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Iterative Nonlinear Control of a Semibatch Reactor. Stability Analysis

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***Abstract*— This paper presents the application of Iterative Nonlinear Model Predictive Control, INMPC, to a semibatch chemical reactor. The proposed control approach is derived from a model-based predictive control formulation which takes advantage of the repetitive nature of batch processes. The proposed controller combines the good qualities of Model Predictive Control (MPC) with the possibility of learning from past batches, that is the base of Iterative Control. It uses a nonlinear model and a quadratic objective function that is optimized in order to obtain the control law. A stability proof with unitary control horizon is given for nonlinear plants that are affine in control and have linear output map.**

The controller shows capabilities to learn the optimal trajectory after a few iterations, giving a better fit than a linear non-iterative MPC controller. The controller has applications in repetitive disturbance rejection, because they do not modify the model for control purposes. In this application, some experiments with a disturbance in inlet water temperature has been performed, getting good results.

I. INTRODUCTION

Batch and semibatch processes experience continuous transitions and are usually highly nonlinear, involving complex reaction mechanisms and model-plant mismatch. Batch operation is done under unsteady state and reference trajectories are frequently time-varying, making process variables change over wide ranges and exhibiting therefore significant nonlinear behavior. This leads to time-invariant models being unsuitable for describing the process and consequently control strategies based upon linear models can drive to significant errors. On the other hand, the repetitive way of operation allows the extraction of information from past batches in order to improve the new batch. In batch mode of operation, batch-to-batch variations can be significant and are of primary concern. In most industrial cases, the batch-to-batch variations are strongly auto-correlated, providing the possibility of using previous batch results to adjust the recipe of a subsequent batch. The error that cannot be removed by on-line feedback control can be eliminated or reduced by the so called *batch-to-batch* or *run-to-run* control. This can be done by means of Iterative Learning Control (ILC) [18] which refers to a body of methodologies that attempt to improve the control performance of a repeated run based on the results from previous runs.

Because feedback control can respond to disturbances immediately and batch-to-batch control can correct any bias left uncorrected by the feedback controller, which may be due to unmodelled disturbances, parameter errors and dynamics, a combined scheme can potentially allow these to complement each other to render the benefits of both. The idea of combining batch-to-batch control with feedback control appeared in [3]. In [19], a combination of GPC (Generalized Predictive Control) and ILC has been successfully applied to robotic manipulators.

Notice that, in this case, the problem is not easy to solve since the feedback control of the on-going run is a difficult problem itself, because it involves a nonlinear controller. The inclusion of data collected during the on-going batch run (in addition to those from the past runs) makes the feedback control strategy capable of responding to new disturbances that occur during the run.

The paper presents the application of a nonlinear iterative controller to a multivariable semibatch reactor. This controller is called Iterative Nonlinear Model Predictive Control (INMPC) and was presented in [11] ([6] for monovariable plants). This controller tries to improve existing strategies by the use of a nonlinear controller devised along the last-run trajectory as well as by the inclusion of filters. Tracking the setpoint profile is tackled by a nonlinear controller based on EPSAC (Extended Predictive Self-Adaptive Control) [17] while its iterative nature improves the performance at each batch. This papers extends the results to multivariable plants and performs a stability analysis.

The paper is organized as follows. In section II, the plant is described. Nonlinear and linear models for control purposes are obtained and identified. INMPC controller is summarized in section III, and a convergence result for unitary horizons are given in section III-B. Simulations are presented in section IV, where a comparison with a linear MPC and a disturbance test is performed. Finally, in section V the major conclusions are drawn.

II. PLANT DESCRIPTION

The plant is an example of a semibatch process that is suitable to be implemented in laboratory equipment. This plant has been used as a benchmark by several authors (see, for example, [1], [2]). It is assumed to be composed of a reaction vessel, where a chemical reaction is performed, and a cooling loop. The idea is to transform the material via an exothermic chemical reaction. A multivariable controller is necessary in order to achieve control of temperature and reactant concentration during the process duration.

The difference between batch and semibatch processes in this example is clear. Batch process means that, once the reaction has started, there is no input of more reactant into the vessel. Therefore, the product concentration cannot be controlled, and the system would be a single input-single output one.

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In the case study, the process is semibatch. At initial time there is a fixed reactant concentration (lower than initial concentration in an equivalent batch process), but it is possible to add more material after the chemical reaction has started. It makes the control more difficult (multivariable) because the reactant concentration can be controlled. For this reason, semibatch processes can usually reach a better performance than batch processes. The control objective is to followa given reference trajectory of temperature and product concentration. This reference is computed externally in some optimal way minimizing some cost function. The reactant concentration set point at the end of the batch is null in order to minimize the reactant that can not be transformed.

A. Continuous-time model

It can be assumed that the mass inside the tank, m, is constant since the inlet reactant flow, u_c, is small enough (ie. high reactant concentration). The equations describing the system have the form [3]:

$$\begin{cases} dT/dt &= \frac{F}{m}(T_e - T) + \frac{Q}{mC} \\ dC_A/dt &= -k_0 e^{-E/RT} C_A^2 + u_c \end{cases} \tag{1}$$

$$Q = (-\Delta H)\, V k_0 e^{-E/RT} C_A^2 \tag{2}$$

$$F = a_f v + b_f \tag{3}$$

$$\beta = a_i F + b_i (T_{e_w} - T) + c_i \tag{4}$$

$$T_e - T = \beta (T_{e_w} - T) \tag{5}$$

$$\begin{cases} T(0) &= T_0 \\ C_A(0) &= C_{A_0} \end{cases} \tag{6}$$

$$0 \le t \le T_s \cdot N \tag{7}$$

where the controlled variables are the temperature inside the tank (T) and the reactant concentration (C_A), and the manipulated variables are valve opening (v) and inlet reactant flow (u_c). System (1) describes the plant dynamics, equations (2)-(5) are auxiliary static equations, describing the generated heat inside the vessel, Q, the cooling water flow, F, and the heat exchanger efficiency, β. Equation (6) represents the (constant) initial batch conditions, and (7) defines the batch duration, which in this case is considered to be constant. When this time is variable (i.e. in a time span optimization), several authors [4], [5] have proposed some methods to convert the problem into a constant duration one.

Fig. 1 presents a graphical description of the plant. Parameters are enumerated in Table I. Values of a_f, b_f, a_i, b_i and c_i are identified from a laboratory plant, in order to perform real experiments later. Finally the measured temperature has a delay of d seconds because of the sensor placement.

The generated heat inside the vessel could be emulated using, for example, an electrical resistance in a stirred tank. It has been done, for an equivalent monovariable batch reactor, in [6] and, for another example, in [7]. A disturbance can be easily introduced modifying the inlet cooling water temperature, for example.

This plant seems to be a good candidate for testing nonlinear multivariable control techniques. The two state variables are strongly coupled by an exponential term depending on temperature and the square of product concentration (1)-(2). The effect of valve opening on the dynamics is quadratic because of the definition of valve characteristics (3) and heat exchanger efficiency (4).

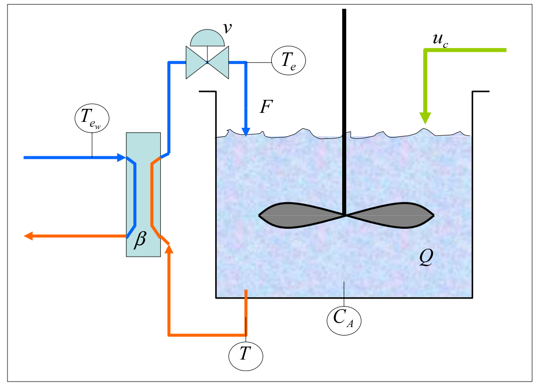

Fig. 1. Multivariable 2x2 plant

TABLE I
PLANT PARAMETERS

Variable	Units	Value
E/R	K	13550
k_0	$l/(mol \cdot s)$	$1.16 \cdot 10^{17}$
m	kg	29.6
C	$kJ/(kg \cdot K)$	4.18
$\frac{(-\Delta H)V}{mC}$	$K \cdot l/mol$	20
T_0	K	308
C_{a_0}	mol/l	0.5
T_{e_w}	K	298
a_f	$kg/(s \cdot \%)$	6.252
b_f	kg/s	5.35
a_i	s/kg	$-879 \cdot 10^{-6}$
b_i	K^{-1}	$-243 \cdot 10^{-6}$
c_i	-	0.964
d	s	30

Therefore, the control of this plant is a difficult task. The product concentration tends to zero quickly because of the quadratic term, and the cooling water and reactant flows are constrained between strict physical limits. In practical non-simulated applications additional problems of sensor noise and plant disturbances will be found. These issues have been partially addressed in this work by introducing small disturbances in inlet cooling water temperature.

B. Transformation into an affine system and discretization

For stability issues, plant equations are better written in discrete-time in a form that is affine in control and linear in output (see section III-B). The controller may be applied directly to plant equations (1)-(7), but the stability analysis requires that the plant has the form given by

$$\begin{cases} x_{t+1} &= f(x_t) + g(x_t) u_t \\ y_t &= C x_t \end{cases} \tag{8}$$

The way to do this transformation is by defining a new state equation and a new input u:

$$\dot{v} = u \tag{9}$$

The state variables are now T, C_A and v, while the inputs are u and u_c. The affine plant, described by (1)-(5) and (9), is discretized using, for simplicity, Euler method with a sampling time T_s. Hence, the model is given by (2)-(4), (8),

$$f(x_t) = \begin{pmatrix} T + T_s\left[\frac{F}{m}\beta\left(T_{e_w} - T\right) + \frac{Q}{mC}\right] \\ C_A - T_s k_0 e^{-E/RT} C_A^2 \\ v \end{pmatrix}, \quad (10)$$

$$g(x_t) = \begin{pmatrix} 0 & 0 \\ T_s & 0 \\ 0 & T_s \end{pmatrix} \quad (11)$$

Finally, the model for control (see section IV) must take into account the plant delay d, which is equal to 2 when the sampling time is 15 seconds. Hence, the plant description is modified to

$$f_m(x_t) = \begin{pmatrix} f(x_t) \\ T_1 \\ T_2 \end{pmatrix}, \quad g_m(x_t) = \begin{pmatrix} g(x_t) \\ 0 \\ 0 \end{pmatrix} \quad (12)$$

and

$$C = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix} \quad (13)$$

where the two last state variables (T_1 and T_2) denote the delayed temperatures.

C. Identification of a linear model

In this section we address the problem of the computation of an approximated linear model in order to make experiments with linear MPC (section IV). A good linear model cannot be found because of the process nonlinearity.

Step responses of this 2-input linear batch process can be computed via 3 open loop experiments with constant input [3]. Firstly, an experiment with constant input ($v = 40$ % and $u_c = 3600\ mol/s$) is performed. The other experiments are obtained modifying only one of the constant inputs ($v = 80$ % and $u_c = 7200\ mol/s$, respectively). The step responses are computed as the difference between the obtained trajectories in the first experiment and the obtained trajectories in the other experiments. Using this simple approach, the repetitive disturbance term is completely removed into the step responses.

These obtained step responses are plotted in Fig. 2. It is used to identify a linear model for MPC control purposes [8]. Reactant concentration response to a step in reactant flow has an integrator effect, that cannot be appreciated in this figure because of the finite batch duration.

III. ITERATIVE NONLINEAR MODEL-BASED PREDICTIVE CONTROL (INMPC)

A. Controller description

It has already been observed in section II that the plant dynamics are complex and nonlinear. Even a nonlinear controller may have problems when controlling this plant. Moreover, not every reference trajectory is reachable and special care has to be taken in order to choose a correct reference trajectory.

Michalska and Mayne [9] propose a suboptimal NMPC for continuous processes that employs an initial feasible solution which is improved iteratively. This idea can be adapted to deal with batch processes. Indeed, the inherent repetitiveness of these processes is an advantage, because the controller has more information about the process, obtained from past batches. It makes the achievement of a trajectory refinement that improves the control at every batch possible.

In order to address the problem Iterative Nonlinear Model Predictive Control (INMPC) is used. This controller [6] combines a nonlinear model based controller with iterative learning capabilities. In this paper, the multivariable application of this controller is presented.

The controller belongs to the predictive type. It means that it computes a prediction of the output variables, which is optimized in order to get the control law. In this case, the problem is formulated using batch incremental variables. Denoting the batch number with a superindex, variables are defined by $\tilde{x}(t) = x^k(t) - x^{k-1}(t)$. Automatically, repetitive and additive disturbances appearing in the process are cancelled into the incremental variables model. Moreover, if the difference from one batch to next one is not large, superposition principle holds, and prediction can be divided into a forced response plus a free response:

$$y = Gu + f \quad (14)$$

where $u \in \mathbb{R}^{N_u \cdot m}$ and $y \in \mathbb{R}^{N_y \cdot p}$ are vectors containing future values of the variables.

Free response f is computed iterating the nonlinear model (8) and considering that the future value of the input is equal to the last batch input at the same instants of time. In the case that the plant is stable, free response will tend to approximate to last batch trajectory. At the first time instant, it will coincide with that trajectory, since it is assumed that there is no variation in initial conditions. When incremental variables are being used, this free response will be null at the first instant of time.

In order to compute the forced response, a model linearization has to be performed. This is done not around an equilibrium point, but around last batch trajectory. A dynamic matrix [8], which is different at every time instant of every batch, is computed, so an accurate nonlinear prediction can be known.

A standard objective function is minimized

$$J = \|y - r\|_Q^2 + \|\tilde{u}\|_R^2 \quad (15)$$

possibly subjected to constraints of types

$$\begin{cases} y_{\min} \le y \le y_{\max} \\ u_{\min} \le u \le u_{\max} \\ \delta u_{\min} \le u^k - u^{k-1} \le \delta u_{\max} \\ \Delta u_{\min} \le u_t - u_{t-1} \le \Delta u_{\max} \end{cases} \quad (16)$$

where

$$u = \begin{pmatrix} u_{t|t} & u_{t+1|t} & \cdots & u_{t+m-1|t} \end{pmatrix}^t \quad (17)$$

$$y = \begin{pmatrix} \hat{y}_{t+d+1|t} & \hat{y}_{t+d+2|t} & \cdots & \hat{y}_{t+d+p|t} \end{pmatrix}^t \quad (18)$$

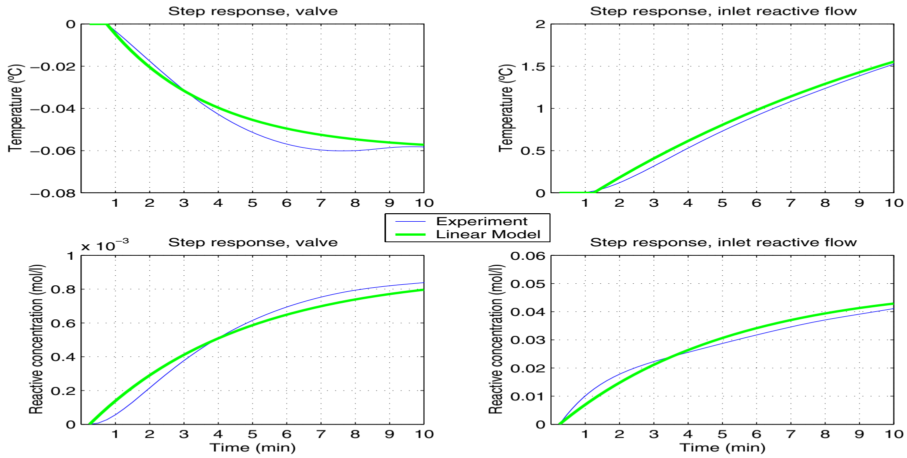

Fig. 2. Step response of the plant

Only the values of the predicted output after the system delay d are considered into the objective function. The solution of (15)-(16) gives the control variable u. Only the first element computed along the control horizon is applied to the plant, as it is done with any receding horizon strategy.

Note that in a batch process, initial conditions are constant. Closed-loop stability properties are different than in MPC for continuous processes because the starting point is fixed. In these conditions, a stability proof can be found without the requirement of a terminal cost or constraint [10], see section III-B.

The number of controller parameters is relatively small (see Table II), similar to the number of parameters in MPC. The major complexity comes from other point. It is the necessity of an accurate plant model (8). Partial derivatives of the functions involved on the model (f and g) are also required by the controller in order to build the linearized model, notably increasing computational load requirements.

B. Stability analysis

A stability analysis of the INMPC controlled system without constraints can be done. A stability proof of a different constrained linear model based controller (Batch MPC or BMPC) is shown in [3].

Assume that the plant can be exactly described by equations (8). They can have a repetitive disturbance term v_t (i.e. it does not depend on the batch index). An iterative controller will deal with this disturbance term and there is no need to include it into the model, assuming that $v_t = v_t^{k-1}$ and that it appears in additive form into the model (8) [11].

The controller is a function of variables at time t in the current batch, variables at every time in the last batch $k-1$, and the future estimated output along the prediction horizon

$$u_t^k = u_t^{k-1} + \Phi\left(x_t^k, x_{t+1}^{k-1}, x_t^{k-1}\ldots\right)\left(\mathbf{r}_t - \mathbf{f}_t^k\right) \qquad (19)$$

Note that $\mathbf{f}_t^k$ is the free response of this system, and it is computed assuming $u_{t+i}^k = u_{t+i}^{k-1}$. At $t=1$, the free response coincides with last batch trajectory $\mathbf{y}_t^{k-1}$, if identical initialization conditions hold. The first control law term u_t^{k-1} is the manipulated variable at time t in the last batch and it appears in most iterative controllers, when batch deviation variables are used. The model for an iterative controller does not need to consider the repetitive disturbances because the control law does not depend on these disturbances.

It should be noted that many plants can be written or transformed, via an output linearization approach [12] or other procedure, in the form of equation (8). Moreover, the controller can be applied to a fully nonlinear plant, but stability is only guaranteed in this concrete case. If we can write the system in the equation (8) form, it is possible to find a stabilizing iterative controller.

In general, stability properties are quite sensitive to the choice of the system delay d. The underestimation of this value may lead to instability. For example, consider the discrete-time ILC (Iterative Learning Controller) law:

$$u_t^k = u_t^{k-1} + k\left(r_{t+1} - y_{t+1}^{k-1}\right) \qquad (20)$$

If the plant delay is 2, the control law would try to compensate the error at $t=1$ increasing continuously the control variable at initial time. The closed loop system would be unstable. Therefore, special care has to be taken into account in the estimation of this value, because most iterative control laws are extremely sensitive to it.

A certain robustness is achieved with respect to errors in the estimation of the smooth functions $f(x)$, $g(x)$, the output matrix C, or even when the terms v or w are not exactly repetitive (i.e. they depend on the batch index) or additive. These facts have been addressed in simulation studies and laboratory applications [11].

1) Multivariable analysis with control and prediction horizons $m=p=1$: Assume that we fix the time $t=1$ and take $Q=I, R=\Lambda$. Ignoring the repetitive terms, plant equations (8) take the form

$$\left\{\begin{array}{ll} x_1^k & = f(x_0) + g(x_0)\,u_0^k = f_0 + g_0 u_0^k \\ y_1^k & = C x_1^k = C g_0 u_0^k + C f_0 \end{array}\right. , \qquad (21)$$

where $G_1 = Cg_0$, $u \in \mathbb{R}^{N_u}$, $x \in \mathbb{R}^{N_x}$ and $y \in \mathbb{R}^{N_y}$. The control law is given by

$$u_0^k = u_0^{k-1} + \left(G_1^T G_1 + \Lambda\right)^{-1} G_1^T \left(r_1 - y_1^{k-1}\right), \qquad (22)$$

where r_1 is the vector of reference values. Note that y_1^{k-1} is equal to the free response of the system, which is obtained when $u_0^k = u_0^{k-1}$, or equivalently, when $\tilde{u}_0^k = 0$. This can be only assured if identical initialization condition holds. Therefore the controller is suitable to be applied in iterative control, but not in repetitive control, where state is not reset from one batch to next one.

G_1 is, in the general case, the dynamic matrix of the linearized system around last batch trajectory at time $t = 1$. In this simplified case, it is equal to Cg_0. $u_\mathbf{0}^\mathbf{k}$ contains only control moves at initial time, because the control horizon m is assumed to be 1. Substituting the input-output relation (21) into (22), we have

$$u_0^k = u_0^{k-1} + \left(G_1^T G_1 + \Lambda\right)^{-1} G_1^T \left(r_1 - b_1 - G_1 u_0^{k-1}\right) \qquad (23)$$

And using some matrix algebra, equation (23) can be written in the form

$$u_0^k = \left(G_1^T G_1 + \Lambda\right)^{-1} \Lambda u_0^{k-1} + constant \qquad (24)$$

This equation can be regarded as a fixed point iteration $x = F(x)$. It is assumed that set point is reachable, that is, there exists u_0^* such that $r_1 = Cg_0 u_0^* + Cf_0$ is verified. It must be proven that the fixed point of (23) is stable. Absolute stability concepts [14] for discrete-time systems [15] may be applied in order to prove stability with nonlinear output map. Here, we apply Banach theorem. It gives stability of the fixed point if it is possible to find $\rho < 1$, such that

$$\|F(x) - F(y)\| \leq \rho \|x - y\|, \qquad \forall x, y \in \mathbb{R}^{N_u} \qquad (25)$$

Using (24) and induced matrix norms, the desired expression is obtained

$$\begin{aligned} \|F(x) - F(y)\| &= \left\| \left(G_1^T G_1 + \Lambda\right)^{-1} \Lambda (x - y) \right\| \qquad (26) \\ &\leq \left\| \left(G_1^T G_1 + \Lambda\right)^{-1} \Lambda \right\|_i \|x - y\| \end{aligned}$$

Now, we use the fact that Λ is a diagonal matrix, and G_1 is full-rank (ie. the system has to be controllable). Then, $G_1^T G_1$ is symmetric positive definite and, therefore, it is orthogonally diagonalizable, say $G_1^T G_1 = P \Omega P^T$, where Ω is diagonal with nonzero elements. Applying some matrix algebra (see for example [16]) and taking norm 2, we have

$$\begin{aligned} \rho &= \left\| \left(P \Omega P^T + \Lambda\right)^{-1} \Lambda \right\|_i = \left\| \left[P (\Omega + \Lambda) P^T\right]^{-1} \Lambda \right\|_i \\ &= \left\| P (\Omega + \Lambda)^{-1} \Lambda P^T \right\|_i \leq \frac{1}{1 + \frac{\Omega_{\min}}{\Lambda_{\max}}} < 1 \qquad (27) \end{aligned}$$

and it is concluded that system is convergent in $t = 1$. The same reasoning can be argued to get a stability proof in $t+1$. Assuming functions f and g are of class C^1 (continuous and differentiable), system equations at time $t+1$ can be written:

$$\left\{ \begin{aligned} x_{t+1}^k &= f\left(x_t^k\right) + g\left(x_t^k\right) u_t^k \\ &= f_t + g_t u_t^k + \varepsilon\left(x_t^k - x_t^*\right) \\ y_{t+1}^k &= C x_{t+1}^k \end{aligned} \right. \qquad (28)$$

TABLE II

NONLINEAR INMPC CONTROLLER PARAMETERS

Parameter	Symbol	Value
Sample time	T_s	15 s
Batch duration	$T_s \cdot N$	900 s
Control horizon	m	1
Prediction horizon	p	5
Roll-off factor	α	0.1
Control weighting matrix	Q	diag 10^{-4} 10^{-3}
Error weighting matrix	R	diag 1 50
Valve limits	%	0 100
Reactant limits	$mol/(l \cdot s)$	0 36000
Reactant concentration limits	mol/l	0 1

TABLE III

LINEAR MPC CONTROLLER PARAMETERS

Parameter	Symbol	Value
Roll-off factor	α	0.5
Control weighting matrix	Λ_{MPC1}	diag 10^{-4} 10^{-3}
Control weighting matrix	Λ_{MPC2}	diag 10^{-4} 10^{-6}

being x_t^* the equilibrium point, $f_t = f(x_t^*)$ and $g_t = g(x_t^*)$. The same stability analysis is applicable, because the term $\varepsilon\left(x_t^* - x_t^k\right)$ tends to zero when the batch index k increases. It is concluded that disturbed system (28) is also asymptotically stable at every time instant t.

IV. RESULTS

Simulation results are presented, showing a comparison between a classical linear MPC and INMPC controllers applied to the multivariable semibatch reactor described in section II. The idea is to improve the performance of the MPC controller in this semibatch process. In order to achieve that, a learning INMPC controller is used.

Equations (1)-(7) have been implemented on a computer, and integrated using a Runge-Kutta method. Parameters are given in Table I. In the first simulations, MPC is used to control this plant. The linear approximated model is obtained performing several experiments with constant inputs, as shown in section II-C. Controller parameters are given in Table III and the result is presented in Fig. 3, where two simulations with different values for the control weighting matrix Λ are shown. It is clear from these experiments that

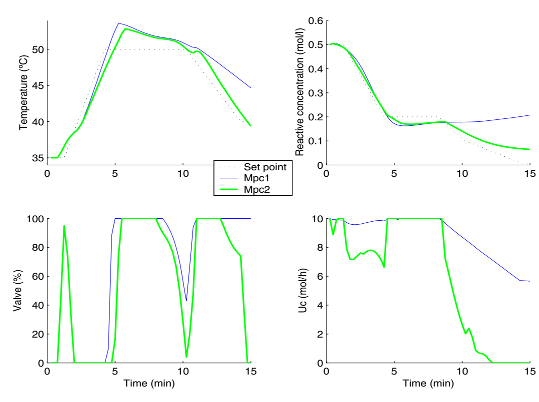

Fig. 3. Experiments with linear MPC, different values of λ

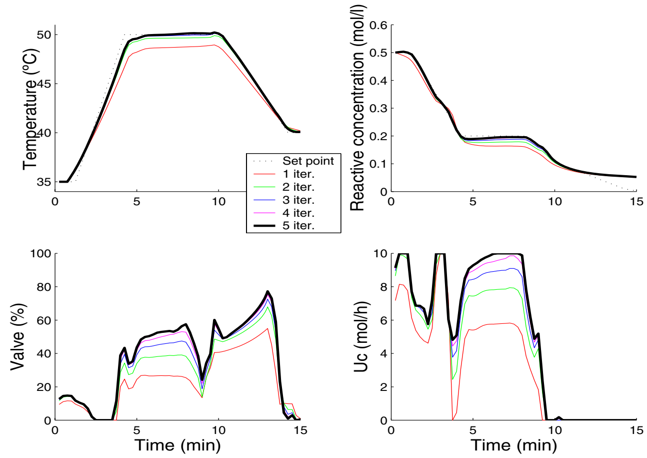

Fig. 4. Experiments with INMPC

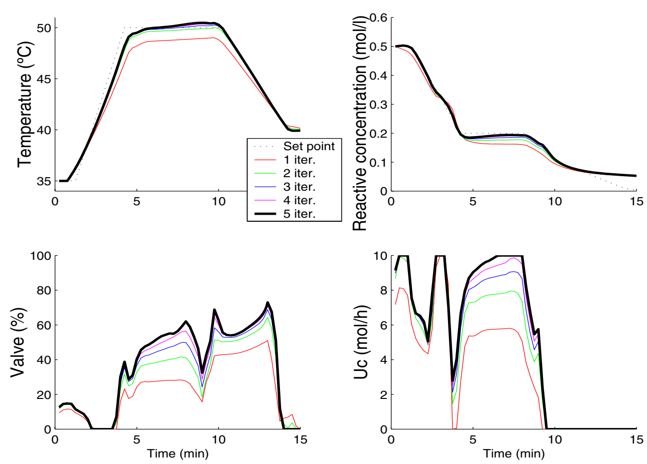

Fig. 5. Experiments with INMPC with a disturbance in inlet cooling water temperature

linear MPC is not a quite good method in this concrete case, even modifying the controller parameters. The mismatch between the linear model and the real one is too large, therefore, the controller cannot achieve better trajectory tracking errors.

Later, INMPC controller is tested, using parameters given in Table II and unitary horizons that guarantee stability. Some batches are presented in Fig. 4. System trajectories are quite close to reference trajectories after only three iterations. It must be said that perfect tracking is not possible in this case, because of the presence of physical constraints. The controller is able to minimize the tracking error after several batches.

A disturbance test is also realized. A variable inlet water temperature is introduced into the plant. The result is presented in Fig. 5. The disturbance amplitude is around 6^oC. It cannot be much bigger, mainly because of the actuator saturation, which would produce an unreachable reference trajectory. Nevertheless, the controller is able to compensate repetitive disturbances quite well. Notice that unitary horizon are used to guarantee stability as proven in Section III-B and better results could be obtained with longer values of it.

V. Conclusions

An iterative nonlinear multivariable constrained MPC controller has been tested in a simulated semibatch chemical reactor. The controller has shown capabilities to learn the optimal trajectory after a few iterations, giving a better fit than a linear non-iterative MPC controller.

The controller has applications in repetitive disturbance rejection, which are adequately cancelled. If these disturbances are not additive, they have to be small enough. In this application, a disturbance in inlet water temperature has been studied, getting acceptable results with the INMPC controller.

A stability proof for unitary control horizon is given.

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