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Special Theme Research Article

Nonlinear parametric predictive control. Application to a continuous stirred tank reactor

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ABSTRACT: This paper presents a nonlinear model-based controller based on the ideas of parametric predictive control applied to a continuous stirred tank reactor (CSTR) process unit. Controller design aims at avoiding the complexity of implementation and long computational times associated with conventional NMPC while maintaining the main advantage of taking into account process nonlinearities that are relevant for control. The design of the parametric predictive controller is based on a rather simplified process model having parameters that are instrumental in determining the required changes to the manipulated variables for error reduction. The nonlinear controller is easy to tune and can operate successfully over a wide range of operating conditions. The use of an estimator of unmeasured disturbances and process-model mismatch further enhances the behavior of the controller. © 2009 Curtin University of Technology and John Wiley & Sons, Ltd.

KEYWORDS: nonlinear model predictive control; parametric predictive control; reactor control; load estimation

INTRODUCTION

After its successful introduction in the petrochemical industry in the 1980s, model-based predictive controllers (MPCs) have gradually gained acceptance in many other fields. The main reason for this success is the ability of MPCs to optimally control multivariable systems with constraints. In each sampling period the MPC algorithm calculates a sequence of adjustments of the manipulated variables that optimize the future behavior of the plant. Then, the first value of the optimal sequence is sent to the plant and the whole calculation is repeated in every subsequent sampling period (refer to Refs [1–4] among various sources on MPC fundamentals and history).

Even though most of the continuous processes are inherently nonlinear, most of the predictive control applications carried out until the present are based on linear dynamic models based mainly on the step or impulse response of the process. The following are some of the main reasons for using these models.

- Linear empirical models can be easily obtained directly from plant data.
- Most of the MPCs have been applied to the petroleum refine industry in which linear models are accurate enough for many purposes.
- Using a linear model and a quadratic objective function, the control algorithm is reduced to a quadratic programming (QP) problem with constraints. There are fast and reliable solutions for this problem using software existing in the market and this is important because the solution should converge to the optimal point in a short time in order to be used in real-time systems.

As the range of application expands, there exist many cases where the nonlinear characteristics of the processes must be taken into account, especially when the process has to work over a range of operational points or when a high performance is required. In such cases a nonlinear model predictive controller (NMPC) should be used. An NMPC is simply a kind of MPC with a nonlinear internal model. There are several alternative types of models that can be used in NMPC, including empirical models (Volterra series, NARX, neural network, etc.), first principles models and a hybrid thereof (grey-box models). First principles models are preferred as they can be reliable outside the range of the experiments performed for identification and tuning is very robust, which is not guaranteed with

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the black-box modeling approach.[4] The advantages of NMPC are well known, as well as its main difficulties in industrial implementation: complex and specialized software demanding long computational times. The introduction of a nonlinear model leads, in the general case, to the lost of convexity of the cost function to be minimized and to a considerable increase in the calculations. This means that it is more difficult to find a solution in a short time and once found, cannot always be guaranteed to be globally optimum (the solution found can be a local minimum).

In recent years, there have been important contributions aimed at solving these problems. For instance in Ref. [5] the use of multiple shooting optimization algorithms is shown to give very good results in the control of a pilot plant distillation column. Also in Ref. [6] the NMPC is solved at every sampling time as a series of linearized models by QP saving computation time. Other approaches[7] consider the use of piece-wise affine models and multiparametric optimization methods in order to pre-compute off-line a control law that can be applied then on-line as a function of the current values of the state and the control signal. In Ref. [8] there is an assessment of different strategies for the application of sequential quadratic programming (SQP) optimization algorithms to NMPC, using an isothermal continuous stirred tank reactor (CSTR) as a case study.

NMPC methods involve, either on-line or off-line, a lot of computation and are not always suitable for 'low cost' applications. In this paper we explore an alternative approach, based on the ideas of parametric predictive control (PPC) proposed by J. Richalet,[9] oriented to facilitate its implementation on standard industrial controllers, which could be a distributed control system (DCS) or a programmable logic controller (PLC). A PPC maintains an internal model of the MPC controller based on first principles, thus capturing the main nonlinearities of the process while providing a rather simple solution able to be implemented in commercial DCS or PLC software modules. For this purpose, instead of relying on a nonlinear programming (NLP) optimization of a cost function for computing the manipulated variables, it uses the 'coincidence point' approach. The proposed design method is intended for processes involving a reduced number of variables in which either a significant nonlinearity is present or the controller has to operate over a wide range of operating conditions, as it happens with slave controllers in cascades.

The main idea is to use a PPC as a low-level nonlinear controller when no explicit constraints are required, replacing a proportional-integral-derivative (PID) controller with some advantages; the PID can get detuned when some or all of the conditions mentioned above are present. Another main advantage of this approach is that the closed loop behavior of the portion of the process controlled by the PPC is seen as if it were linear from the upper control layer point of view. So, it is perfectly feasible to use a cascade with a linear constrained model predictive controller (LMPC) as the master closed loop plant controller, as usually occurs in current MPC industrial applications, operating in cascade over a PPC in a lower layer. The upper LMPC will calculate the set point of the PPC taking into account the cost function (for economic optimal control) and all the constraints, while the PPC will cope with the main nonlinearities and parameter changes of the process.

In this paper, the PPC controller has been developed for the particular case of an exothermic continuous stirred tank reactor, a common process unit that can exhibit a strong nonlinear behavior. The topic of temperature control using a predictive functional control (PFC) was addressed in previous works, dealing with batch reactors with no significant reaction heat,[9] heat exchangers,[10], or CSTR with jacket system.[11]. In Ref. [12] there is another approach to the control of a CSTR using an observer-based NMPC, which uses an augmented state fuzzy Kalman filter (ASFKF) as a state estimator.

The proposed PPC is extended to any kind of reactor considering explicitly the heat reaction which is estimated on-line in the same context. A comparison with a PID and a pure NMPC approach is presented to help evaluate a PPC in terms of performance and computational times.

The paper is organized as follows: after the introduction, the section on Operating Principles gives a brief review of the basic ideas of parametric predictive control. Then, in the section on A Case Study: CSTR, the case study of the CSTR is presented as well as the derivation of the nonlinear controller. The results of some simulated experiments are shown in the section on Results in addition to several alternatives for removing steady-state errors, including disturbance estimation. The paper ends with some brief conclusions.

OPERATING PRINCIPLES

The parametric predictive controller (PPC)[9,13] shares many characteristics of the current MPC:

- The use of an internal model to predict the future behavior of the process
- The use of a reference trajectory
- A structure of the control law
- On-line calculation of a control sequence based on a target aim
- A receding horizon strategy

Figure 1 shows its operating principle. The aim of the controller is finding a control sequence $u(t)$ such that, at time $t + N$ in the future, the current error $(w - y_p)$ is

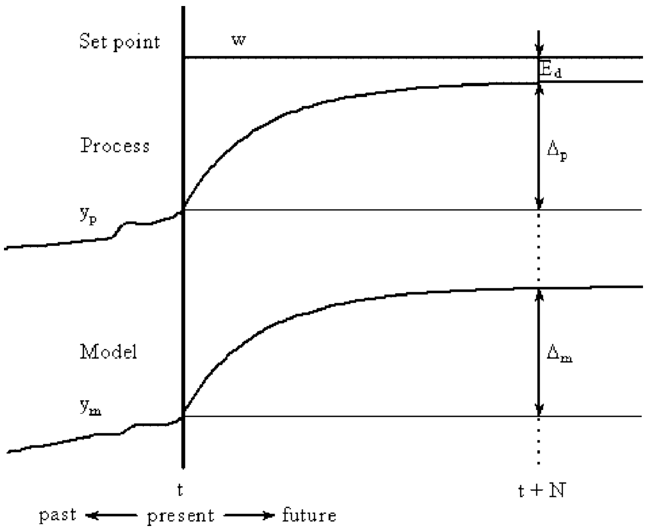

Figure 1. Operating principle of the PPC.

reduced to a certain value E_d, according to the following expression:

$$E_d = \lambda^N \left(w - y_{\mathrm{p}}(t)\right) \quad (1)$$

with $0 \le \lambda < 1$.

In this equation λ^N is the reduction factor and λ is a tuning parameter that establishes the magnitude of the reduction and, thus, the speed of response of the output. Values near 1 provide smoother responses, while values of λ near 0 give faster responses, but with a bigger control effort. The value of N also can be used as a tuning parameter and its value must be chosen according to the desired closed loop response of the system. Normally, its value will fix the closed loop steady state time T_{ss}. This is similar to setting up a first order internal reference trajectory.

Notice that the change in the process output required to reduce the error to E_d at time $t + N$, Δ_{p}, can be derived from Fig. 1, obtaining:

$$\Delta_{\mathrm{p}} = \left(1 - \lambda^N\right)\left(w - y_{\mathrm{p}}(t)\right) \quad (2)$$

The controller makes use of a reduced order independent model, based on first principles, in order to compute the control signal u that would give a change Δ_{m} in its output equal to the required change in the process Δ_{p}. Then, in order to achieve the control objective, the following equality is enforced:

$$\Delta_{\mathrm{p}} = \Delta_{\mathrm{m}}(u) \quad (3)$$

Equations (1)–(3) above are the basis of the PPC design method. In particular, notice that Δ_{p} can be obtained from process measurements, so that Eqn (3) can be used to compute the control action u. An explicit expression of $\Delta_{\mathrm{m}}(u)$ can be obtained under certain conditions:

- When dealing with a linear model
- When the nonlinear model can be reformulated as an expression of a linear system with coefficients that are function of the manipulated variable. For instance, for a first order linear system:

$$\varphi(u)\frac{dx}{dt} + \varepsilon(u)\, x = \Psi(u) \quad (4)$$

Equation (4) is basically nonlinear, but may become linear when $u(t)$ is constant. In this case, if the control horizon is chosen as $N_u = 1$, for the prediction horizon $u(t)$ will be constant so that Eqn (4) reduces to a linear differential equation with constant coefficients, so that an analytical expression can be found for $\Delta_{\mathrm{m}}(u)$.

In Eqn (3) the only unknown is then the control action u that can be computed every sampling time solving this nonlinear algebraic equation. Extensions to other values of N_u and higher order equations can be made at the expense of solving additional equations similar to Eqn 3 for every value of N_u. Obviously, the PPC depends on the model (linear or nonlinear) and has to be obtained for each particular process.

A CASE STUDY: CSTR

In order to solve Eqn (3) at each time step, a process model is needed. As mentioned in the Introduction, a CSTR has been considered as a case study. In the reactor, a continuous flow of reactant A is converted into product B by means of an exothermic reaction, where H stands for the enthalpy of reaction. In order to remove the reaction heat and help maintain the operating temperature T_1 in the reactor, a jacket filled with a refrigerant is used.

A low-level PPC multiple-input single-output (MISO) type controller was developed for the CSTR, as shown in Fig. 2, where the controlled variable is the temperature T_1 and the manipulated variable is the refrigerant

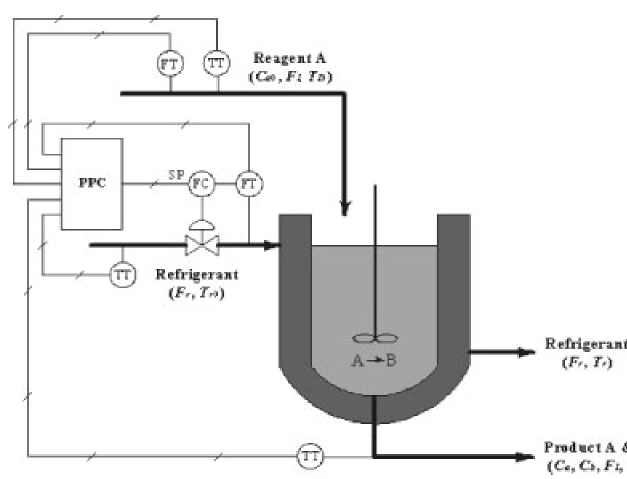

Figure 2. Scheme of the PPC MISO controller for the CSTR.

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flow rate F_r. As measured disturbances we can mention the reagent flow rate F_l, the reagent temperature T_{l0} and the refrigerant liquid input temperature T_{r0}. As an unmeasured disturbance we have the input concentration of the reagent A, C_{a0}.

Model of the plant

A mathematical model for the CSTR can be obtained from mass and energy balances in the reactor and the jacket assuming a homogeneous distribution of temperatures and concentrations in the vessel. The model can be expressed as a set of four differential equations for the two temperatures of the reactor T_l and jacket T_r and the two concentrations C_a and C_b of products A and B respectively. The liquid goes out of the reactor by overflow, so that the volume V_l can be considered as constant. An additional equation, the Arrhenius law, gives the speed of reaction k as a function of the temperature. The differential and algebraic equations of the model are:

$$\frac{dT_l}{dt} = \frac{F_l \rho_l Cp_l (T_{l0} - T_l) - U\ S(T_l - T_r) + V_l k C_a H}{V_l \rho_l Cp_l} \tag{5}$$

$$\frac{dT_r}{dt} = \frac{F_r \rho_r Cp_r (T_{r0} - T_r) + U\ S(T_l - T_r)}{V_r \rho_r Cp_r} \tag{6}$$

$$\frac{dC_b}{dt} = \frac{V_l k C_a - F_l C_b}{V_l} \tag{7}$$

$$\frac{dC_a}{dt} = \frac{F_l (C_{a0} - C_a) - V_l k C_a}{V_l} \tag{8}$$

with

$$k = A e^{-E_a/R(T_l + 273)} \tag{9}$$

Development of the nonlinear PPC controller

In order to develop a useful model for the controller, some simplifications can be performed. Assuming that the dynamics of the jacket is faster than the one in the reactor, Eqn (6) can be equated to zero; T_r can be obtained from this equation and replaced in Eqn (5). Note that this assumption is grounded on the fact that the tank hold-up is much bigger than the jacket volume. Thus, a simplified model of the reactor temperature is:

$$\frac{dT_{l,m}}{dt} = k_1(F_r) T_{l,m} + k_2(F_r) \tag{10}$$

$$k_1(F_r) = \frac{-1}{V_l \rho_l Cp_l} \left(F_l \rho_l Cp_l + \frac{F_r \rho_r Cp_r U\ S}{F_r \rho_r Cp_r + U\ S} \right) \tag{11}$$

$$k_2(F_r) = \left(F_l \rho_l Cp_l T_{l0} + \frac{F_r \rho_r Cp_r T_{r0} U\ S}{F_r \rho_r Cp_r + U\ S} + \Delta E \right) \times / V_l \rho_l Cp_l \tag{12}$$

The term $\Delta E = V_l k C_a H$ represents the heat generated by the exothermic reaction by unit time and the index m in $T_{l,m}$ is used to stress the fact that it refers to the model temperature.

Equation (10), which can be used to compute predictions of the reactor temperature as a function of the future values of the manipulated variable F_r, is nonlinear, so that it may be difficult to integrate. Nevertheless, it has the structure of a linear Eqn (4) with time varying parameters $k_1(F_r)$ and $k_2(F_r)$. Note that the manipulated variable F_r is included in both parameters $k_1(F_r)$ and $k_2(F_r)$. To carry out an analytical integration of the model, a couple of assumptions are made. First, the control horizon of the controller is kept equal to 1 ($N_u = 1$) meaning that in order to make predictions F_r is considered constant in the future. Secondly, notice that Eqns (11), (12) depend on a set of parameters, disturbances, and ΔE. In MPC, future values of the disturbances are considered usually constant and equal to their current values, but updated every sampling time. Perhaps one of the few drawbacks of the PPC approach is that it requires an analytical solution of the differential Eqn (10). Equation (12) includes the term ΔE, which is a function of T_l through the Arrhenius law. Unfortunately, no analytical solution of Eqn (10) can be found if we consider this term as it is. To deal with this problem ΔE is also considered as a disturbance and it is treated in the same way, that is, assumed constant but its value is recalculated on each sampling time. Accordingly, $k_1(F_r)$ and $k_2(F_r)$ are constant parameters and the model expressed by Eqn (10), at time instant t, can be considered as linear and its future evolution can be computed as the solution to Eqn (10). An analytical solution can be found integrating it between t and $t + NT_s$, T_s being the sampling period:

$$T_{l,m}(t + N\,T_s) = e^{k_1(F_r) N\ T_s} T_{l,m}(t) + \frac{k_2(F_r)}{k_1(F_r)} \left(e^{k_1(F_r) N\,T_s} - 1 \right) \tag{13}$$

From this equation, the change in the reactor temperature $\Delta T_{l,m}$ in the time interval NT_s corresponding to a value of the manipulated variable can be derived:

$$\Delta T_{l,m} = \left(e^{k_1(F_r) N\,T_s} - 1 \right) \left(\frac{k_2(F_r)}{k_1(F_r)} + T_{l,m}(t) \right) \tag{14}$$

In order to realign the output of the model with the process output at each sampling period, the following replacement is carried out in Eqn (14), $T_{l,m}(t) = T_{l,p}(t)$, being $T_{l,p}(t)$ the present value of the temperature in the process. The final controller equation is obtained from Eqns (2), (3) and (14).

$$\left(1 - \lambda^N\right)\left(w - T_{l,p}(t)\right) = \left(e^{k_1(F_r) N\,T_s} - 1 \right) \left(\frac{k_2(F_r)}{k_1(F_r)} + T_{l,p}(t) \right) \tag{15}$$

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This is an implicit equation in F_r, which must be solved every sampling period by a numerical method in order to find the value of F_r, which will reduce by a factor λ^N the temperature error in N sampling times. Notice that the solution of Eqn (15) requires the knowledge of the model parameters as well as the flow of product A and input temperatures of the refrigerant and the reagent A, which can be measured easily. The parameters of the model (ρ_l, Cp_l, ρ_r, Cp_r) can be determined off-line or obtained from the literature. The product US can be also determined with the appropriate experiments. The more problematic value is ΔE; so, a procedure for the estimation of ΔE should be provided.

Notice also that Eqn (15) is valid regardless of the particular chemical reaction $A \to B$. Different types of reaction kinetics will lead to the same controller but with a different ΔE. Further, the assumption of a control horizon $N_u = 1$ is key for analytical integration but longer control horizons can be used if an explicit integration formula at different future time intervals is applied. The only penalty is a more complex controller. For instance, for $N_u = 2$, the equivalent expression to Eqn (14) is:

$$\begin{aligned}\Delta T_{l,m}(t + N\ T_s) &= \left(e^{k_1(F_{r2})(N-1)T_s}\right.\\ &\quad \left. e^{k_1(F_{r1})T_s} - 1\right)\ T_{l,m}(t)\\ &\quad + \frac{e^{k_1(F_{r2})(N-1)T_s}\ k_2(F_{r1})}{k_1(F_{r1})}\left(e^{k_1(F_{r1})T_s} - 1\right) +\\ &\quad + \frac{k_2(F_{r2})}{k_1(F_{r2})}\left(e^{k_1(F_{r2})(N-1)T_s} - 1\right) \qquad (16)\end{aligned}$$

It is noteworthy that now there are two unknowns: $F_r(t)$ and $F_r(t + 1)$ so that, in order to compute both, two coincidence points have to be provided instead of one, which lead to a set of two implicit algebraic equations similar to Eqn (15).

Thus, the PPC controller solves every sampling time an algebraic equation like Eqn (15) or (16) in order to compute the current manipulated variable, instead of solving a dynamic optimization problem. The main features of the PPC controller are the following:

- Nonlinear control based on first principles.
- Based on a reduced order model of the process.
- It combines the simplicity of a linear controller with the essential nonlinearities of the process.
- It can be used as a low-level nonlinear controller, with no optimization or restrictions treatment.
- In the case of an MISO controller with measured disturbances, a feed-forward compensation is introduced naturally by the model.
- The computation required for the PPC controller, solving a nonlinear algebraic equation, is easy to implement using any regular programming language, either on a commercial DCS or PLC.

The PPC algorithm, as presented up to this point, does not incorporate the typical mechanisms that avoid steady-state errors in MPC. So, no explicit integral action is included in the controller, as happens on regular MPCs. The absence of integral action produces steady-state errors when there is model mismatch or unmeasured disturbances. Thus, integral action must be added in order to cope with model inaccuracies or unknown disturbances. The steady-state errors can be eliminated in different ways: adding an explicit integral term to the PPC controller, using a PI controller in a cascade upstream the PPC controller or including in the PPC algorithm an adequate estimator. In this case, an estimator of ΔE (the exothermicity term) has been derived from the model, as stated below.

Estimation of ΔE

An estimator of ΔE can be developed using the reduced model of the CSTR and past measurements of $T_{l,p}$. The operating principle of the estimator is illustrated in Fig. 3.

Using Eqn (14), and considering $N = 1$, the actual value of k_2, denoted k_{2r}, can be computed as follows, assuming that our model in a sampling interval starts in $T_{l,p}(t - 1)$ forcing it to reach $T_{l,p}(t)$:

$$\begin{aligned}\Delta T_{l,p} &= T_{l,p}(t) - T_{l,p}(t-1) = \left(e^{k_1 T_s} - 1\right)\\ &\quad \left(\frac{k_{2r}}{k_1} + T_{l,p}(t-1)\right) \qquad (17)\end{aligned}$$

$$k_{2r} = \frac{k_1}{e^{k_1 T_s} - 1}\left(T_{l,p}(t) - T_{l,p}(t-1)\ e^{k_1 T_s}\right) \qquad (18)$$

Here k_1 is computed with the value of F_r corresponding to the previous sampling period which is known at time t. Equating Eqn (18) with Eqn (12), the estimated value of ΔE can be obtained:

$$\begin{aligned}\Delta\hat{E} &= \frac{V_l \rho_l Cp_l k_1}{e^{k_1 T_s} - 1}\left(T_{l,p}(t) - T_{l,p}(t-1)e^{k_1 T_s}\right)\\ &\quad - F_l \rho_l Cp_l T_{l0} - \frac{F_r \rho_r Cp_r T_{r0} U\ S}{F_r \rho_r Cp_r + U\ S} \qquad (19)\end{aligned}$$

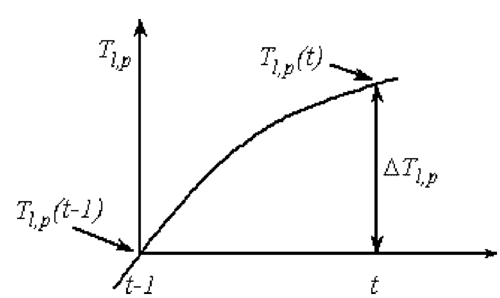

Figure 3. Operating principle of the estimator.

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Again, all variables in Eqn (19) correspond to the previous sampling period. In order to smooth the estimation, a first order filter is applied to (19):

$$\Delta\hat{E}^*(t) = \alpha\ \Delta\hat{E}^*(t-1) + (1-\alpha)\Delta\hat{E} \qquad (20)$$

where $\Delta\hat{E}^*$ is the filtered value of $\Delta\hat{E}$ and $0 < \alpha < 1$ is the parameter of the filter.

RESULTS

In order to test the PPC controller, several experiments were carried out in a simulated environment using the nonlinear model Eqns (5)–(9) as process. The sampling time T_s was set to 1 min. Four cases were considered:

- ΔE is known
- ΔE is assumed as a constant in the model.
- A PID controller is used in a cascade in order to eliminate steady-state errors.
- ΔE is estimated with Eqns (19), (20) every sampling time.

In each of the four cases, the response of the closed loop system to changes in the set point covering a rather wide range of operation conditions were computed using $N = 15$ and $\lambda = 0.8$ as tuning values. This particular case is a kind of continuous process where the set point normally is not changed very often; so, the range of temperatures used in the experiments is considered adequate. Anyway, the PPC controller has the nonlinear model of a generic process that is valid in the whole range of operation, and similar results can be obtained under other operating conditions or reactions. Also, the response to disturbances in measured and unmeasured variables, maintaining the set point constant, was considered in the fourth case.

Case 1 – ΔE known

The value of ΔE is calculated considering that the concentration of the reagent A can be measured. It is seen from Fig. 4 that the temperature T_l follows fairly well the set point changes. Figure 5 illustrates the evolution of the manipulated variable F_r, where the nonlinear behavior of the controller can be seen in the gain.

Case 2 – ΔE left constant

The concentration of reagent A is considered not measurable and the value of ΔE is calculated with an estimated constant value C_{a0}. As the controller does not have an embedded integral action, steady-state errors arise, as shown in Fig. 6.

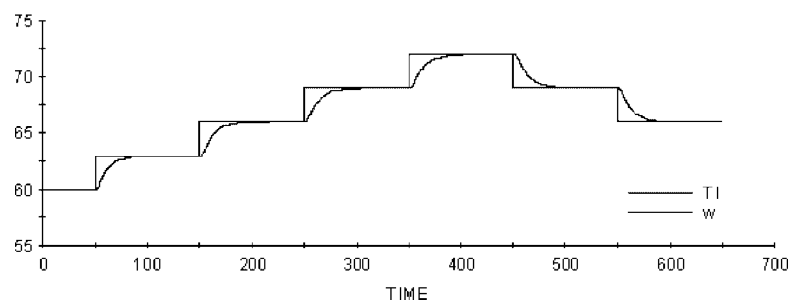

Figure 4. Case 1 – ΔE is calculated – evolution of $T_{l,p}$ with $N = 15$ and $\lambda = 0.8$.

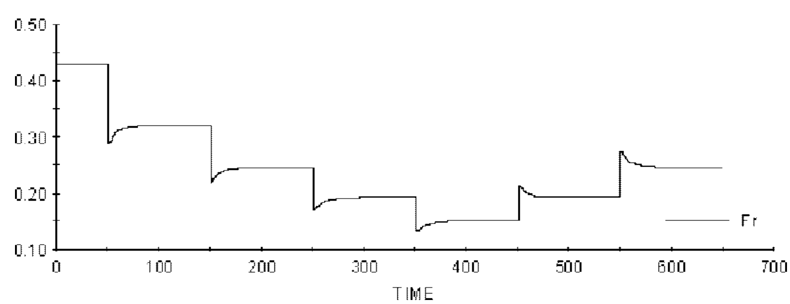

Figure 5. Case 1 – ΔE is calculated – evolution of the manipulated variable F_r.

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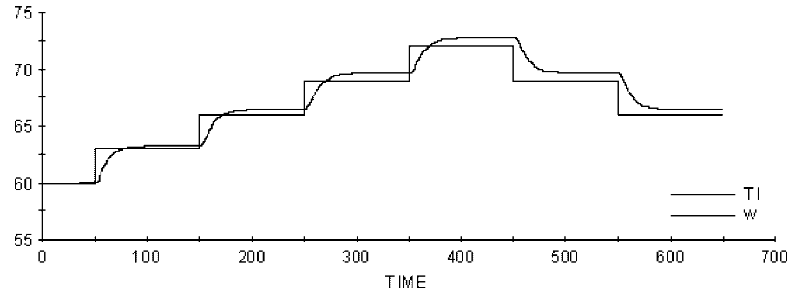

Figure 6. Case 2 – ΔE is left constant – evolution of $T_{\mathrm{l,p}}$. A steady-state error appears.

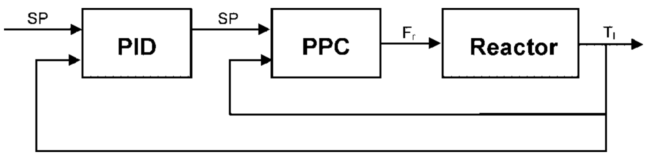

Figure 7. Case 3 – ΔE is left constant – a cascaded PID + PPC are used.

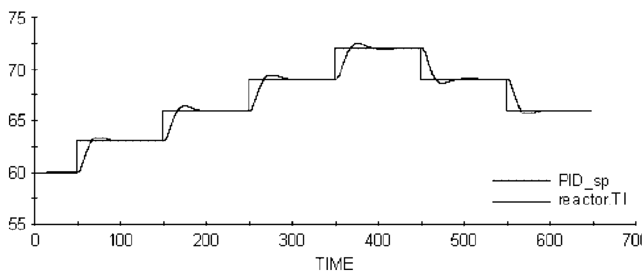

Figure 8. Case 3 – evolution of $T_{\mathrm{l,p}}$ and the set point of the PID.

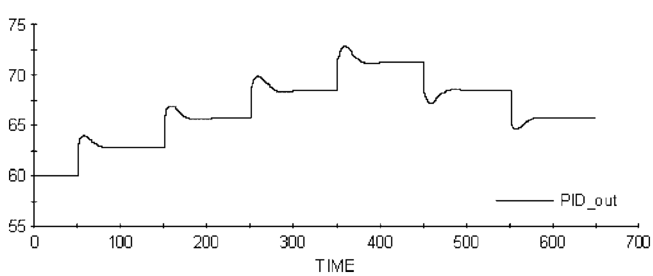

Figure 9. Case 3 – output of the PID controller (linear).

Case 3 – ΔE is left constant and a PID controller is added

As a first approach to eliminate the steady-state error, a PID controller is added in cascade with the PPC controller, as shown in Fig. 7. It is seen from Fig. 8 that the PID controller compensates steady-state errors, being the output of the PID linear (Fig. 9). The PPC controller takes into account the nonlinearities of the process, as revealed in Fig. 10. The PID controller

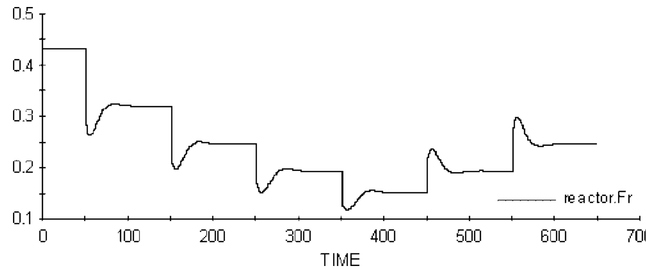

Figure 10. Case 3 – output of the PPC controller (nonlinear).

tuning parameters are $K_{\mathrm{p}} = 0.9$; $T_{\mathrm{i}} = 6$ min and $T_{\mathrm{d}} = 1.25$ min. Even though the performance of the combined PID + PPC controllers is quite good, the main drawback of this approach is the necessity of tuning two controllers. This tuning required several tests in order to obtain a good response.

Case 4 – ΔE is estimated

The value of ΔE is estimated using Eqns (19) and (20). Figure 11 shows the evolution of the temperature in the reactor in this case and Fig. 12 illustrates the evolution of the manipulated variable. As can be seen, the process follows the set point in a uniform manner in spite of the changes in the operating point. Figure 13 depicts the computation time of the PPC controller, which has a peak value of 14.6 μs and a mean time of 6.61 μs. In addition to the set point changes, Figs 14 and 15 show the disturbance rejection of the controller when the following disturbances are considered (the values indicate the applied increments/decrements to the current value and the time):

$$T_{\mathrm{r0}} \longrightarrow +5\,^{\circ}\mathrm{C} \text{ at } t = 50 \text{ and } T_{\mathrm{r0}}$$
$$\longrightarrow -10\,^{\circ}\mathrm{C} \text{ at } t = 100$$
$$T_{\mathrm{l0}} \longrightarrow +5\,^{\circ}\mathrm{C} \text{ at } t = 200 \text{ and } T_{\mathrm{l0}}$$
$$\longrightarrow -10\,^{\circ}\mathrm{C} \text{ at } t = 300$$
$$F_{\mathrm{l}} \longrightarrow +0.05 \text{ l/ min at } t = 400 \text{ and } F_{\mathrm{l}}$$

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$$\longrightarrow -0.1\ \text{l/min at } t = 500$$

$$C_{a0} \longrightarrow +0.2\ \text{kg\_mol/m}^3 \text{ at } t = 600 \text{ and } C_{a0}$$

$$\longrightarrow -0.4\ \text{kg\_mol/m}^3 \text{ at } t = 700$$

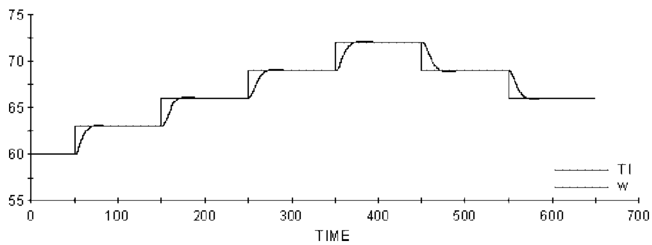

Figure 11. Case 4 – ΔE is estimated – evolution of $T_{l,p}$.

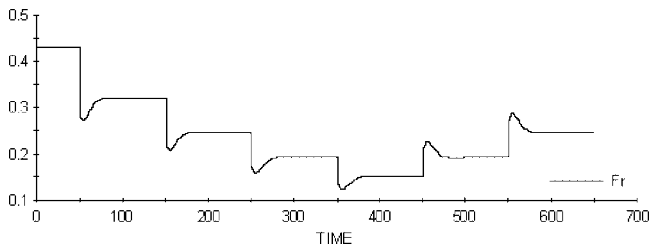

Figure 12. Case 4 – Output of the PPC controller (nonlinear).

Again, the controller has a good response when measured and unmeasured disturbances are applied. Figure 16 shows how the PPC controller with an estimator can compensate a model mismatch. In this case, the heat transmission coefficient (U) has a difference of 15% between the value used in the PPC controller and the value used in the simulation of the continuous model. The estimator here has an implicit integral action which not only compensates the disturbances but also compensates a significant model mismatch.

Comparisons with other controllers

In addition, for the sake of comparison, a full nonlinear predictive controller was applied to the same process considering the same manipulated and controlled variables. The NMPC controller uses the process model Eqn (5)–(9) as the internal one and computes the control action in the usual manner minimizing a quadratic function of the prediction errors. An SQP algorithm and a sequential approach were used in the optimization.

In order to compare the performance obtained with the PPC nonlinear controller, some simulations results are presented below. First, a discrete PID controller is used to control the temperature of the reactor and then a regular NMPC controller is used for the same task.

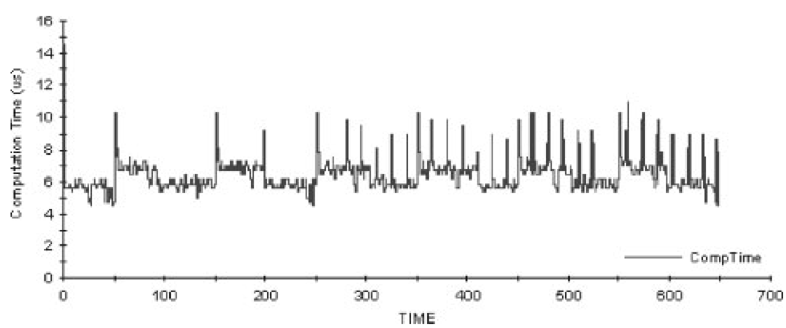

Figure 13. Case 4 – computation time (μs); max time = 14.6 μs, mean time = 6.61 μs.

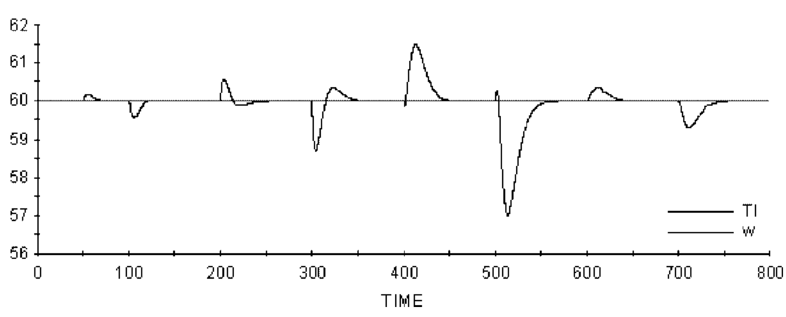

Figure 14. Case 4 – ΔE is estimated – disturbance rejection – evolution of $T_{l,p}$.

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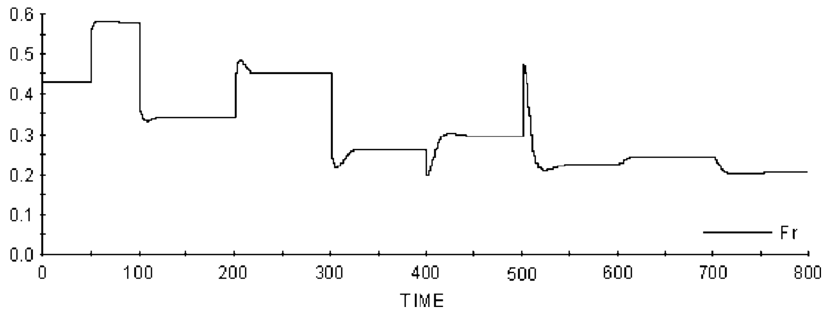

Figure 15. Case 4 – ΔE is estimated – disturbance rejection – evolution of F_r.

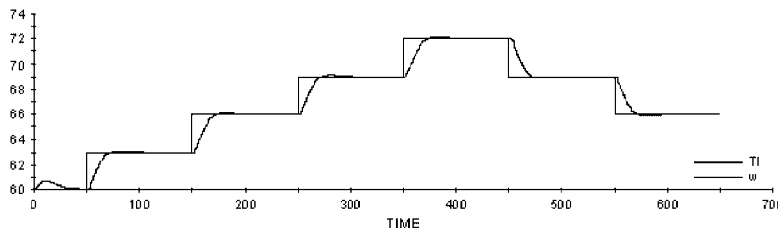

Figure 16. Case 4 – compensation of a model mismatch in the heat transmission (15%).

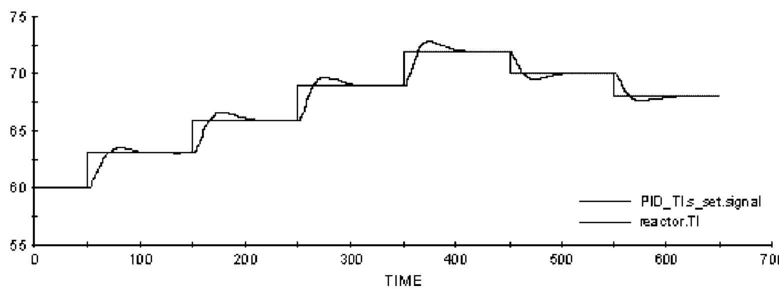

Figure 17. Evolution of T_l with a discrete PID controller.

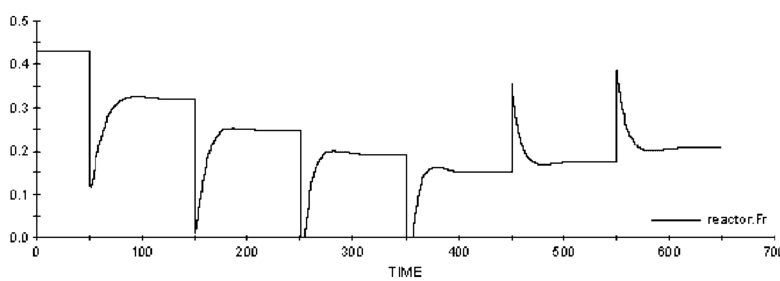

Figure 18. Output of the discrete PID controller.

With a PID controller

A discrete incremental PID controller is used to control T_l. The PID controller used has the proportional and integral terms as a function of the error, and the derivative term as a function of the controlled (or process) variable. Besides, the internal calculations are carried out in percent of the range, as industrial PID controllers do. The parameters of the PID controller are: $K_p = -0.1$, $T_i = 16$ s and $T_d = 4$ s. Figure 17 displays the time evolution of the reactor temperature T_l when the set point of the controller changes and Fig. 18 shows the evolution of the manipulated variable F_r in this case. As can be observed, the PID controller is slower than the PPC controller and it has a bigger overshoot.

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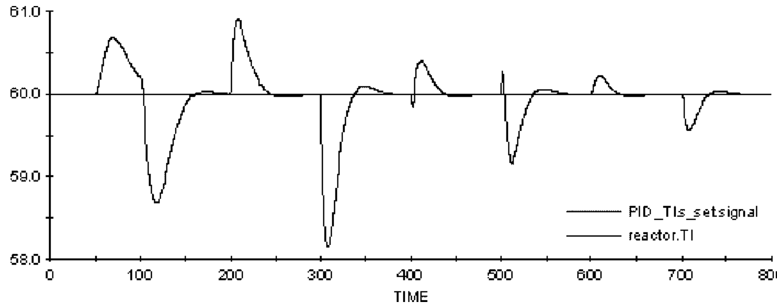

Figure 19. PID controller – disturbance rejection – evolution of T_l.

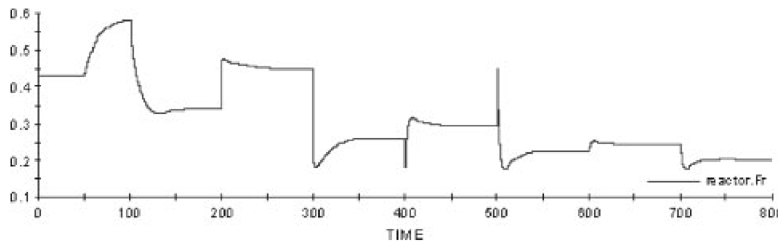

Figure 20. PID controller – disturbance rejection – evolution of F_r.

Besides, the manipulated variable F_r goes to saturation in some parts of the experiment. The steady-state is reached in $50 \sim 60$ min in this case, while the PPC controller reaches the same point in about $20 \sim 30$ min. Figures 19 and 20 present the PID controller response against the same disturbances mentioned in the section on Case 4 – ΔE Is Estimated.

With a NMPC controller

In this case an NMPC controller using as internal model the nonlinear equations (5)–(9) and a prediction error minimization criterion is used. The cost function J penalizes deviations of the predicted controlled output $y(t)$ from a reference trajectory $r(t)$, which for the SISO case, will lead to:

$$J = \int_{t_k}^{t_k+t_p} [\hat{y}(\tau) - r(\tau)]^2 d\tau \qquad (21)$$

The manipulated variable is discretized over the prediction horizon $t_p = N_p \times T_s$, where T_s is the sampling interval of the controller. Controls are assumed to have a piece-wise constant form such as $u(t) = u(k)$, $kT_s \leq t \leq (k+1)T_s$ and $u(k) = u(N_u - 1)$, $k \geq N_u$.

The dynamic optimization problem associated to the NMPC controller is solved keeping the continuous formulation of the model process Eqns (5)–(9) used to calculate the predictions $\hat{y}$ needed for the minimization of Eqn (21) and the value of J, by means of a dynamic simulator (Fig. 21).

An NLP optimization problem must be solved on-line at each sampling period to generate the control moves. An SQP algorithm is used for the optimization.

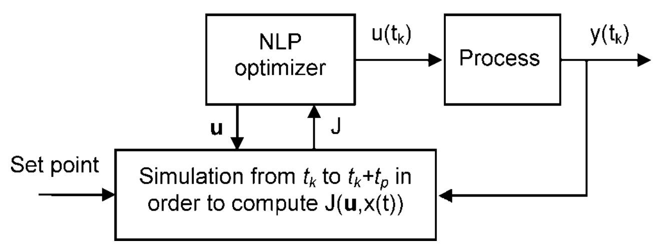

Figure 21. NMPC – continuous implementation framework.

The successful implementation of the mentioned control technique requires the knowledge of the current state of the nonlinear system at each time interval. In order to reconstruct the present state of C_{a0} from the measured outputs, the receding horizon estimation (RHE) approach has been adopted, maintaining the same nonlinear model as in the controller.

Figure 22 displays the time evolution of the reactor temperature when the set point of the controller changes and Fig. 23 shows the evolution of the manipulated variable F_r in this case. In order to facilitate the comparison with the PPC controller, the same prediction and control horizon were chosen. The response is similar to the one obtained with the PPC controller in Fig. 11. The simulation was performed in a 1.83 GHz computer with 1 GB of RAM and the time required to solve the predictive control problem every sampling time is represented in Fig. 24. Also, Figs 25 and 26 show the NMPC controller response against the same disturbances mentioned in the section on Case 4 – ΔE Is Estimated.

The response is better in the NMPC case as might be expected: The temperature reacts quicker so that most of

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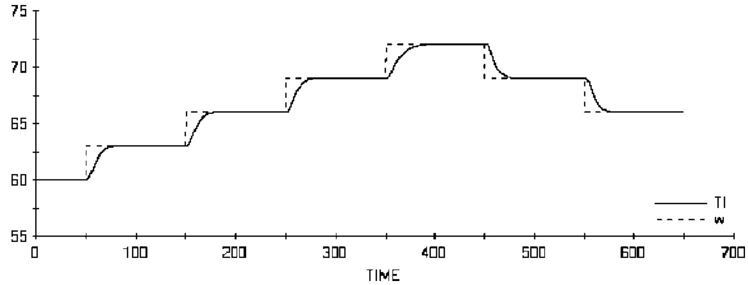

Figure 22. NMPC with an internal first principles model – evolution of $T_{l,p}$.

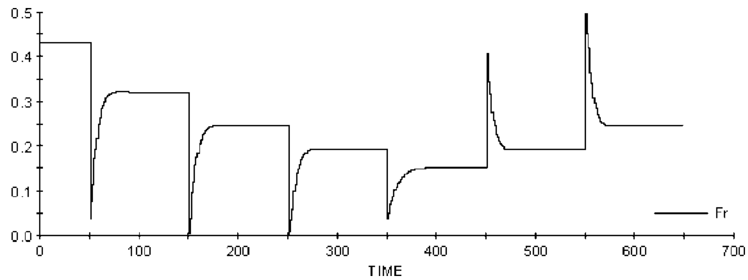

Figure 23. NMPC with an internal first principles model – evolution of F_r.

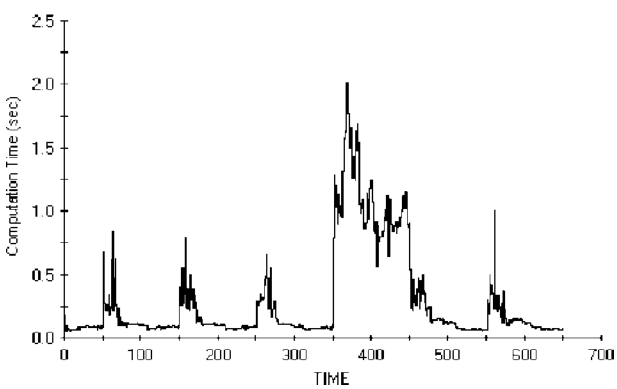

Figure 24. Computation time (s); max time = 2 s, mean time = 0.29 s.

the disturbances are reduced a bit faster. Nevertheless, because the PPC controller incorporates a nonlinear model of the process capturing in this way its main nonlinearities, the quality of the response of the PPC is similar to the one obtained with the NMPC. The main difference is observed in the computation time which is in the order of a few microseconds (mean time = 6.61 μs) in the PPC controller versus a fraction of a second in the conventional NMPC controller case (mean time = 0.29 s). So, the mean time used to compute the conventional NMPC algorithm is 50 000 times longer than the PPC. If we combine the simplicity of implementation, tuning, and computation speed, the PPC controller is appealing for industrial environments, especially for applications where a commercial PLC or DCS is used.

CONCLUSIONS

In this paper, a reduced order PPC for a CSTR was developed. Its main characteristics are its nonlinear nature based on a first principles model. It uses a reduced order model of the process and combines the simplicity of a linear controller with the essential nonlinearities of the process, providing a good alternative for 'low cost' NMPC, easy to be implemented in a commercial PLC or DCS.

Results for different cases obtained in a simulated environment have been shown. The experiments were carried out modifying the set point and introducing changes in different variables in order to simulate measured and unmeasured disturbances. Due to the lack of integral action in the controller, steady-state errors that are not compensated arose. Two of the possible solutions to this problem were shown: a cascaded PID controller and an estimator for the reaction heat. In both cases steady-state errors and model mismatch could be compensated efficiently.

The controller demonstrates a remarkable capacity to deal with the process nonlinearities. As an advantage, besides its simplicity and speed, the tuning is easy to achieve and it does not need retuning after the desired response is obtained, adapting itself to the different operating points. The tuning parameters (N, λ) and the filter parameter (α) are used to set the response behavior of the system.

As a disadvantage, this kind of controllers needs a special formulation for each case. The controller takes

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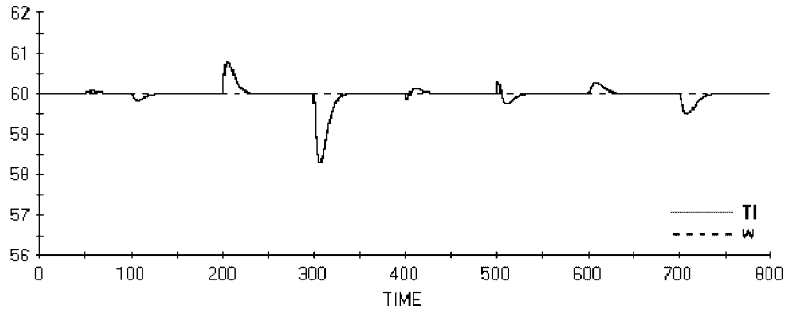

Figure 25. NMPC with an internal first principles model – disturbance rejection – evolution of $T_{l,p}$.

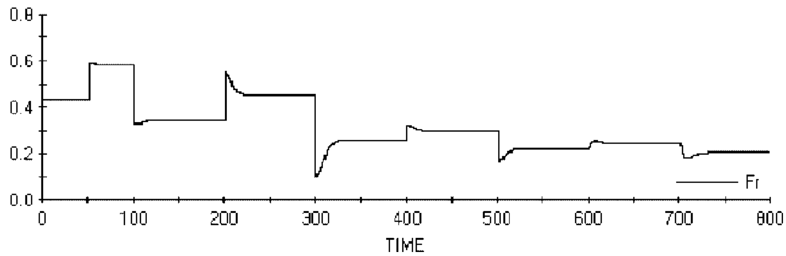

Figure 26. NMPC with an internal first principles model – disturbance rejection – evolution of F_r.

advantage of the structure of the first principles model of this kind of processes. Extensions to other typical process systems will be investigated in the future, as well as a MIMO controller of this process, in order to control T_l and the concentration of C_a in the final product, if good measurements of C_a could be obtained on-line.

NOMENCLATURE

ρ_l Density of the liquid in the tank
Cp_l Specific heat of the liquid in the tank
ρ_r Density of the refrigerant liquid
Cp_r Specific heat of the refrigerant liquid
U Heat transmission global coefficient
S Heat interchange surface
V_l Tank volume
V_r Jacket volume
C_a A concentration
C_b B concentration
E_a Activation energy
R Universal constant of the gases
H Reaction heat
A Reaction rate coefficient
T_{r0} Input temperature of the refrigerant liquid
T_{l0} Input temperature of the reagent
C_{a0} Input concentration of the reagent

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