predictive Control (STQGPC). These adaptive controllers are algorithms coupled to the identification Recursive Least Square (RLS) procedure. Different control strategies, to know, feedback, feedforward or both strategies together were implemented and analysed. Thus, a reasonable group of control algorithms and strategies were evaluated allowing to obtain a larger understanding of the nature and the main characteristics of the reactor in close loop, and moreover to identify which controllers and strategy were more suitable to operate the reactor in an efficient and safe way.

2. Three-Phase Slurry Catalytic Reactor

The model consisted of mass and energy balance equations, which beyond the predictions of the concentrations and temperature profile, allows for the evaluation of the effect of the phase change of the reacting medium (flash) and the variation of the physical properties and the coefficients of heat and mass transfer. This work considered the hydrogenation of o-cresol on Ni/SiO$_2$ catalyst, which is typical of many hydrogenation processes of industrial interest. More details on the hypotheses adopted to the dynamic model, kinetic equation, numerical solution of model dynamic and the flash multicomponents calculations are given in Vasco de Toeldo et al. (2001) and Vasco de Toledo and Maciel Filho (2002).

**Fluid Phase:**

**Mass balance of reactant A in the gas phase:**

$$
\frac{D_a}{L} \left( \frac{\partial^2 FA}{\partial \xi^2} + \frac{\partial FA}{\partial \xi} \right) = u_i \left( (FA_{zi} - 0) - FA_{zi} \right) - \left( \frac{\partial FA}{\partial \xi} \right)_{\xi=0} = 0
$$

**Mass balance of reactant A and B and product C in the liquid phase:**

$$
\begin{align*}
\frac{D_a}{L} \left( \frac{\partial^2 FA}{\partial \xi^2} + \frac{\partial FA}{\partial \xi} \right) &= u_i \left( (FA_{izi} - 0) - FA_{izi} \right) - \left( \frac{\partial FA}{\partial \xi} \right)_{\xi=0} = 0 \\
\frac{D_a}{L} \left( \frac{\partial^2 FB}{\partial \xi^2} + \frac{\partial FB}{\partial \xi} \right) &= u_i \left( (FB_{izi} - 0) - FB_{izi} \right) - \left( \frac{\partial FB}{\partial \xi} \right)_{\xi=0} = 0 \\
\frac{D_a}{L} \left( \frac{\partial^2 FC}{\partial \xi^2} + \frac{\partial FC}{\partial \xi} \right) &= u_i \left( (FC_{izi} - 0) - FC_{izi} \right) - \left( \frac{\partial FC}{\partial \xi} \right)_{\xi=0} = 0
\end{align*}
$$
Energy balance in the fluid (gas + liquid) phase:
\[
\left(\varepsilon_e \rho_e C_p + \varepsilon_i \rho_i C_p\right) \frac{\partial T}{\partial t} = \left(\varepsilon_e \rho_e \tilde{u}_e + \varepsilon_i \rho_i \tilde{u}_i\right) \frac{\partial T}{\partial \tilde{z}} + \partial_z \left[ h_a (T_i - T_e) + \frac{4U}{D_0} \left(T - T_e\right) - Q_{\text{flash}}\right] - \frac{Q}{L}
\]
\[
\left(\varepsilon_e \rho_e C_p - \varepsilon_i \rho_i C_p\right) \frac{\partial T}{\partial \tilde{z}} = \left(\varepsilon_e \rho_e \tilde{u}_e + \varepsilon_i \rho_i \tilde{u}_i\right) \left(T_{z=0} - T_e\right)
\]
\[
\frac{\partial T}{\partial \tilde{z}} \bigg|_{\tilde{z}=0} = 0
\]

Solid Phase:
Mass balance of reactants A and B and product C in the solid phase:
\[
\varepsilon_r \frac{\partial FA}{\partial t} = \frac{D_{as}}{R_p^2} \left(\varepsilon_r \frac{\partial (FA)}{\partial r}\bigg|_{r=p}\right) - \rho_i Q_{as}(FA_i, FB_i, T_i) - \left(K_{gl}\right) \left(FA - FA_s(r_p - 1)\right) \frac{\partial FA}{\partial r} \bigg|_{r=p} = 0
\]
\[
\varepsilon_r \frac{\partial FB}{\partial t} = \frac{D_{as}}{R_p^2} \left(\varepsilon_r \frac{\partial (FB)}{\partial r}\bigg|_{r=p}\right) + \rho_i Q_{as}(FA_i, FB_i, T_i) - \left(K_{gl}\right) \left(FB - FB_s(r_p - 1)\right) \frac{\partial FB}{\partial r} \bigg|_{r=p} = 0
\]
\[
\varepsilon_r \frac{\partial FC}{\partial t} = \frac{D_{as}}{R_p^2} \left(\varepsilon_r \frac{\partial (FC)}{\partial r}\bigg|_{r=p}\right) + \rho_i Q_{as}(FA_i, FB_i, T_i) - \left(K_{gl}\right) \left(FC - FC_s(r_p - 1)\right) \frac{\partial FC}{\partial r} \bigg|_{r=p} = 0
\]

Energy balance in the solid phase:
\[
\rho_i \frac{\partial T}{\partial t} = \frac{\lambda}{R_p^2} \left(\varepsilon_r \frac{\partial (T)}{\partial r}\bigg|_{r=p}\right) + \varepsilon_r \left(T - \left(-\Delta H_R \right) R_p(FA_i, FB_i, T_i) \right) - \left(T - \left(-\Delta H_R \right) R_p(FA_i, FB_i, T_i) \right) \frac{\partial T}{\partial r} \bigg|_{r=p} = 0
\]

where agl and als are gas-liquid and liquid-solid interfacial areas respectively, m\(^{-1}\); FA, molar flow of the component A, kmol/h; FA*, solubility of the component A, kmol/h; C\(_p\), heat capacity, kj/kg.K; D\(_{gl}\), effective diffusivity, m\(^2\)/s; D\(_{as}\), reactor diameter, m; h\(_s\), heat transfer coefficient, kj/m\(^2\).s.K; K\(_{gl}\) and K\(_{ls}\), are mass transfer coefficients gas-liquid and liquid-solid respectively, m/s; L, reactor length, m; Q\(_{\text{flash}}\), heat of change phase of the reacting medium, kj/m\(^3\); Q\(_{l}\), volumetric flow of the liquid phase, m\(^3\)/s; r\(_p\), dimensionless particle radial position; R\(_p\), radius particle, m; \(R_{\text{W}}\), rate of hydrogenation of o-cresol, kmol/kg-cat.s; T, temperature, K; t, time, s; u, linear velocity, m/s; U, reactor to wall heat transfer coefficient, kj/m\(^2\).s.K; z, dimensionless reactor axial position; \(\Delta H_R\), heat of reaction, kj/kmol; \(\lambda\), thermal conductivity, kj/m.s.K; \(\rho\), density, kg/m\(^3\); \(\varepsilon\), porosity. Subscripts: g, gas phase; fo, feeding; l, liquid phase; i, initial value (reactor inlet); p, particle; r, coolant fluid; s, solid; Superscripts: s, catalyst surface.

3. Control

The developed model and solution procedure allowed to predict the main characteristics of the dynamic behaviour of reactor. It was used for the analysis of the performance of different control strategies (feedback, feedforward or both strategies) and algorithms.
The control action of the feedforward strategy was generated by a parametric model of the controlled and manipulated variables, which was developed by the application of the full factorial design method. The application this technique is a new and powerful procedure. In the case of digital algorithms, it was used the classic PI, the predictives QDMC and QGPC (model predictive controls with restrictions using optimisation routine, SQP), and the adaptive STQDMC and STQGPC (predictive algorithms coupled to the identification algorithm RLS), Clarke et al. (1987), Garcia and Morshedi (1986), Zafirou and Marchal (1991). Among the digital controllers considered, the classical algorithm was chosen due to its large use in industry and easy implementation, and its performance was be compared to more sophisticated control algorithms. The other controllers were chosen by their robustness, flexibility of tune due to the presence of several parameters and indications in literature. Thus, it was possible to understand the reactor dynamic behaviour in closed loop for different control strategies and algorithms. Therefore, the model allowed to analyse the performance of advanced controllers and different control strategies in thermal control of the reactor, that consists of problems of set point changes and disturbance in the operational parameters of the reactor. These controllers make use of advanced numerical techniques that able an effective control of the process, due mainly to the several available adjustment parameters, and to their adaptive characteristic that allows one to accompany the changes which happen in the process.

4. Results

The results obtained show that the model allowed the prediction of the main characteristics of the dynamic behaviour of the reactor in face of several changes in the operational parameters. This knowledge is fundamental for the elaboration of an efficient control strategy, as well as for reactor start-up and shut-down procedure. In order to illustrate the open-loop reactor behaviour, in Figure 1 a dynamic profile of the reactor temperature is represented along the axial length for a perturbation in the reactant fluid feed temperature, $T_{fo}$. In Figure 2 the dynamic behaviour of the reactor is observed in relation to perturbation in the temperature of the coolant fluid, $Tr$. From these two figures, it is observed that the reactor is very sensitive to changes in these operational parameters, and it has a typical asymptotic dynamic behaviour. More details can be seen in Vasco de Toledo et al. (2001). In Figure 3 it is showed the effect of the phase change of the reacting medium in the dynamic behaviour of the reactor after a step perturbation in $Tr$. This phenomenon gave rise to steep temperatures gradients within the reactor due to the heat involved in the phase change determined by the flash calculation. As a result, temperature increased when condensation occurs and it decreased as the reacting medium vaporizes. Thus the reactor showed an oscillatory dynamic behaviour.

The control objective was to maintain the reactor temperature at desired level (as an inference for concentration control) in spite of changes in set point and disturbances in the operational variables.
For the reactor control, the manipulated variables were the temperature of the refrigerant fluid, $T_{fr}$, and the reactant fluid feed temperature, $T_{fo}$. Depending upon the control problem considered, $T_{fo}$ was used as manipulated variable and $T_{fr}$ as disturbance variable and vice-versa, for other cases.

In Figure 4, a SISO regulatory control of the reactor using $T_{fo}$ as manipulated variable is shown. In this case, the control of the reactor is made considering the phase change of the reacting medium. The good performance of the controller was verified when the desired operation conditions of the reactor were re-established after a step perturbation in $T_{fr}$. The strategies was to avoid the system to achieve conditions where the phase change occurs, which would make difficult or unfeasible the operation of the reactor in a safe and efficient way as in open for closed loop.

In Figures 5 and 6 a SISO servo and a regulatory control are observed while $T_{fo}$ and $T_{fr}$, respectively, were chosen as manipulated variables. The best performance of the controllers QGPC and STQGPC can be observed in relation to other controllers in these figures. Also it has to be pointed out that the mixed control strategy (feedforward+feedback (STQGPC)) presented a better performance than others because this strategy combined velocity and precision to reach the desired setpoint.
5. Concluding remarks

The deterministic reactor model was able to predict the main dynamic characteristics of the slurry catalytic reactor as for open as closed loop. Considering the reactor control, results showed that adaptive (STQGPC) and predictive (QGPC) controllers had a better servo and regulatory performance than the other controllers. Analysing the performance of the considered strategies, it can be observed that the mixed (feedforward + feedback (STQGPC)) strategy achieved better results.

Thus, the great variety of control strategies and algorithms evaluated allowed to obtain an understanding of the reactor dynamic behaviour in closed loop. Moreover, it was possible to identify that predictive and adaptive controllers implemented though the mixed strategy were more suitable to operate the reactor in an efficient and safe way.

References


