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Evaluation of control algorithms for three-phase hydrogenation catalytic reactor

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Abstract

The present work deals with the proposition and evaluation of easy to implement control structures for a hydrogenation industrial size reactor. The used mathematical model formulation is a detailed deterministic and previously validated one, which was made focusing on the hydrogenation reaction of *o*-cresol to obtain the 2-methyl-cyclohexanol, in the presence of a Ni/SiO_2 catalyst. A simplified model, generated through factorial design statistical tool, is also used for stationary states predictions, providing very quick solution, suitable for on-line applications. Five different control structures, based on the feedback and feedforward classic structures and on combinations of them, are evaluated both concerning to the ability of the controller to maintain (regulatory control) or to change the controlled variable to the new set-point (servo control) in a reasonable action time. The study shows that, in the analyzed operation range, the combined structure is the best one to be used for this reactor, both for the servo and regulatory control problems. The calculation of control actions is significantly reduced by the use of simplified models. However, since an offset is present in the regulatory problem when the simplified model is used, this model is not suggested to be used in the regulatory problem.

Keywords: Hydrogenation; Dynamic modeling; Simulation; Optimization; Model-based controller

1. Introduction

Three-phase reactors can be found in several important applications, including hydrogenation and oxidation processes. Hydrogenation reactions are industrially widely applied, usually for commodities production, with large production scale. It consists of a highly non-linear process, multivariable, with exothermic reactions taking place. The high performance operation of large-scale industrial units is one of the most difficult and dangerous in chemical industries, especially when reactors are considered. A competitive advantage in such kind of systems is the operation at an optimal level of performance, even at very high throughputs. In the last decade, model predictive control (MPC) algorithms have been widely studied and applied in many chemical processes. Unfortunately, reports on control of three-phase catalytic reactors are relatively scarce when compared to other types of catalytic reactors [1]. High conversion and selectivity are usually required and more recently, after the 1990s, a full conversion of the limiting reactant (for instance, higher alcohols) are demanded for environmental sake. At this point it is interesting to draw attention to some typical aspects of such reactors. They are usually very large units (above 100 tonnes/h with length in the range of several dozen of meters) with a quite complex behavior due to phase change and strong interactions among heat and mass transfer, involving the gas, liquid and solid phases.

An overview of commercially available MPC technologies (LQG, linear quadratic Gaussian; IDCOM, model predictive heuristic; DMC, dynamic matrix control; QDMC controllers, constrained dynamic matrix control) is given by Qin and Badgwell [2]. This did not change in the last one to two years, if an overview of the industrial implementation is made [3]. The history of evolution of unconstrained to constrained algorithms and some applications of such algorithms are reported by Qin and Badgwell. A lot of work in literature that applies MPC in a variety of chemical processes can be found. The state-of-art of controller performance monitoring, including both feedforward and feedback control, has been reviewed by Hoo et al. [4]. These

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Nomenclature

a_{gl} and a_{ls} gas–liquid and liquid–solid interfacial areas, respectively (m^{-1})
A^* solubility of the component A (kmol/m^3)
A_0 pre-exponential factor (kmol/(kg catalyst s))
A_1 pre-exponential factor (m^3/mol)
A_2 pre-exponential factor (m^3/mol)
A_g A component concentration in the gas phase (kmol/m^3)
A_l A component concentration in the liquid phase (kmol/m^3)
A_{gfo} A component concentration in the gas phase in the reactor feed (kmol/m^3)
A_{lfo} A component concentration in the liquid phase in the reactor feed (kmol/m^3)
B_l B component concentration in the liquid phase (kmol/m^3)
B_{lfo} B component concentration in the liquid phase in the reactor feed (kmol/m^3)
C_A concentration of the component A (kmol/m^3)
C_B concentration of the component B (kmol/m^3)
Cp heat capacity (kJ/(kg K))
D_e effective diffusivity (m^2/s)
D_t reactor diameter (m)
E_0, E_1 and E_2 activation energies (J/mol)
F_i molar flow of ith component (kmol/s)
h convective heat transfer coefficient (kJ/(m^2 s K))
ΔH_r heat of reaction (kJ/(k mol))
k kinetic constant (kmol/(kg catalyst s))
K_{gl} and K_{ls} mass-transfer coefficients between the gas–liquid and liquid–solid phases, respectively (cm/s)
K_A and K_B constants of adsorption to components A and B, respectively (m^3/kmol)
L reactor length (m)
r_p dimensionless particle radial position
R universal gas constant (J/(mol K))
R_p particle radius (m)
R_W rate of hydrogenation of *o*-cresol (kmol/(kg catalyst s))
T temperature (K)
T_{fo} temperature in the feeding (K)
T_r temperature of the coolant fluid (K)
t time (s)
u linear velocity (m/s)
U global heat-transfer coefficient (kJ/(m^2 s K))
W catalyst concentration ((kg catalyst)/m^3)
z dimensionless reactor axial position

Greek letters
ε_g gas phase hold-up
ε_l liquid phase hold-up
ε_s solid porosity
λ thermal conductivity (kJ/(m s K))
ν stoichiometric coefficient
ρ density (kg/m^3)
τ tortuosity

Subscripts
A component A
B component B
g gas phase
fo feeding
l liquid phase
i initial value (reactor inlet)
p particle
s solid
r coolant fluid

Superscript
s catalyst surface

two control strategies were demonstrated both in a case study of an ideal continuous-stirred tank reactor (CSTR) and in an industrial polymer reactor. Additionally, it was shown that minimum variance control is usually undesirable because of issues such as model/plant mismatch. Thornhill et al. [5] also worked with a CSTR, but with a pilot scale one. They examined factors that influence the minimum variance performance measure of a SISO control loop and discussed the reasons why performance during set-point changes differs from the regulatory performance during operation at a constant set-point. The results demonstrated how regulatory performance is influenced by the nature of the disturbances, and that correlations of signals within a control loop can indicate whether the disturbances are random or deterministic. For controller performance purposes, the correlation coefficients between the manipulated variable (MV) and movements of MV (i.e. the increments in the manipulated variable) should be below 0.41 to ensure that MV movements are not too aggressive. Pannocchia [6] developed a novel robust model predictive control (RMPC) algorithm for the feedback temperature control of a CSTR. Offset removal in the controlled variables for set-points changes was achieved.

Although the possible advantages of advanced nonlinear model-based control methods over classical methods, Utz et al. [7] accredit the relatively low number of real industrial applications of such advanced control to the time-consuming optimization as well as the difficulty to model suitably nonlinear processes. In order to contribute with industrial applications, the authors presented a comparative evaluation of nonlinear model predictive control (NMPC) and a two-degree-of-freedom control-scheme with flatness-based feedforward control design and decentralized PI-controllers (FB-2DOF). The studies are carried with a set-point transition using a class of chemical CSTR that functions as a benchmark process for nonlinear control, to know, the Klatt–Engell reactor. Based on an analysis of simulation scenarios, the controllers are compared with respect to controller performance, robustness criteria, and implementation issues. NMPC exhibits performance advantages when

it comes to time-efficient set-point transitions when there is no plant-model mismatch, which is mostly due to the higher number of design parameters of this controller. In FB-2DOF control, the relatively few design parameters are a limiting factor, especially when it comes to tight performance requirements or when constraints have to be considered. NMPC allows direct incorporation of process models and constraints, but, it employs computationally expensive online optimization. Robustness properties of the two controllers are found to be quite comparable for the chosen and investigated transition time. NMPC is relatively simple to be implemented. For FB-2DOF, the software implementation itself is very simple. However, the control design can require high engineering efforts when parametrising the system by the flat output or guaranteeing adherence of the trajectories to constraints. Wang el al. [8] proposed the original open loop unstable plants to be first stabilized using a state feedback strategy followed by the local linearization within a regime classified by a gap metric measure. In order to make a smooth transition between regimes and to make the control free of offset, a Kalman filter is implemented. The advantages of the NMPC proposed approach were demonstrated in two case studies: robust control of a CSTR and of a *Zymomonas mobilis* fermentor.

Thornhill et al. [9] applied the principles of the minimum variance controller (MVC) for the controller performance evaluation, as introduced by Bezergianni and Georgakis [10] and extended by the same authors in 2003 [11], when the calculation of the relative variance index was suggested. Thornhill et al. [9] reported 12 single-input-single-output (SISO) MVC controllers in refinery plant with positive results. The calculation of the MVC assumes that the process can be represented adequately by a linear time-invariant (LTI) transfer function model with additive disturbances. The control loop performance assessment (CLPA) algorithm has several parameters (number of terms in the model, sampling interval, data ensemble length and the prediction horizon) that have to be adjusted correctly to give the best results. The aim of the paper was to recommend default numerical settings for these parameters that are suitable for most refinery control loops. Procedures were described for selecting these parameters which made it feasible to implement the algorithm on a refinery-wide scale.

A lot of work is also found in control applications in fluid catalytic cracking units. A methodology for the evaluation of strategies control and for the preliminary assessment of controllability of nonlinear systems was proposed by Maya-Yescas and Aguilar [12] for chemical reactors (FCC regenerators). The results obtained when evaluating the control strategies proposed in four different situations were coherent with industrial practice and operating experience. Alvarez-Ramirez et al. [13] presented the design of multivariable feedback control configurations for control of the riser output for FCC units. Numerical simulations were performed to show the effectiveness of several multivariable control configurations under disturbances and uncertainty parameters. Vieira et al. [14] implemented and evaluated the performance of a neural network-based model predictive control (MPC) applied to a FCC converter. The studies were carried out by dynamic simulation, where the simulator output signals were disturbed by random noise. To simulate usual procedures in the FCC industrial plant, a servo-regulatory control problem was implemented, as well as a regulatory one. According to the authors, the neural model predictive control is a powerful alternative tool to bring the process under control for both servo and regulatory problems. The neural network MPC response showed to be even smoother than that obtained from DMC algorithm. The predictions from the neural model and from the optimal control calculations could be obtained in a few seconds when the control horizon was equal to 1 or 2.

Alpbaz et al. [15] provide the comparison of DMC and PID controllers applied to a packed distillation column. The reflux ratio was chosen as the manipulated variable to control the overhead product temperature. The dynamic behavior of the column was observed at various step changes in the feed composition. Numerical results obtained from theoretical model are compared with experimental data. The performance of these control systems was tested using the integral square error (ISE) index. The simulations results showed that the performance of DMC controller for tracking a temperature set-point is better than that of conventional PID controller.

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. The outlet concentration is not easily measured on-line, so it can be inferred (estimated) from the available temperature measurements.

In the area of tubular reactors, Wu and Chen [16] implemented an analytic optimization algorithm connected to the measurement-based predictive control framework on an exothermic tubular reactor system (PFR). The exit reactor temperature is used as the controlled variable and the coolant flow rate and coolant temperature in the feed are treated as manipulated variables. They proposed two predictive control strategies denominated nondistributed model predictive control without sensing state information and with sensing state information at the prescribed location. The first scheme is a nondistributed output feedback controller. It manipulates a distributed reactor system using the steady-state optimization approach and an open-loop observer while state/input constraints and unknown inlet disturbances are being considered simultaneously. In this scheme structure, treated as a feedback-based implementation one, there are two models: one steady-state model, used in optimization calculations, and a so-called lumped difference model, which predicts the output with respect to the input constraints. The second scheme, a measurement-based predictive control algorithm controller design, can induce the stable and no-offset output regulation at the outlet of the reactor. Results show that the second scheme presented better tracking than the first one, but more-oscillating responses were detected.

Dechechi et al. [17] developed a novel adaptive control algorithm based on dynamic matrix control (DMC) philosophy with

adaptive features for application in an industrial hydrogenation catalytic multiphase reactor. This process has complex heat transfer mechanisms and fast dynamic behavior. The on-line internal model adaptation was carried out successfully using recursive least square method with an ARMA (autoregressive moving average)-based model. This algorithm showed a very good performance leading the reactor to be operated safely in large range of operation conditions. The results also showed the high efficiency of the developed multivariable controller when applied to this industrial process under normal operation. There were five controlled variables (the most important one was the temperature along the reactor length) and six manipulated variables (cooling flow rate of each jacketed tubes of the reactor).

Costa and Maciel Filho [18] evaluated the performance of a non-linear predictive controller applied to a three-phase catalytic reactor using a functional link network as internal model. The exit reactor temperature is controlled and the feed temperature is the manipulated variable. It was shown that the functional link structure represented accurately the dynamic and static behavior of the process, having, therefore, good performance as internal model of the control algorithm. The performance of the non-linear controller was tested for load disturbances and set-point changes with good results.

Rezende et al. [19] investigated the DMC performance on the feedback control of a multi-phase reactor, evaluating the impact of controller parameters. These authors proposed and analyzed a simple to use and easy to implement control structure (DMC), using SISO control approach in two separate studies, one for the control of the desired product concentration and the other for the control of temperature at the reactor exit.

In the present work, the control problem is formulated as the thermal control of the reactor, controlling concentration in an indirect way. The emphasis here is given to relative easy to implement control structures. For the establishment of the control strategy of the considered hydrogenation reactor, it is necessary, besides to define its operational objective and the manipulated(s) variable(s), to develop a model that predicts the main characteristics of the reactor dynamic behavior. Once these items are defined, suitable control structures may be proposed. In the implementation of the control loop, it is necessary to know the physical and operational limitations of the reactor manipulated and controlled variables. This appears to be obvious but it rarely is explicitly taken into account in control studies evaluation. Here the difficulties to implement, for instance, a control scheme which requires a temperature profile establishment along the reactor length, are considered in the control strategy propositions, because clearly there are physical limitations to be successfully implemented in industrial plants. The control strategies evaluated in this work are possible and relatively easy to implement with the existing resources in many typical industrial plants, especially those in where a regulatory control layer based on PID controller is available. Most of hydrogenation plants have this already on due to safety reasons. This information is essential to define a suitable and feasible control strategy, especially when on-line optimization is required. In such situations, the optimizer finds out the best operational values for the process variables and these values are used as controller(s) set-point(s).

2. Hydrogenation reactor: modeling and characteristics

The system used as study case is a multiphase reactor with industrial size, where the hydrogenation reaction of *o*-cresol takes place. This is representative of many industrially important processes, as phenol and vegetable oils hydrogenation reactors, where very exothermic reactions occur. The deterministic model here used takes into account the heterogeneous dynamic behavior of the system, and consists of mass and energy balance equations for the reactants in gas, liquid and at solid phase [20]. The kinetic law considers the hydrogenation reaction of *o*-cresol to obtain 2-methyl-cyclo-hexanol, in the presence of the catalyst Ni/SiO_2 [20]. The utilized scheme to represent the reactor is shown in Fig. 1.

The hydrogenation of *o*-cresol to 2-methyl-cyclohexanol on Ni/SiO_2 can be represented by Eq. (1):

$$3H_2(g) + C_6H_4OHCH_3(l) \rightarrow C_6H_{10}OHCH_3(l) \quad (1)$$

$$A(g) + \nu B(l) \rightarrow \nu C(l) \quad (2)$$

Eq. (2) is a generic representation of three-phase hydrogenation reactions. In this study case, A stands for hydrogen, B for *o*-cresol, C for 2-methyl-cyclohexanol and ν is the stoichiometric coefficient (equal to 1/3).

Eq. (3) has been obtained for the reaction rate of *o*-cresol hydrogenation reaction [21], where C_i is the concentration of the component i (kmol/m^3):

$$R_W = k\frac{K_A K_B C_A C_B}{(1 + K_A C_A)(1 + K_B C_B)} \quad (3)$$

The kinetic constants are functions of temperature, based on the Arrehnius' law:

$$k = A_0 \exp\left(-\frac{E_0}{RT}\right) \quad (4)$$

$$K_A = A_1 \exp\left(-\frac{E_1}{RT}\right) \quad (5)$$

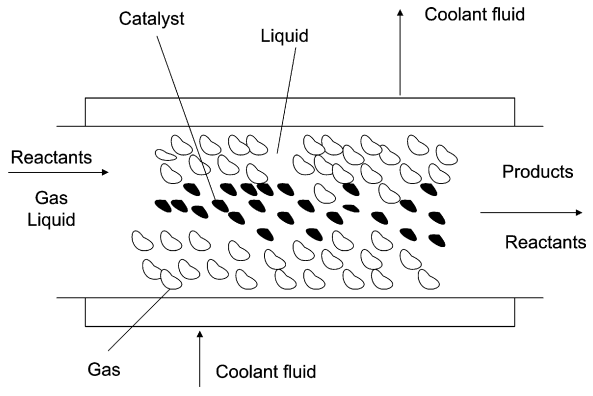

Fig. 1. Three-phase reactor.

$$K_B = A_2 \exp\left(-\frac{E_2}{RT}\right) \tag{6}$$

The kinetic parameters for Eqs. (4)–(6) are: $A_0 = 5.4 \times 10^5$ kmol/(kg catalyst s), $A_1 = 10.55\ m^3/mol$, $A_2 = 7.54 \times 10^{-3}\ m^3/mol$, $E_0 = 82220$ J/mol, $E_1 = 5003$ J/mol and $E_2 = 16325$ J/mol.

The following hypothesis were adopted for the model development [20,22]: (a) negligible pressure variations; (b) reaction of the type: $A(g) + \nu B(l) \rightarrow \nu C(l)$, occurring at the catalyst and with a kinetic that is dependent on the concentrations of A and B; (c) no phase change in the system. The operational parameters of the reactor, mass and energy balance coefficients, and physical properties have been considered constant. Some of these parameters were generated by empirical correlations [22].

The model equations, Eqs. (7)–(27), are differential ones and are built-up through the mass and energy balance for all substances in all system phases, i.e. in gas, liquid and adsorbed at the catalyst particles. The model equations are as follow:

1. Fluid phase:
   - Mass balance of reactant A in the gas phase:

$$\varepsilon_g \frac{\partial A_g}{\partial t} = \frac{D_{eg}}{L^2}\frac{\partial^2 A_g}{\partial z^2} - \frac{u_g}{L}\frac{\partial A_g}{\partial z} - (K_{gl})_A a_{gl}(A^* - A_l) \tag{7}$$

$$\left.\frac{D_{eg}}{L}\frac{\partial A_g}{\partial z}\right|_{z=0} = u_g(A_g - A_{gfo}) \tag{8}$$

$$\left.\frac{\partial A_g}{\partial z}\right|_{z=1} = 0 \tag{9}$$

   - Mass balance of reactant A in the liquid phase:

$$\varepsilon_l \frac{\partial A_l}{\partial t} = \frac{D_{el}}{L^2}\frac{\partial^2 A_l}{\partial z^2} - \frac{u_l}{L}\frac{\partial A_l}{\partial z} + (K_{gl})_A a_{gl}(A^* - A_l) - (K_{ls})_A a_{ls}(A_l - A_s^s) \tag{10}$$

$$\left.\frac{D_{el}}{L}\frac{\partial A_l}{\partial z}\right|_{z=0} = u_l(A_l - A_{lfo}) \tag{11}$$

$$\left.\frac{\partial A_l}{\partial z}\right|_{z=1} = 0 \tag{12}$$

   - Mass balance of reactant B in the liquid phase:

$$\varepsilon_l \frac{\partial B_l}{\partial t} = \frac{D_{el}}{L^2}\frac{\partial^2 B_l}{\partial z^2} - \frac{u_l}{L}\frac{\partial B_l}{\partial z} - (K_{ls})_B a_{ls}(B_l - B_s^s) \tag{13}$$

$$\left.\frac{D_{el}}{L}\frac{\partial B_l}{\partial z}\right|_{z=0} = u_l(B_l - B_{lfo}) \tag{14}$$

$$\left.\frac{\partial B_l}{\partial z}\right|_{z=1} = 0 \tag{15}$$

   - Energy balance in the fluid phase:

$$(\varepsilon_g \rho_g C_{pg} + \varepsilon_l \rho_l C_{pl})\frac{\partial T}{\partial t} = \frac{\varepsilon_g \lambda_g + \varepsilon_l \lambda_l}{L^2}\frac{\partial^2 T}{\partial z^2} - \frac{\varepsilon_g \rho_g C_{pg} u_g + \varepsilon_l \rho_l C_{pl} u_l}{L}\frac{\partial T}{\partial z} + h_s a_{ls}(T_s^s - T) - \frac{4U}{D_t}(T - T_r) \tag{16}$$

$$\left.\frac{\varepsilon_g \lambda_g + \varepsilon_l \lambda_l}{L}\frac{\partial T}{\partial z}\right|_{z=0} = (\varepsilon_g \rho_g C_{pg} u_g + \varepsilon_l \rho_l C_{pl} u_l)(T - T_{fo}) \tag{17}$$

$$\left.\frac{\partial T}{\partial z}\right|_{z=1} = 0 \tag{18}$$

2. Solid Phase:
   - Mass balance of reactant A at the solid phase:

$$\varepsilon_s \frac{\partial A_s}{\partial t} = \frac{D_{ea}}{R_p^2}\frac{1}{r_p^2}\frac{\partial}{\partial r_p}\left(r_p^2 \frac{\partial A_s}{\partial r_p}\right) - \rho_s R_W(A_s, B_s, T_s) \tag{19}$$

$$\left.\frac{D_{ea}}{R_p}\frac{\partial A_s}{\partial r_p}\right|_{r_p=1} = (K_{ls})_A(A_l - A_s^s) \tag{20}$$

$$\left.\frac{\partial A_s}{\partial r_p}\right|_{r_p=0} = 0 \tag{21}$$

   - Mass balance of reactant B at the solid phase:

$$\varepsilon_s \frac{\partial B_s}{\partial t} = \frac{D_{eb}}{R_p^2}\frac{1}{r_p^2}\frac{\partial}{\partial r_p}\left(r_p^2 \frac{\partial B_s}{\partial r_p}\right) - \nu\rho_s u_l R_W(A_s, B_s, T_s) \tag{22}$$

$$\left.\frac{D_{eb}}{R_p}\frac{\partial B_s}{\partial r_p}\right|_{r_p=1} = (K_{ls})_B(B_l - B_s^s) \tag{23}$$

$$\left.\frac{\partial B_s}{\partial r_p}\right|_{r_p=0} = 0 \tag{24}$$

   - Energy balance for the solid phase:

$$\rho_s C_{ps}\frac{\partial T_s}{\partial t} = \frac{\lambda_s}{R_p^2}\frac{1}{r_p^2}\frac{\partial}{\partial r_p}\left(r_p^2 \frac{\partial T_s}{\partial r_p}\right) + \rho_s(-\Delta H_R)R_W(A_s, B_s, T_s) \tag{25}$$

$$\left.\frac{\lambda_s}{R_p}\frac{\partial T_s}{\partial r_p}\right|_{r_p=1} = h_s(T - T_s^s) \tag{26}$$

$$\left.\frac{\partial T_s}{\partial r_p}\right|_{r_p=1} = 0 \tag{27}$$

The numeric solution of this model was obtained by using the method of lines in conjunction with orthogonal collocation,

which showed to be an effective procedure for the space discretization in conjunction with the DASSL algorithm for the integration over time [20].

The open-loop dynamic behavior of multiphase reactors was observed by Vasco de Toledo et al. [20]. The reactor is a typical non-linear distributed parameter system and has its behavior even more complex due to mass transfer resistance among phases. The dynamic behavior of the reactor was observed for disturbances in the reactant fluid feed temperature, T_{fo}, and in the feed temperature of the coolant fluid, T_r .It is observed that the reactor is very sensitive to changes in T_{fo} and in T_r. An asymptotic dynamic behavior is exhibited by the temperature of the reactor and an oscillatory behavior by the coolant fluid temperature, which is a typical characteristic of distributed parameter systems. The system is very sensitive to changes in T_r due to the fact that this model has a large complexity in the catalyst particle model, which generates great sensibility in relation to changes in the operational parameters. This sensibility of the dynamic behavior of the reactor in relation to changes in the coolant fluid is observed mainly in industrial situations.

In the present work, for the reactor control, the tested manipulated variables were the temperature of the coolant fluid, T_r, and the reactants feed temperature, T_{fo}. This is coherent with the operating strategies of many existing hydrogenation plants [3]. As already mentioned, the controlled variable is the reactor exit temperature.

3. Proposition of control structures

In this work, the performance analysis of different control strategies (feedback, feedforward and a combination of both strategies) is made. As mentioned, emphasis is given to relative easy to implement control structures.

In theory, feedback strategy is a more guaranteed one because the controller will always take an action if the controlled variable changes from the set-point value. However, due to process dynamics, this action can last longer until the process returns to the set-point.

The feedforward strategy, on the other hand, is able to take an action earlier in the process, since it measures the perturbation and not the controlled variable. The feedforward strategy, however, frequently suffers from several inherent difficulties: it requires the identification of the disturbance, and a very good model of the process. If a non-measured perturbation takes place, the feedforward controller is unable to take an action. These requirements lead to difficulties for many systems in the chemical industry, mainly due to the fact that the changes in the process parameters cannot be compensated, unless a reliable estimation procedure is incorporated into the model.

In this way, this work proposes to evaluate both isolated structures and a composition of them for the *o*-cresol hydrogenation reactor. The feedback structure makes use of the dynamic matrix control (DMC). The way the composed weighted action (feedback and feedforward) can be formulated is also analyzed, i.e., the best weight for both actions is studied.

In this work, possible model mismatch is not considered in the evaluation, but this is not a limitation, since a comparison among control structures is made with the same model prediction quality.

3.1. Quadratic dynamic matrix control (QDMC)

The feedback strategy is here implemented by the predictive QDMC (quadratic dynamic matrix control), a model predictive control (MPC) with constraints. The QDMC is based on the solution of an optimization problem, here based on the method of successive quadratic programming (SQP) [22–24].

Among the digital controllers, the QDMC was chosen based on its robustness and flexibility. Some tests with PID have shown that a considerable effort need to be done to tune the parameters and this is a drawback for its implementation. Melo et al. [1] compared the performance of two advanced controllers (QDMC and STQDMC: self tuning quadratic dynamic matrix control) for the two-layers optimization and feedback control of the *o*-cresol hydrogenation reactor and concluded that both controllers presented good performance. However, STQDMC requires longer computational calculation times because of its adaptive mechanism. In this way, the QDMC algorithm was preferable in the studied case and it was selected for the present study.

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 in a control horizon (smaller or equal to the prediction horizon)[25]. The predicted behavior is calculated using a process model, convolution one, obtained by the standard procedure for dynamic matrix-based controllers. 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 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, and when constraints are considered in the controlled and manipulated variables, it is necessary to use optimization algorithms, because, in this case, there is no analytical solution for the control problem. In this work, the controller performance criterion is expressed as

$$J = \min_{\Delta u}\phi = \frac{1}{2}\Delta u^T H \Delta u + c^T \Delta u, \quad \text{where } H = A^T W^T W A, \quad c^T = -E'^T W^T W A$$
$$\text{subjected to the following operational constraints : } \quad y_{min} \le y \le y_{max} \quad u_{min} \le u \le u_{max}, \Delta u_{min} \le \Delta u \le \Delta u_{max} \tag{28}$$

In these equations, W is the weighting factor matrix (composed of 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, y is the controlled variable (with y_{max} and y_{min} as minimal and maximal values respectively) and u is the manipulated variable (with u_{max} and u_{min} as maximum and minimum values, respectively).

A matrix is the dynamic matrix, generated by the classic method, with the system response to a step, using the convolution (or parametric) model, which linearly relates manipulated and controlled variables. W is the diagonal matrix with the suppression factors, which are control tuning parameters. Both matrices were generated by open-loop simulations [26].

It is important to emphasize that in order to generate the W and A matrixes, a dynamic model of the process is required. This model for the *o*-cresol hydrogenation reactor is composed by Eqs. (3)–(27).

It is worthwhile mentioning that this controller, associated with optimization algorithm, is able to consider more sophisticated control problems. Usually the benefits obtained in this approach justify the inherent increase of complexity (computational efforts for instance) when it is compared to analytical methods of solution, since a better performance may be obtained. DMC controllers are relatively easy to be developed and implemented and usually present good results for specific range of operation.

The use of DMC-based algorithms is also justified since many companies usually have the controller license available, although sometimes not in use due to the lack of deeper studies on the controller performance of large-scale systems, including monitoring difficulties and reliable control strategies evaluation.

3.2. Feedforward strategy

The objective of a feedforward controller is basically to generate anticipated corrective actions to compensate measured input disturbances. The idea here is to adopt a different approach for the control strategy regarding the action of manipulated variable and the dynamic response. The general concept of classic feedforward is used to formulate the control strategy. The feedforward action is therefore calculated aiming to minimize the quadratic error, which is a measure of the difference between the calculated exit reactor temperature and set-point for this process variable. This objective function for the feedforward controller may be written as in Eq. (29), in which either T_{fo} or T_r is selected as manipulated variable:

$$\begin{aligned} &\min_{T_{fo}}((T - T_{set\,point})^2) \\ &\text{s.t.:} \quad T_{fo\,min} \le T_{fo} \le T_{fo\,max} \\ &\text{or} \\ &\min_{T_r}(T - T_{set\,point})^2 \\ &\text{s.t.:} \quad T_{r\,min} \le T_r \le T_{r\,max} \end{aligned} \tag{29}$$

Both T_{fo} and T_r are analyzed as manipulated variable, which means that, when T_{fo} is used as manipulated variable, the first optimization problem of Eq. (29) is solved and when T_r is selected as manipulated variable, the second optimization problem is considered. At Section 5, the use of these two variables as practically feasible manipulated variables is discussed. It is worthwhile mentioning that, for practical implementation, changes in the coolant temperature are difficult to be used, since usually thermal fluids have as characteristic high heat capacity. This means that a large effort, in terms of heat exchanger designs and operation, has to be made to change the temperature of large amount of fluid in a reasonable time interval. This feature is taken into account in the analysis of results.

The Levenberg–Marquardt algorithm was used to implement this methodology: it finds out the manipulated variable value, knowing the desired set-point and the process disturbances.

Since this feedforward strategy does not require a dynamic model (no prediction horizon is part of the model), a simplified model, calculated for stationary states, can be used. It is expected that a simplified model is easier to be implemented and of fast computation calculation. In this way, two alternatives were used in this work for the reactor exit temperature (T) calculation to be used in Eq. (29): the detailed deterministic model (Eqs. (3)–(27)) and a simplified one, generated with use of a statistical tool (factorial design). The application of the factorial design to generate a simplified stationary working model for control purposes is a new procedure introduced in this work and that seems to be a powerful procedure, due to its simplicity and good predictions capabilities, as illustrated in Section 4.

3.3. Evaluated control strategies

This work evaluated five control strategies, to know:

(a) Single feedback (FB) – in fact, a DMC controller, as described in Section 3.1.
(b) Single feedforward, coupled with deterministic model (FF_deterministic).
(c) Single feedforward, coupled with simplified statistical model (FF_statistical).
(d) Combination of feedback and feedforward, with deterministic model for both ones (FF_deterministic + FB).
(e) Combination of feedback and feedforward, with simplified statistical model for feedforward action calculation (FF_statistical + FB).

The coupling of feedback and feedforward control (strategies d and e above) is made by a weighted action, as depicted in Eq. (30):

$$\begin{aligned} &u\_(\text{feedback} + \text{feedforward}) \\ &\quad = \beta \times u\_\text{feedforward} + (1 - \beta) \times u\_\text{feedback}, \quad 0 \le \beta \le 1 \end{aligned} \tag{30}$$

It is expected that the combined action (feedback combined with feedforward, Eq. (30)), presents part of the advantages of both isolated strategies, and decreases the drawbacks of isolated strategies. Section 5 demonstrates the advantages of such combined action.

Two situations exist in which a control system can be required. In the first one, called regulatory control problem, the disturbance, also called load, change in an unexpected way and

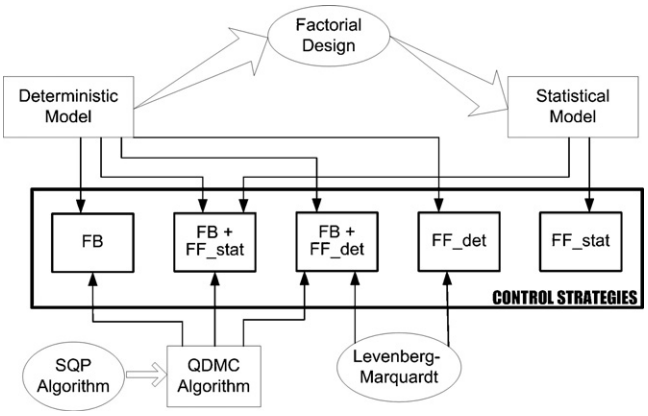

Fig. 2. Schematic diagram of the control strategies.

the control objective is to keep the exit at a desired value (set-point). This is a typical problem in many hydrogenation plants due to changes in the hydrogen supply with impact in the reactor pressure and behavior. In the second situation, a change in the value of the desired stationary state (set-point) is made and the objective of the control is to bring the controlled variable to the new stationary state. This situation is called a problem of servo control.

All five strategies (a–e) are evaluated both in a controller functioning as a servo and a regulatory one, which means that it was evaluated the ability of the controller to maintain (regulatory control) or to change the controlled variable to the new set-point (servo control) in a reasonable action time and to not cause sharp perturbations in the manipulated variable. In order to evaluate the performance of these strategies, perturbations both in operational variables (which means to cause perturbations inputs to the hydrogenation reactor) and in set-point values were introduced. Fig. 2 represents, in a schematic way, the five strategies studied in this work.

4. Development of the simplified statistical model

The development of a simplified model is here made with the aid of the factorial design statistical tool. This tool is useful in the identification of the most significant variables (called factors) in a response. The tool also allows the generation of a simplified model, valid in the studied range of variables. More details about factorial designs may be found in Box et al. [27].

The aim of this section is to generate a simplified model for the reactor exit temperature (T) as a function of the feed hydrogen concentrations in gas and liquid phases (A_{gfo} and A_{lfo}, respectively), *o*-cresol concentration (B_{lfo}), the reactants feed temperature (T_{fo}) and coolant temperature (T_r). In order to achieve this purpose, the deterministic model (Eqs. (7)–(27)) is used as virtual plant that gives the system steady-state responses to different input values to the reactor. The factorial design is used to guide both in which inputs should be supplied to the virtual plant as also in how to compute the input variables influence on the reactor exit temperature.

For the development of the simplified model, therefore, reactor exit temperature (T) is the response and the factors are the feed hydrogen concentrations in gas and liquid phases (A_{gfo} and A_{lfo}, respectively), *o*-cresol concentration (B_{lfo}), the reactants feed temperature (T_{fo}) and coolant temperature (T_r).

A factorial central composite design, composed by 43 computational simulations, was made in order to evaluate the influence of each independent variable on the stationary state reactor exit temperature and, with this information, to generate the required simplified model. These simulations included 32 (2^5) factorial points, 1 central point and 10 axial points (totalizing 43 runs). Table 1 presents the factor levels used in the factorial design study and Table 2 brings the central composite simulation results (the 43 runs) for the reactor exit temperature at the reached stationary state.

The software Statistica (Statsoft, v.7) was used to analyze the results and to generate a simplified linear model for temperature as a function of the five studied factors. The choice to generate a linear model was made because of the simple and useful model structure it derives. Table 3 brings the coefficients of this model with real (not coded) values for factors.

In this way, the reactor exit temperature at steady-state is given by Eq. (31) (units as in Nomenclature section):

$$T = -62.50498 + 355.6215(A_{gfo}) + 3.836649(A_{lfo}) + 143.4759(B_{lfo}) + 0.676911(T_{fo}) + 0.428379(T_r) \quad (31)$$

It is worthwhile to mention that Eq. (31) is valid only for the variables ranges described by Table 1. However, this does not mean a limitation of the procedure, since, if a larger range is necessary, another model can be easily generated.

The very good quality of the simplified model can be checked in Fig. 3, in which the reactor exit temperatures predicted by the deterministic model (Eqs. (3)–(27)) are compared to the values

Table 1
Variables and levels for central composite design

Factor	Level				
	−2.38[a]	−1	0	1	2.38[a]
A_{gfo} (kmol/m^3)	0.01140	0.01350	0.01500	0.01650	0.01860
A_{lfo} (kmol/m^3)	0.00838	0.00990	0.01100	0.01210	0.01360
B_{lfo} (kmol/m^3)	0.18300	0.21600	0.24000	0.26400	0.29700
T_{fo} (K)	476.00	513.00	540.00	567.00	604.00
T_r (K)	381.00	450.00	500.00	550.00	619.00

[a] $\pm 2.38 = \pm(2^5)^{1/4}$ (axial point).

Table 2
Central composite design for the steady-state reactor exit temperature as response

Simulation	A_{gfo} (kmol/m^3)	A_{lfo} (kmol/m^3)	B_{lfo} (kmol/m^3)	T_{fo} (K)	T_r (K)	T (K)
1	0.01350	0.00990	0.21600	513.00	450.00	512.60
2	0.01350	0.00990	0.21600	513.00	550.00	557.08
3	0.01350	0.00990	0.21600	567.00	450.00	550.83
4	0.01350	0.00990	0.21600	567.00	550.00	592.10
5	0.01350	0.00990	0.26400	513.00	450.00	518.72
6	0.01350	0.00990	0.26400	513.00	550.00	563.89
7	0.01350	0.00990	0.26400	567.00	450.00	557.61
8	0.01350	0.00990	0.26400	567.00	550.00	599.19
9	0.01350	0.01210	0.21600	513.00	450.00	512.62
10	0.01350	0.01210	0.21600	513.00	550.00	557.08
11	0.01350	0.01210	0.21600	567.00	450.00	550.84
12	0.01350	0.01210	0.21600	567.00	550.00	592.11
13	0.01350	0.01210	0.26400	513.00	450.00	518.74
14	0.01350	0.01210	0.26400	513.00	550.00	563.90
15	0.01350	0.01210	0.26400	567.00	450.00	557.62
16	0.01350	0.01210	0.26400	567.00	550.00	599.20
17	0.01650	0.00990	0.21600	513.00	450.00	514.18
18	0.01650	0.00990	0.21600	513.00	550.00	557.89
19	0.01650	0.00990	0.21600	567.00	450.00	551.69
20	0.01650	0.00990	0.21600	567.00	550.00	592.49
21	0.01650	0.00990	0.26400	513.00	450.00	520.83
22	0.01650	0.00990	0.26400	513.00	550.00	564.98
23	0.01650	0.00990	0.26400	567.00	450.00	558.78
24	0.01650	0.00990	0.26400	567.00	550.00	599.73
25	0.01650	0.01210	0.21600	513.00	450.00	514.19
26	0.01650	0.01210	0.21600	513.00	550.00	557.89
27	0.01650	0.01210	0.21600	567.00	450.00	551.70
28	0.01650	0.01210	0.21600	567.00	550.00	592.50
29	0.01650	0.01210	0.26400	513.00	450.00	520.84
30	0.01650	0.01210	0.26400	513.00	550.00	564.99
31	0.01650	0.01210	0.26400	567.00	450.00	558.78
32	0.01650	0.01210	0.26400	567.00	550.00	599.73
33	0.01140	0.01100	0.24000	540.00	500.00	556.20
34	0.01860	0.01100	0.24000	540.00	500.00	558.76
35	0.01500	0.00838	0.24000	540.00	500.00	557.91
36	0.01500	0.01360	0.24000	540.00	500.00	557.93
37	0.01500	0.01100	0.18300	540.00	500.00	549.66
38	0.01500	0.01100	0.29700	540.00	500.00	566.20
39	0.01500	0.01100	0.24000	476.00	500.00	512.41
40	0.01500	0.01100	0.24000	604.00	500.00	599.21
41	0.01500	0.01100	0.24000	540.00	381.00	504.08
42	0.01500	0.01100	0.24000	540.00	619.00	606.55
43	0.01500	0.01100	0.24000	540.00	500.00	557.92

calculated by the simplified one (Eq. (31)). As it can be observed, the statistical model may be used without any restriction in the range in which it was generated because the predicted values are practically the same as the ones obtained with the deterministic model.

The ANOVA (analysis of variance) is another way to check the quality of the model. Table 4 shows that the statistical model is very representative, since, the F-test, indicates a calculated value for F (1032.91) almost 500 times greater than the tabulated value for F at 95% confidence level ($F_{0.95;20;22} = 2.07$).

The use of the statistical simplified model in the feedforward strategy is made expressing the manipulated variable (feed reactant temperature, T_{fo}, or the coolant temperature, T_r) as a function of the reactor exit temperature (controlled variable, whose value is defined by the set-point) and of the other factors. In this way, when the simplified model is used in control strategies (i.e., in FF_statistical and FF_statistical + FB), the manipulated variable is calculated as in Eqs. (32) and (33).

Table 3
Regression coefficients for steady-state exit temperature

Factor	Regression coefficient
Mean (interception)	−62.50498
A_{gfo}	355.6215
A_{lfo}	3.836649
B_{lfo}	143.4759
T_{fo}	0.676911
T_r	0.428379

Table 4
Analysis of variance (ANOVA) ($R^2 = 0.99894$)

Source of variation	Sum of squares	Degrees of freedom	Mean square	F-Value
Regression	34846.33	20	1742.32	1032.91
Error	37.11	22	1.6868	
Total	34883.44	42		

T_{fo} as manipulated variable:

$$T_{fo} = \frac{T_{set\ point} - (-62.50498 + 355.6215(A_{gfo}) + 3.83664(A_{lfo}) + 143.4759(B_{lfo}) + 0.428379(T_r))}{0.676911} \quad (32)$$

T_r as manipulated variable:

$$T_r = \frac{T_{set\ point} - (-62.50498 + 355.6215(A_{gfo}) + 3.83664(A_{lfo}) + 143.4759(B_{lfo}) + 0.676911(T_{fo}))}{0.428379} \quad (33)$$

5. Results and discussions

5.1. Evaluation of weights for weighted (mixed) strategies

The first step for the implementation of the five proposed control strategies is the analysis of the β weight in Eq. (30) in order to decide the best value to be used in the mixed strategies. The mixed strategy with deterministic model being used in the feedforward action calculation (FF_deterministic + FB) was used for the evaluation of the best weight value. Five values for β were tested, to know, 0.1, 0.3, 0.5, 0.7 and 0.9. Since the boundary values (0 and 1) represent single feedback and single feedforward actions, respectively, these values were not included in this section.

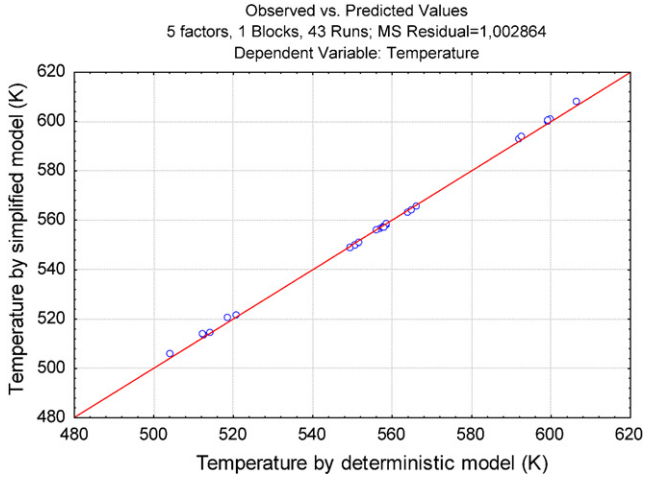

Fig. 3. Comparison between the prediction of steady-state exit reactor temperature for the deterministic and statistical (simplified) models.

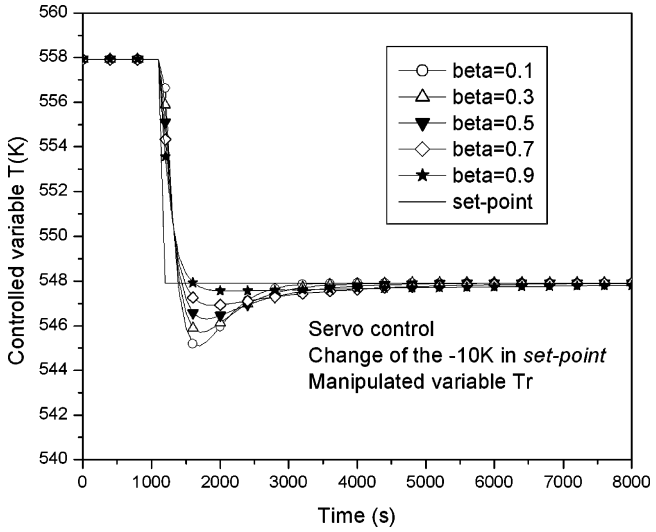

Fig. 4. Controlled variable profile for different β values for mixed strategy (FF_deterministic + FB) in a servo control.

The decision upon the best β value was made based both on minimization of errors and on controlled and manipulated variable profiles.

5.1.1. Servo control

Figs. 4 and 5 bring the reactor exit temperature (controlled variable) and coolant fluid temperature (manipulated variable) profiles for the mixed strategy for a servo control, in which a

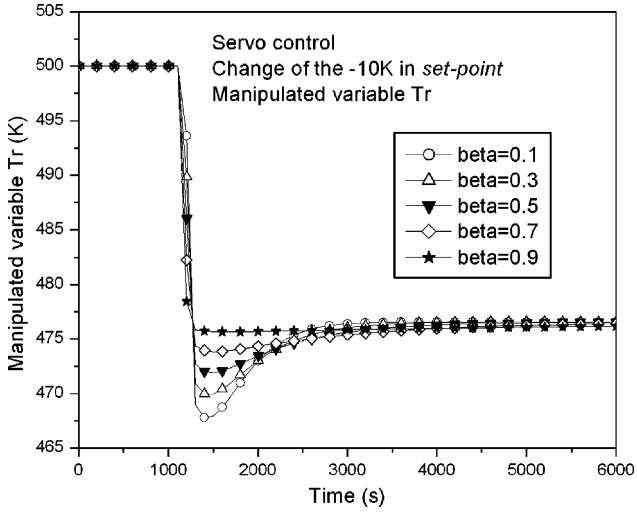

Fig. 5. T_r manipulated variable profile for different β values for mixed strategy (FF_deterministic + FB) in a servo control.

perturbation of −10 K in the original set-point was introduced at time = 1100 s.

From Fig. 4, both $\beta = 0.9$ and 0.7 (values that means a greater contribution of the feedforward action than the feedback one) give rise to acceptable controlled variable profiles: the controlled variable is brought to the new set-point value in reasonable action time and without having a significant undershoot. However, Fig. 5 demonstrates that none of β values causes a smooth behavior of the manipulated variable, i.e., high coolant temperature decrease rates are necessary to make the control of reactor exit temperature when the set-point is decreased by 10 K. This is an important point of concern, since very large coolant temperature decrease rates are very difficult to achieve, due to the high heat capacity of thermal fluids. This would require more sophisticated and certainly more expensive heat design strategies, maybe not fully justified for commodities. Analogous results are observed if reactants feed temperature (T_{fo}) is used as manipulated variables (behavior not shown for the sake of brevity). Nonetheless, although the decrease rates are also high for T_{fo}, it represents a situation easier to be implemented in practice.

In order to decide for the best weight for the weighted strategy for the servo control, the integral of absolute error (IAE) values for each β value are compared, both for T_{fo} and T_r as manipulated variable. Table 5 shows that the smaller error are obtained for $\beta = 0.7$. In this way, for the servo control, $\beta = 0.7$ is selected for the mixed strategy. The comparison among all five control strategies explained in Section 3.3 are made in Section 5.2 (with $\beta = 0.7$ for the mixed strategy for servo control).

5.1.2. Regulatory control

Figs. 6 and 7 bring the reactor exit temperature (controlled variable) and reactants feed temperature (manipulated variable) profiles for the mixed strategy for a regulatory control, in which step perturbations of 10% in A_{gfo}, A_{lfo}, B_{lfo} and T_r were introduced at time = 1100 s.

From Fig. 6, $\beta = 0.9$ (almost pure feedforward action) is, without doubt, the best weight value, since the controlled variable is little disturbed from the set-point and the steady-state is once more faster achieved. Table 6 (IAE table) really indicates that $\beta = 0.9$ produces a IAE value much smaller than the ones for other β values. However, once more the behavior of the manipulated variable is not smooth for any β (Fig. 7).

In Section 5.2, therefore, all five strategies are compared for the regulatory control with $\beta = 0.9$ for the mixed strategy.

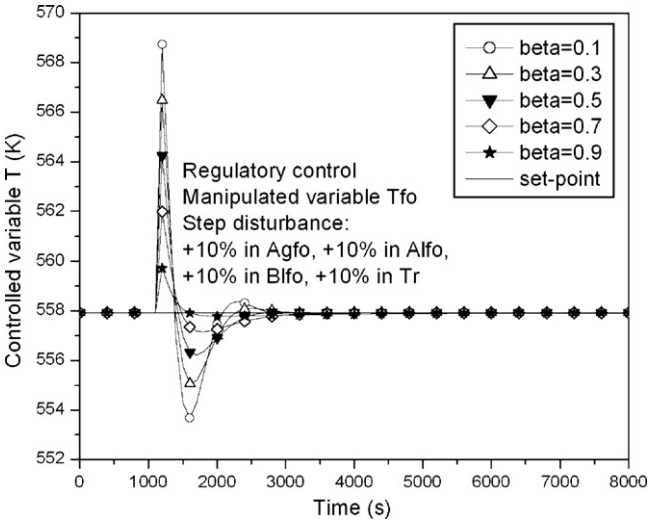

Fig. 6. Controlled variable profile for different β values for mixed strategy (FF_deterministic + FB) in a regulatory control.

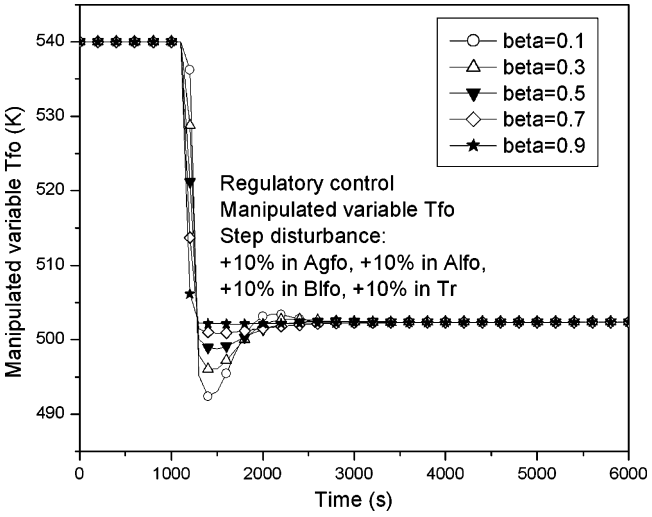

Fig. 7. T_{fo} manipulated variable profile for different β values for mixed strategy (FF_deterministic + FB) in a regulatory control.

5.2. Evaluation of the control strategies

The performance for the studied strategies (feedback, feedforward and mixed feedforward and feedback) is shown in Figs. 8–12. In order to decide for the best strategy in each case, the used criterion was to observe the changes both in the manipulated (T_{fo}, since implementation of the required changes in T_r

Table 5
IAE values for servo control for the various β values

Weight value (β)	IAE value	
	Manipulated T_{fo}	Manipulated T_r
0.1	4050.91	3917.09
0.3	3872.72	3759.41
0.5	3717.65	3629.90
0.7	3661.58	3584.78
0.9	3829.54	3745.88

Table 6
IAE values for regulatory control for the various β values

Weight value (β)	IAE value	
	Manipulated T_{fo}	Manipulated T_r
0.1	3400.84	4746.41
0.3	2641.52	3576.52
0.5	2010.38	2527.39
0.7	1368.31	1475.12
0.9	675.67	280.48

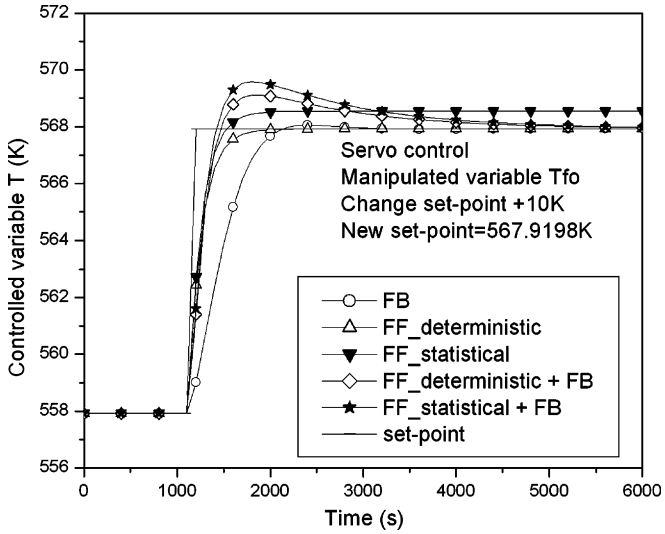

Fig. 8. Exit reactor temperature (controlled variable) profile for a 10 K change in set-point value—SISO servo control.

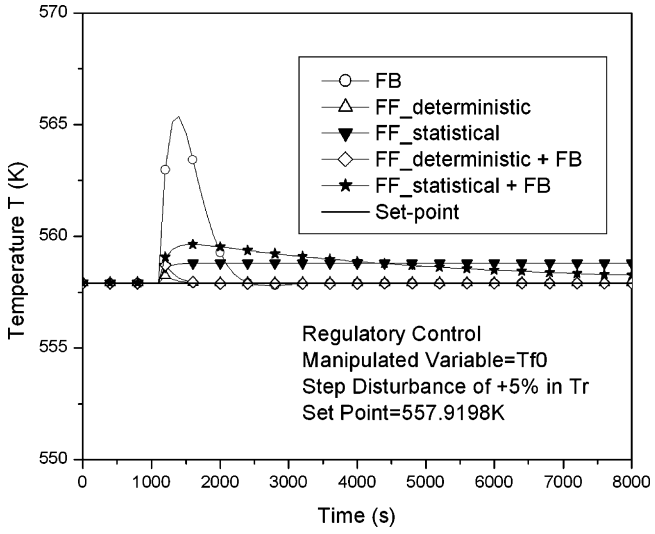

Fig. 10. Exit reactor temperature (controlled variable) profile for a 5% step disturbance in T_r—SISO regulatory control.

would be economically hardly justified) and in the controlled variables.

The SISO servo control performance for all five strategies are shown in Figs. 8 and 9 for both the controlled and manipulated variables profiles.

From Fig. 8, the pure feedforward strategy, calculated by the deterministic model (up triangle mark) seems to be the best one, but the challenge is to have a suitable way to implement drastic changes in the feed reactant temperature, as indicated in Fig. 9: large manipulated variable rates, such as around 0.8 K/s, are required. This rate in large-scale production units, such as the studied reactor, in which mass flow rates of 180 tonnes/h are common, may represent indeed a difficult job. In Fig. 9, the only strategy that presents smoother changes in the manipulated variable is the pure feedback strategy. However, the time demanded by this controller to bring the process to the new set-point (Fig. 8) is unacceptable, given the characteristic high mass flow rates.

It has to be born in mind that the successful implementation of the pure feedforward strategy demands an excessive care in maintaining all the others variables in a strict control. This points out that, for the implementation in large-scale systems, in which it is not expected to have the state variables fully measured, it is more convenient and even safer to adopt strategies with feedback information. In this sense, the weighted feedback and feedforward (calculated by statistical model) strategy (star mark) appears to be suitable for practical implementation because, although a larger overshoot occurs, the decaying time is quite acceptable when compared to the offset presented by the pure feedforward (calculated by statistic model) strategy (dark down triangle mark). Such offset may be due to the model limitations in predicting the process behavior, when compared to the detailed deterministic model. The feedback action in the sta-

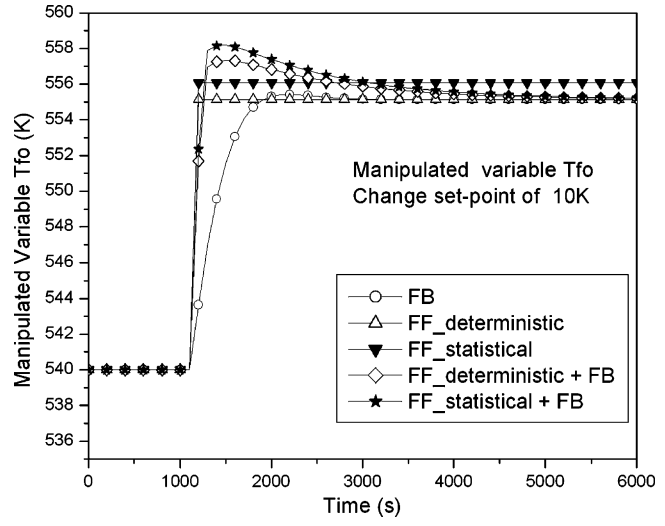

Fig. 9. Reactant feed temperature (manipulated variable) profile for a 10 K change in set-point value—SISO servo control.

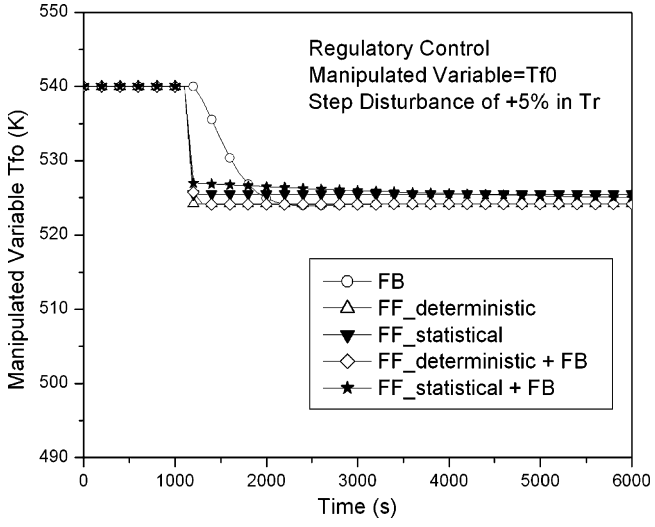

Fig. 11. Reactant feed temperature (manipulated variable) profile for a 5% step disturbance in T_r—SISO regulatory control.

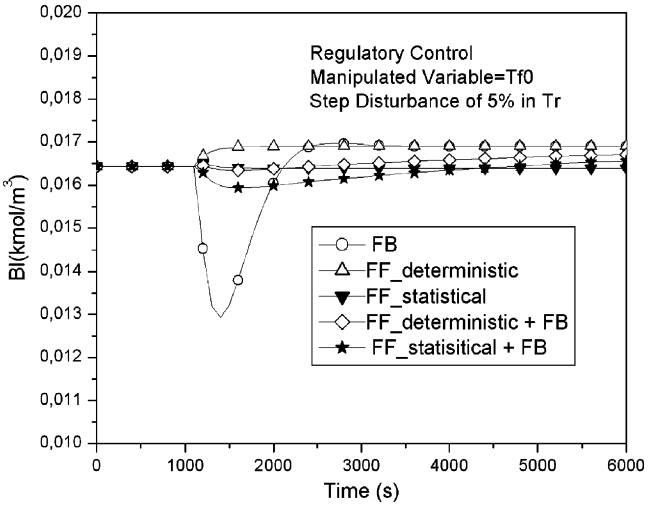

Fig. 12. Exit *o*-cresol concentration in the liquid phase profile for a 5% step disturbance in T_r—SISO regulatory control.

tistical weighted feedback and feedforward strategy is able to eliminate such offset.

An important point to be considered is the computational time. Extensive simulations indicate that, while the deterministic approach takes around 6 min (in an AMD 2.08GHz 768MB RAM computer) to complete the full calculations, the weighted approach, calculated with statistical model (star mark), takes only few seconds.

Bearing all this consideration in mind, the weighted approach, calculated with statistical model (star mark), appears to have the largest potential to be implemented in large-scale systems, which is not expected to be fully monitored.

For the SISO regulatory control (Figs. 10–12), the pure feedback strategy is of poor performance (large overshoot and large time demanded to bring the process back to the set-point, which may hamper the efficient and safe operation of the reactor). The strategies based on statistical model cause offset. In this way, the statistical model could not bring considerable benefits for the regulatory control problem.

In reality, almost all strategies present overshoot, but the deterministic pure feedforward (up triangle mark) and the deterministic weighted (rhombus mark) strategies seem to be very suitable, due to the small presented overshoots and to the small time required for bringing back the system to the set-point. However, due to the already mentioned need to adopt strategies with feedback information, the deterministic weighted (rhombus mark) strategy is selected as the best one for the SISO regulatory control considered in this work. Once more, due to the large manipulated variable rates, a specific design for the heat exchange for the feed reactant temperature (T_{fo}) is required.

In order to illustrate the impact of the suggested strategies in the *o*-cresol conversion, the profile of *o*-cresol concentration at liquid phase at the reactor exit is presented in Fig. 12. It is straightforward to check the good quality of the deterministic weighted strategy in fast bringing back this outlet concentration to the original one (original steady-state).

6. Conclusions

In this work, the use of easy to implement control structures is considered for the control of a three-phase catalytic reactor, where the hydrogenation of *o*-cresol occurs. The process is non-linear, has large-scale production rates and possesses a model of high dimension. Since online concentration measurements are difficult to obtain, the thermal control of the reactor is made. The feedback considered action is based on the dynamic matrix control and feedforward actions are calculated both with deterministic and simplified statistical models. Weighted actions (coupling feedback and feedforward actions) are analyzed and the best weights for both servo and regulatory controls show a greater contribution of feedforward action.

Coolant temperature does not seem to be an economically fully justified manipulated variable for this process control, due to the large decrease rates demanded for the exit reactor temperature control, when set-point and load disturbances are present. In this way, feed reactant temperature was selected as manipulated variable, with the remaining challenge to have a suitable way to accomplish drastic changes in the feed reactant temperature.

The results showed that it was possible to evaluate different control strategies for the solution of the multiphase reactor control. The mixed configuration (feedforward + feedback) appears to have a great potential since good control performance was obtained. In regard to simplified statistical model, it significantly reduced the calculation of control actions, but its use led to offset. However, the combination of feedback action with the statistical feedforward action in the servo control eliminated this offset.

In conclusion the mixed strategies, combining feedback and feedforward actions, showed to be the best ones for the regulatory and servo control problems. The deterministic model should be used both for feedback and feedforward actions calculations in the regulatory problem, but the statistical model should be conveniently used for feedforward calculations in the mixed strategies for the servo control problem.

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References

[1] D.N.C. Melo, M.M. Santos, E.C. Vasco de Toledo, S.D.M. Hasan, M.R. Wolf Maciel, R. Maciel Filho, Comput. Chem. Eng. 29 (2005) 2485–2493.
[2] S.J. Qin, T.A. Badgwell, Control. Eng. Pract. 11 (2003) 733–764.
[3] R. Maciel Filho. Personal Communication from Industries and Controller Suppliers (2007).
[4] K.A. Hoo, M.J. Piovoso, P.D. Schnelle, D.A. Rowan, Int. J. Adapt. Control Signal Process. 17 (2003) 635–662.
[5] N.F. Thornhill, B. Huang, S.L. Shah, Int. Adapt. J. Control Signal Process. 17 (2003) 709–727.
[6] G. Pannocchia, J. Process. Control 14 (2004) 927–937.
[7] T. Utz, V. Hagenmeyer, B. Mahn, J. Process. Control 17 (2007) 129–141.
[8] F.Y. Wang, P. Bahri, P.L. Lee, L.T. Cameron, Comput. Chem. Eng. 31 (2007) 410–418.

[9] N.F. Thornhill, M. Oettinger, P. Fedenczuk, J. Process. Control 9 (1999) 109–124.
[10] S. Bezergianni, C. Georgakis, World Congress of IFAC, Beijing, China, 1999.
[11] S. Bezergianni, C. Georgakis, Int. Adapt. J. Control Signal Process. 17 (2003) 527–552.
[12] R. Maya-Yescas, R. Aguilar, Chem. Eng. J. 92 (2003) 69–79.
[13] J. Alvarez-Ramirez, J. Valencia, H. Puebla, Chem. Eng. J. 99 (2004) 187–201.
[14] W.G. Vieira, V.M.L. Santos, F.R. Carvalho, J.A.F.R. Pereira, A.M.F. Fileti, Chem. Eng. Process. 44 (2005) 568–855.
[15] M. Alpbaz, S. Karacan, Y. Cabbar, H. Hapoğlu, Chem. Eng. J. 88 (2002) 163–174.
[16] W. Wu, C.W. Chen, Ind. Eng. Chem. Res. 46 (2007) 2064–2076.
[17] E.C. Dechechi, L.A.C. Meleiro, R. Maciel Filho, Proceedings of the 11th European Symposium on Computer Aided Process Engineering, vol. 9, Kolding, 2001.
[18] A.C. Costa, R. Maciel Filho, Can. J. Chem. Eng. 81 (2003) 1109–1118.
[19] M.C.A.F. Rezende, A.C. Costa, R. Maciel Filho, Int. J. Chem. React. Eng. 2 (2004) A21.
[20] E.C. Vasco de Toledo, P.L. Santana, M.R. Wolf Maciel, R. Maciel Filho, Chem. Eng. Sci. 56 (2001) 6055–6061.
[21] H. Hichri, A. Armand, J. Andrieu, Kinetics and slurry-type reactor modeling during catalytic hydrogenation of *o*-cresol on Ni/SiO_2, Chem. Eng. Process. 30 (1991) 133–140.
[22] E.C. Vasco de Toledo, R. Maciel Filho, Proceedings of 14th European Symposium on Computer-Aided Process Engineering, vol. 18, Lisbon, 2004.
[23] C.E. Garcia, A.M. Morshedi, Chem. Eng. Commun. 46 (1986) 73–87.
[24] E. Zafiriou, A. Marchal, AIChE J. 37 (10) (1991) 1550–1560.
[25] D.Q. Mayne, J.B. Rawlings, C.V. Rao, P.O.M. Scokaert, Automatica 36 (2000) 789–814.
[26] W.L. Luyben, Process Modeling, Simulation and Control for Chemical Engineers, 2nd edition, McGraw-Hill, New York, NY, 1990.
[27] G.E.P. Box, W.G. Hunter, J.S. Hunter, Statistics for Experimenters—An Introduction to Design, Data Analysis and Model Building, John Wiley, New York, 1978.