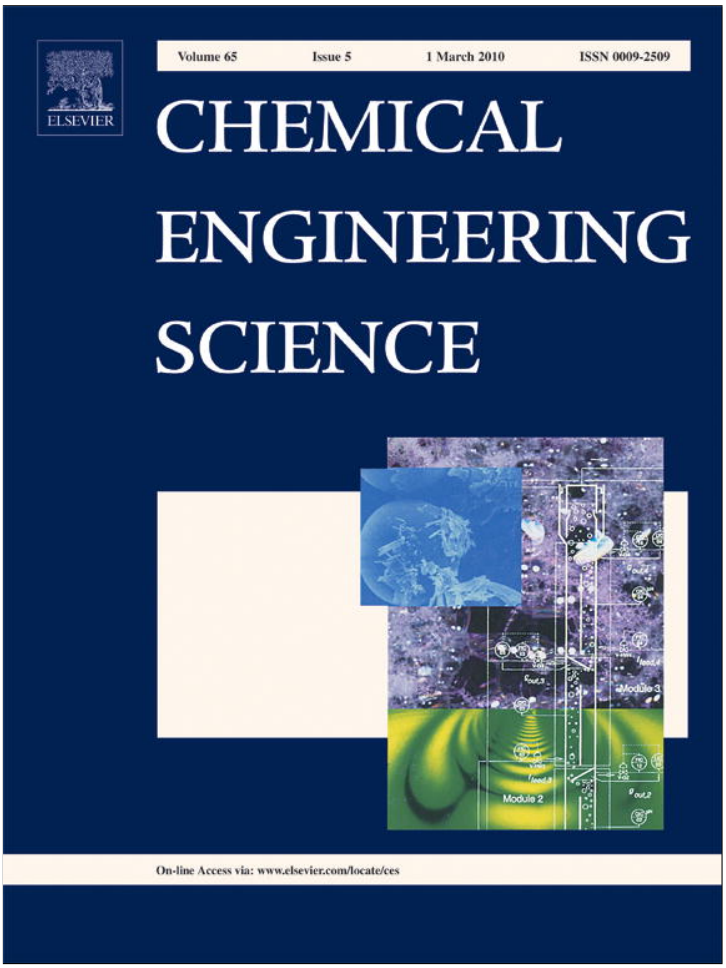

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# Continuous-time Wiener-model predictive control of a pH process based on a PWL approximation

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ABSTRACT

This paper deals with a novel formulation of continuous-time model-predictive control for nonlinear systems. A nonlinear-mapping approximation, employing a PWL approximation, is also an integral part of the control scheme, and thus removes the need for output-function invertibility. The analytical formulation of the control law makes it possible to use the method in practice, especially in the chemical industry. An illustrative experiment is conducted to compare the proposed approach with the method of nonlinear $H_\infty$ control of a pH-neutralization process.



## 1. Introduction

Linear-model predictive control (LMPC) is a well-known and well-established industry standard. The generic term LMPC refers to a class of control algorithms in which a linear dynamic process model is used to predict and optimize process performance. Having its roots in the 1970s, LMPC is nowadays commercially available primarily for controlling constrained multivariable processes (Henson, 1998). However, many processes are sufficiently nonlinear to render the successful application of LMPC impossible. There are two main cases where a nonlinear type of control has to be considered: a moderately nonlinear process with large operating regimes (e.g., multi-grade polymer reactors) and a highly nonlinear process that operates near a fixed operating point (high-purity distillation columns). The need for high-quality control of such processes led to the development of the nonlinear-model predictive control (NMPC) methods. In general, NMPC (and also LMPC) is an optimization-based control strategy where a sequence of control moves is computed to minimize an objective function that includes predicted future values of the controlled outputs. The predictions in each computation step are obtained from a nonlinear process model. The majority of methods rely on the so-called nonlinear receding horizon principle (Mayne and Michalska, 1990; Henson, 1998), where feedback is included by implementing only the manipulated inputs computed for the present time step, then moving the prediction horizon forward one step and repeating the procedure with the new measurements. This strategy yields an open-loop optimal controller. There is a wide variety of existing NMPC methods, for example in Maner et al. (1996), Badgwell (1997) and Norquay et al. (1999) in the discrete-time framework, and in Demircioglu and Gawthrop (1991), Chen et al. (2003) and Magni and Scattolini (2004) in the continuous-time framework. For the state of the art of NMPC methods the reader is referred to the papers by Morari and Lee (1999) and Henson (1998). Issues like the stability and optimality of the NMPC methods were discussed in detail by Mayne et al. (2000).

NMPC requires the availability of a suitable nonlinear dynamic model of the process, and the accuracy of the model is of paramount importance. There are two general classes of nonlinear models used: fundamental models, based on transient mass, energy, and momentum balances, and empirical models, such as Hammerstein, Wiener, Volterra, and fuzzy models, which are derived on the basis of empirical data from the process. The majority of NMPC methods are derived in discrete time, and therefore need discrete-time models. On the other hand, the majority of models are given in continuous form and need to be discretized. The drawbacks of discretizing nonlinear continuous-time models were discussed by Pearson (2003); and they include structural changes, the dependence of the stability on the model's parameters and the initial states, and the inaccurate system intersample behavior (Magni and Scattolini, 2004). Because of this our proposed method is based on a continuous-time model of a

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process, and the model can be obtained either directly from a first-principle nonlinear process model or by identification.

The proposed approach in this paper tackles the control of nonlinear processes using continuous-time nonlinear model-based predictive control. The advantage of the proposed approach is in the continuous-time framework which is used here. This means that the sampling time, when applying the algorithm on digital hardware and the digital redesign is made, can be selected after the analogue control system is designed and, thus the continuous-time closed-loop bandwidth is known. The approach in continuous-time enables also a multi-sampling-rate digital implementation.

Special attention is given to the processes that can be efficiently modelled using a Wiener-type model. The linear dynamics are derived from the first-principle nonlinear model; and the nonlinear output function is calculated from the steady-state equations and approximated by piecewise-linear (PWL) functions. The model-output prediction is calculated using a Taylor-series expansion of the Wiener model. The Wiener-PWL structure makes it possible to form the prediction in an exact analytical form consisting of a constant linear, and a variable nonlinear, part. The former is a constant matrix that can be calculated off-line, and the latter is a scalar product representing the gradient of the PWL-approximation of the nonlinearity in the Wiener model. The receding-horizon strategy was combined with a cost function that minimizes the difference between the future-output-prediction error and the model-prediction error. Consequently, this brings the following benefits to the control-law calculation:

- The law is derived in a closed analytical form, which resolves the issue of nonlinear optimization and achieving the global optimum in each calculation step.
- The reduction of the calculation of the control signal to a scalar product and an inverse of a scalar (everything else can be calculated offline) brings a significant reduction in the computational complexity. This makes it possible to consider the proposed method for practical applications.
- The nonlinearity is inherently included in the law; compared to the method in Norquay et al. (1999); this removes the need to invert the NL approximation.

The outline of the paper is as follows. In Section 2 the PWL functions are introduced and the model-output prediction is formulated in the continuous-time domain. In Section 3 the nonlinear predictive control law is derived, and some stability issues are also discussed. Section 4 presents the pH-neutralization process and gives a comparison of the closed-loop-control results for the proposed approach and a nonlinear $H_\infty$ approach. Section 5 concludes the paper with some directions for future work.

## 2. Problem statement

Let us assume a nonlinear continuous-time system

$$\dot{x}_p(t) = f(x_p(t), u(t)),$$

$$y_p(t) = g(x_p(t)),$$

$$y_p(0) = y_{p0}, \quad y_p(T) = y_{pT}, \tag{1}$$

where $f : \mathbb{R}^n \to \mathbb{R}^n$ and $g : \mathbb{R}^n \to \mathbb{R}$ are smooth functions, $x_p \in \mathbb{R}^n$ is a vector of $n$ state variables, $u \in \mathbb{R}$ is a process input and $y_p \in \mathbb{R}$ is a process output. An optimal control can in general be seen as the solution of

$$\min_{u \in \Omega} J(x_p, y_p, t) = \min_{u \in \Omega} \int_0^T F(x_p, y_p, t)\, dt, \tag{2}$$

where $F \in \mathbb{R}^+$ is a cost function that satisfies the optimality criteria, and $\Omega$ is the set of admissible control signals. In other words, we have to design a controller that asymptotically stabilizes a closed-loop system in such a way that the process output, $y_p(t)$, optimally follows the prescribed reference trajectory, $y_r(t)$, according to the given performance index $J$. However, dealing with nonlinear continuous-time systems, the problem setup in (2) leads to solving the Hamilton–Jacobi–Bellman partial differential equations (Bertsekas, 1995). The solution of the HJB PDE system is usually obtained numerically (Chen et al., 2003), which is computationally too expensive to be considered for practical control applications. As an alternative, in this paper we avoid solving the system of PDE by using the moving-horizon control concept (Mayne and Michalska, 1990; Clarke et al., 1987; Chen et al., 2003). The idea is to calculate the optimal control sequence in each time instant by minimizing the given performance index, which involves open-loop prediction of the model output and the predicted reference signal. The initial conditions are the reference, the model output and the process measured output at the given time instant $t$, and the closed-form analytical solution is open-loop optimal. After applying the calculated input signal $u(t)$, the time-frame is moved to the next time instant.

### 2.1. Dealing with a nonlinearity in a system by using the Wiener model and a PWL approximation

The system's nonlinearity presents an additional difficulty in terms of system modelling and control. This problem can be successfully solved by using a Wiener-type system that has a special structure that facilitates its application to model-based predictive control. The Wiener system has the structure of a dynamic linear block followed by a static nonlinearity

$$\dot{x}(t) = Ax(t) + Bu(t),$$

$$v(t) = Cx(t),$$

$$y(t) = h(v(t)), \tag{3}$$

where $A \in \mathbb{R}^n \times \mathbb{R}^n$, $B \in \mathbb{R}^n$, and $C \in \mathbb{R}^n$ are the state-space matrices, $h : \mathbb{R} \to \mathbb{R}$ denotes the static nonlinear mapping and $y \in \mathbb{R}$ is the process-model output. The variable $v(t) \in \mathbb{R}$ represents the intermediate variable that does not necessarily have a clear physical meaning. Notice also that the functions $h$ from (3) and $g$ from (1) are not necessarily equal because, in general, the static nonlinearity in the model also covers the effects of the nonlinearity in the states of the process. Different approaches to Wiener-model identification are found in the literature. The most frequently used is the nonlinear–linear (N–L) approach, which is the most comprehensible and ensures an accurate description of the static nonlinearity (Gerkšič et al., 2000). This approach requires steady-state data. The excitation signal has to be designed to obtain the information about the steady-state behavior of the system. The steady-state curve of the observed system is obtained from data pairs of the input variable $u$ and the corresponding output variable $y$ during steady-state, $(u_{si}, y_{si})$. The data set of steady-state points is a non-equidistant set of data and it is spread around the nominal static curve. This set of steady-state points is now modelled using PWL approach.

Using the PWL approximation, the process-model output is defined as

$$y(t) = \hat{h}(v(t)) = \Theta^T \Lambda(v(t)), \tag{4}$$

where $\Theta^T \in \mathbb{R}^{\sigma+1}$ and $\Lambda \in \mathbb{R}^{\sigma+1}$. Using this, any nonlinear function $h$ can be uniquely represented by the segmentation of its input domain (Julián, 1999). Let us consider the segmentation into $\sigma$ segments by the boundary parameters $\alpha_i$, with $\alpha_0 \le \alpha_1 \le \cdots \le \alpha_{\sigma-1}$. The elements of the basis functions can be expressed as

$$\Lambda(v) = \begin{bmatrix} 1 \\ \frac{1}{2}(v-\alpha_0+|v-\alpha_0|) \\ \vdots \\ \frac{1}{2}(v-\alpha_{\sigma-1}+|v-\alpha_{\sigma-1}|) \end{bmatrix} \tag{5}$$

and the vector of the parameters is defined as

$$\Theta^T = [\theta_0, \theta_1, \ldots, \theta_\sigma]. \tag{6}$$

The locations of the boundaries are determined according to the data distribution, usually by clustering algorithms (Pal and Bezdek, 1995), and the vector of the parameters can be calculated using common least-square algorithms. By calculating the boundaries and the vector of the parameters the static nonlinear block is defined. Secondly, the linear dynamic block has to be defined. The linear block can be defined, as it has been realized in our case, directly from the mathematical model or by identification from the obtained data. The mathematical model of the pH process has the structure of Wiener type. Therefore, the linear part of the model, can been derived directly from the nonlinear differential equations by linearization around the chosen operating point. This procedure is in more detail given in Section 4. The identification approach requires the data of the input signal $u$ and the output signal $v$. Since the static model was obtained in the steady state and the gain of linear model block is assumed to be unity, the static mapping from $v$ to $y$ (marked with $h$ in (3)) is equivalent to the static mapping from $u_s$ to $y_s$ that is described by the PWL model. To calculate the intermediate variable $v$ from $y$ the inverse static nonlinearity is required. The output variable $y$ is mapped by the inverse static nonlinearity to obtain the estimated intermediate variables $\tilde{v}$. The linear model block is then formed as the relation between the input variable $u$ and the intermediate variable $v$. The parameters of this block are estimated using the identification algorithm on the data pairs $(u, \tilde{v})$.

### 2.2. Continuous-time prediction of the model output

In general the objective of a model-predictive control law is to drive the predicted future output of a system as close as possible to the future reference, subject to the input constraints. In the continuous-time framework this implies that the predictions of the reference and the process output must be either known or estimated. Let us define the reference model by the triple in state-space as $A_r$, $B_r$ and $C_r$, and denote the reference signal $w(t)$. In the moving time frame the model-output prediction at time $\tau$ can be approximated by a truncated Taylor series expansion

$$y(t+\tau|t) = \Gamma^T(\tau)Y(t), \tag{7}$$

where the vectors $\Gamma \in \mathbb{R}^{n_y+1}$ and $Y \in \mathbb{R}^{n_y+1}$ are given by

$$\Gamma(\tau) = \left[1 \;\; \tau \cdots \frac{\tau^i}{i!} \cdots \frac{\tau^{n_y}}{n_y!}\right]^T, \tag{8}$$

$$Y(t) = [y(t) \;\; y^{[1]}(t) \ldots \;\; y^{[i]}(t) \;\; \ldots y^{[n_y]}(t)]^T, \tag{9}$$

where $n_y$ is the output order, and $y^{[i]}(t)$ stands for the $i$th derivative of $y(t)$ with respect to $t$. Analogously, the reference-model output prediction can be defined as

$$y_r(t+\tau|t) = \Gamma^T(\tau) \cdot r \cdot w(t), \tag{10}$$

where the vector of the Markov parameters $r \in \mathbb{R}^{n_y+1}$ is defined as

$$r = [0 \;\; C_rB_r \;\; C_rA_rB_r \;\; \cdots \;\; C_rA_r^{n_y-1}B_r]^T. \tag{11}$$

Let us investigate the model-output prediction (7) in the PWL approximation case. The $i$th derivative of $y(t)$ is defined as

$$y^{[i]}(t) = \Theta^T \frac{d\Lambda(v)}{dv} CA^i x(t) + \Theta^T \frac{d\Lambda(v)}{dv} [CA^{i-1}B \;\; \ldots \;\; CB]U(t), \tag{12}$$

where $U(t)$ stands for

$$U(t) = [u(t) \;\; u^{[1]}(t) \ldots u^{[i]}(t)]^T \tag{13}$$

and where

$$\frac{d\Lambda(v)}{dv} = \begin{bmatrix} 0 \\ \frac{1}{2}(1+\mathrm{sign}(v-\alpha_0)) \\ \vdots \\ \frac{1}{2}(1+\mathrm{sign}(v-\alpha_{\sigma-1})) \end{bmatrix}. \tag{14}$$

Because all of the higher derivatives of the PWL mapping with respect to $v$ are equal to 0 ($d^2\Lambda(v)/dv^2 = \cdots = d^n\Lambda(v)/dv^n = 0$), all of the higher powers of $\dot{v}(t)$ are cancelled as well. Let us define the control order as follows.

**Definition 1.** The control order in the continuous-time predictive control is said to be $n_u$ if the following is valid: $u^{[n_u]}(t+\tau) \neq 0$, $\forall \tau \in [0, T]$ and $u^{[i]}(t+\tau) = 0$, $\forall i > n_u, \tau \in [0, T]$ where $u^{[n_u]}(t+\tau)$ stands for $n_u$ th derivative of $u(t+\tau)$ with respect to $\tau$. The control order defines the allowable set, $\mathcal{U}$, of the optimal control input in the receding horizon frame, and hence imposes the constraints on $u(t+\tau)$.

**Remark 1.** In this paper the output order $n_y$ and the control order $n_u$ are two design parameters. However, in some papers limitations in the choice of $n_y$ are used (Chen et al., 2003). If the relative order of a process is denoted $\rho$, $n_y$ should be at least of the same order as $n_u+\rho$ if the $n_u$ th derivative of the control signal is to appear in the prediction, i.e., $n_y \ge n_u+\rho$. This is due to the fact that $n_u$ defines the highest derivative of the control signal that is assumed to drive the process in the moving-frame horizon, where the minimization of the given cost function takes place.

The control vector $U(t)$ of the $n_u$th order is then defined as

$$U(t) = [u(t) \;\; u^{[1]}(t) \ldots u^{[n_u]}(t)]^T. \tag{15}$$

Combining Eqs. (7)–(9) with (12), the prediction of the model output $y(t+\tau|t)$ at time $\tau$ is given by

$$y(t+\tau|t) = \Gamma^T[Py(t) + q(v)K_qx(t) + q(v)K_hU(t)], \tag{16}$$

where $P \in \mathbb{R}^{n_y+1}$, $K_q \in \mathbb{R}^{n_y+1} \times \mathbb{R}^n$, and $K_h \in \mathbb{R}^{n_y+1} \times \mathbb{R}^{n_u+1}$ are defined as

$$P = [1 \;\; 0 \;\; \ldots \;\; 0]^T, \tag{17}$$

$$K_q = [0 \;\; (CA)^T \;\; (CA^2)^T \;\; \ldots \;\; (CA^{n_y})^T]^T \tag{18}$$

and

$$K_h = \begin{bmatrix} 0 & \cdots & \cdots & 0 \\ CB & 0 & \cdots & 0 \\ CAB & CB & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ CA^{n_y-1}B & CA^{n_y-2}B & \cdots & CA^{n_y-1-n_u}B \end{bmatrix}. \tag{19}$$

The matrices $K_q$ and $K_h$ can be calculated offline as they only depend on the linear-model dynamics. Scalar function $q(v) \in \mathbb{R}$ represents the gradient of the static output mapping, and is

calculated as

$$q(v) = \Theta^T \frac{d\Lambda(v)}{dv}. \tag{20}$$

## 3. Nonlinear Wiener-type model-predictive control

The performance index adopted in this paper is given by

$$V = \int_0^T \|y_r(t+\tau) - y_p(t+\tau|t)\|^2 \, d\tau. \tag{21}$$

This means that in each time instant $t$ the predictions of the reference response $y_r(t+\tau)$ and the process output $y_p(t+\tau)$ are calculated for the prediction horizon $T$. The index is similar to the one in Chen et al. (2003); the difference is that here we use the prediction of the measured process output. This is justified for practical applications where it is necessary for the measured output to follow the reference-model output. The problem is that we cannot assess the future process output from the measurements. Rather, we will estimate its future behavior from the available signals in the time instant $t$,

$$y_p(t+\tau|t) = y_p(t) - y(t) + y(t+\tau|t), \tag{22}$$

following the assumption that the model and the process increments are equal when driven by the same input signal $u(k)$ (cf. the assumptions of predictive functional control in Škrjanc and Matko, 2001). Furthermore, we can inherently force the process output to follow the reference dynamics. This is done by assuming that the future control error is given by

$$e(t+\tau) = \Gamma^T r(w(t) - y_p(t)), \tag{23}$$

implying that the output error should decay exponentially at the rate given by the product $\Gamma^T r$. With this change the proposed control strategy is based on a minimization of the difference between the future control error and the difference between the predicted model output at the time horizon $\tau \in [0, T]$ and the current model output:

$$\varepsilon(t,\tau) = e(t+\tau) - (y(t+\tau|t) - y(t)). \tag{24}$$

The control law will be obtained by minimizing the cost function

$$V = \int_0^T \varepsilon(t,\tau)^T \varepsilon(t,\tau) \, d\tau. \tag{25}$$

Given the prediction of the process-model output in (16), the cost function (25) is

$$V(U,v,t) = \int_0^T (rw - ry_p - qK_hU - qK_qx)^T \Gamma\Gamma^T (rw - ry_p - qK_hU - qK_qx) \, d\tau. \tag{26}$$

Notice that, taking into account the calculation in (16), the product $\Gamma^T P y(t)$ is equal to $y(t)$, and hence cancels the last term of (24). The minimization of the cost function $V(U,v,t)$ according to the control variable $U$ ($\partial V/\partial U = 0$) results in the continuous-time model-predictive control law. The variables $q$, $w$, $y_p$, and $x$ are only evaluated at the beginning of the time frame; therefore, the only variable that depends on $\tau$ is $\Gamma$. Hence, we can define the matrix $\overline{\Gamma} \in \mathbb{R}^{n_y+1} \times \mathbb{R}^{n_y+1}$ as

$$\overline{\Gamma} = \int_0^T \Gamma\Gamma^T \, d\tau. \tag{27}$$

Given that the general term of the symmetric matrix $\Gamma\Gamma^T$ is $T^{i-1+j-1}/((i-1)!(j-1)!)$, Eq. (27) can be rewritten as

$$\overline{\Gamma} = \begin{bmatrix} \gamma_{(1,1)} & \cdots & \gamma_{(1,n_y+1)} \\ \vdots & \ddots & \vdots \\ \gamma_{(n_y+1,1)} & \cdots & \gamma_{(n_y+1,n_y+1)} \end{bmatrix}, \tag{28}$$

where

$$\gamma_{(i,j)} = \frac{1}{(i+j-1)(i-1)!(j-1)!} T^{i+j-1} \tag{29}$$

for every $i,j = 1,\ldots,n_y+1$. The minimization of the cost function $V(U,v,t)$ is given as

$$\frac{\partial V}{\partial U} = -2q(v)K_h^T\overline{\Gamma}[r(w - y_p) - q(v)K_hU - q(v)K_qx] = 0 \tag{30}$$

and the control vector becomes

$$U = q(v)^{-1}(K_h^T\overline{\Gamma}K_h)^{-1}K_h^T\overline{\Gamma}[r(w - y_p) - q(v)K_qx]. \tag{31}$$

However, when we apply the calculated control signal we only need the first element of the control vector. Let us now define the first row of the matrix $(K_h^T\overline{\Gamma}K_h)^{-1}K_h^T\overline{\Gamma} \in \mathbb{R}^{n_u+1} \times \mathbb{R}^{n_y+1}$ as $\kappa$. The control law of the nonlinear Wiener-type model-predictive control is now given by

$$u(t) = \frac{1}{q(v)}\kappa[r(w - y_p) - q(v)K_qx]. \tag{32}$$

What makes this control strategy suitable for practical applications is that the computational load is only on the online calculation of the scalar product $\Theta^T d\Lambda(v)/dv$, whereas $\kappa$, $r$ and $K_q$ can be calculated off-line.

### 3.1. Existence of solution

Investigating the term $\varepsilon(t,\tau)$ in the cost function (25), it is clear that the critical point in the optimization is the difference between the process increment and the model increment, i.e., between $e(t+\tau)$ and $y(t+\tau|t) - y(t)$ in (24). Theoretically, it is possible that both terms go to infinity, the difference stays close to zero, so that the minimum is achieved, and the solution for $u$ does not change. This is why we also have to define the set of admissible output signals corresponding to the given set of admissible controls. However, in practical cases it is not probable that both the process and the model would go to infinity while driven by the same signal $u \in \Omega$.

Solving (31) gives us the optimal vector of the input signal and its derivatives with respect to the open-loop cost function. The key part of the equation is the inverse $(K_h^T\overline{\Gamma}K_h)^{-1}$. To get a unique solution of the optimization problem, the inverse must exist. However, we cannot ensure the existence of the inverse for all possible choices of the design parameters $n_y$ and $n_u$. Furthermore, the products $CA^\zeta B$, where $\zeta$ depends on $n_y$ and $n_u$, can also be equal to zero, depending on the relative order of the process. The existence of the solution of (31) is stated by the following theorem.

**Theorem 1.** *The optimal analytical solution* (32) *of the CWMPC control law with stable linear part exists for any non-zero prediction horizon T if, and only if, the difference between the output and the input prediction order is greater than or equal to the relative order of the linear part of process model, i.e.,* $n_y - n_u \geq \rho$.

**Proof.** In the analytical solution given by (32) the main problem is inversion of the term $K_h^T\overline{\Gamma}K_h$ which is a $(n_u+1)$- by-$(n_u+1)$, where matrix $K_h$ consists of elements of the form $CA^\zeta B$ where $\zeta = 0,\ldots,n_y - n_u - 1$. The relative order $\rho$ of a linear part of process model affects the products $CA^\zeta B$ such that they are zero for $\zeta < \rho - 1$. The matrix $K_h^T\overline{\Gamma}K_h$ is by definition invertible if, and only if, it has a full rank, i.e., $n_u+1$ linearly independent columns.

Considering the case when $n_y - n_u < \rho$. The last element of the $(n_u+1)$ th column in matrix $K_h$, defined as $CA^{\rho-1}B$ is equal zero. The columns in the matrix $K_h$ have increasing exponent $\zeta$. This means that also all the previous elements of the last column in matrix $K_h$ equal zero, and the matrix $K_h$ has at least one zero

column. Since $\overline{\Gamma}$ is symmetrical, the product $K_h^T \overline{\Gamma} K_h$ is singular and the solution to (31) does not exist. □

## 4. Simulation example

The proposed method was tested on a chemical process with marked nonlinearity. A mathematical model of a pH neutralization process was adopted from Galán et al. (2000). The example consists of a neutralization reaction between a strong acid (HA) and a strong base (BOH) in the presence of a buffer agent (BX). The neutralization takes place in a continuous stirred tank reactor (CSTR) with a constant volume $V$. It is a well-known fact that the pH processes are extremely difficult to deal with due to their highly nonlinear behavior with respect to different titration curves.

Fig. 1 shows a scheme of the continuous pH neutralization process. An acidic solution with a time-varying volumetric flow $q_A(t)$ of a composition $x_{1i}(t)$ is neutralized using an alkaline solution with volumetric flow $q_B(t)$ of known composition consisting base $x_{2i}$ and buffer agent $x_{3i}$. Due to the high reaction rates of the acid–base neutralization, chemical equilibrium conditions are instantaneously achieved. Moreover, under the assumption that the acid, base and buffer are strong enough, total dissociation of the three compounds takes place. The process-dynamics model can be obtained by considering the electroneutrality condition (which is always preserved) and through mass balances of equivalent chemical species (known as chemical invariants). For this specific case, the dynamic behavior of the process can be described considering the state variables

$$x_1 = [A^-],$$

$$x_2 = [B^+],$$

$$x_3 = [X^-]. \tag{33}$$

Therefore, the mathematical model of the process can be written in the following way:

$$\dot{x}_1 = \frac{1}{\theta}\cdot(x_{1i}-x_1) - \frac{1}{V}\cdot x_1 \cdot u,$$

$$\dot{x}_2 = -\frac{1}{\theta}\cdot x_2 + \frac{1}{V}\cdot(x_{2i}-x_2)u,$$

$$\dot{x}_3 = -\frac{1}{\theta}\cdot x_3 + \frac{1}{V}\cdot(x_{3i}-x_3)u, \tag{34}$$

$$g(x,\xi) = \xi + x_2 + x_3 - x_1 - \frac{K_w}{\xi} - \frac{x_3}{1+\frac{K_x\xi}{K_w}} = 0, \tag{35}$$

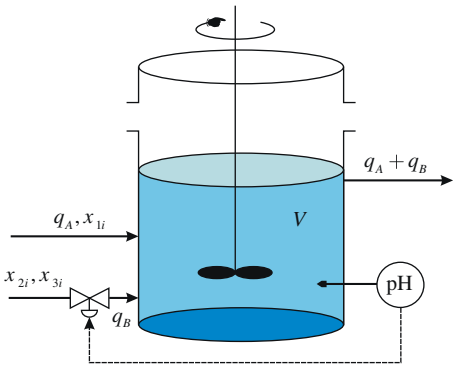


**Fig. 1.** pH-neutralization process.

where $\xi = 10^{-pH}$, $\theta = V/q_A$, and $u = q_A/q_B$. $K_w$ and $K_x$ are the dissociation constants of the buffer and water, respectively. The parameters of the system represented by (34)–(35) are $x_{2i} = 0.0020$ mol NaOH/L, $x_{3i} = 0.0025$ mol $NaHCO_3$/L, $K_x = 10^{-7}$ mol/L, $K_w = 10^{-14}$ mol$^2$/L$^2$ and $V = 2.5$ L. Eq. (35) takes the standard form of the widely used implicit expression that connects pH with the states of the process, and it can also be rewritten to a third-order polynomial form:

$$g(x,\xi) = \xi^3 + (K_w/K_x + x_2 + x_3 - x_1)\xi^2 + (x_2 - x_1 + K_x)\xi - K_w^2/K_x = 0. \tag{36}$$

Before proceeding with the controller design, some important aspects, related to the dynamic behavior of the neutralization reactor, must be pointed out to exploit its particular structure. When mathematical models based on first principles are employed for the design of controllers, the variables involved have a clear physical meaning and their ranges are at least partially known. For the neutralization reactor, due to the instantaneous character of the acid-base reactions, where equilibrium conditions can be justified, it seems that the only dynamics involved is associated with the mixing phenomena. This implies that the concentrations of different chemical species that take part in the reaction vary from zero to a limit value. Therefore, by defining the admissible-input set, the admissible-output set is also defined (cf. Fig. 2).

**Remark 2.** The dynamics of the neutralization reactor resides in a bounded and closed set, where $x_{p,j} \in [0, x_{p,j}^+]$ is the concentration invariant set.

**Remark 3.** Due to the invariance of the concentration set, the output set is also a bounded and a closed set, where $y_p \in [y_p^-, y_p^+]$.

The Wiener model is derived directly from the first-principle model. The approach is particularly appealing for the control of chemical processes because first principles give a straightforward way of obtaining nonlinear continuous-time models. Considering the system in (3), a model in the Wiener form can be obtained by linearization of the functions $f$ and $g$ around a given point, normalizing the model's steady-state gain (the Wiener model should have a steady-state gain equal to 1), and calculating the steady-state solutions of the output function $g$ to get a nonlinear output mapping.

The linear approximation for the nonlinear system (34) and (35) is given by

$$A = \begin{bmatrix} -\frac{1}{\theta}(1+u_s) & 0 & 0 \\ 0 & -\frac{1}{\theta}(1+u_s) & 0 \\ 0 & 0 & -\frac{1}{\theta}(1+u_s) \end{bmatrix},$$

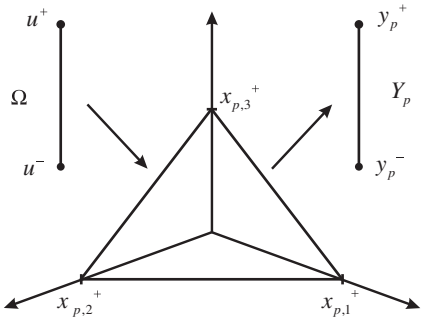


**Fig. 2.** Invariant species concentration set for the neutralization reactor.

$$B=\begin{bmatrix} -\frac{1}{\theta}x_{1,s} \\ \frac{1}{\theta}(x_{2i}-x_{2,s}) \\ \frac{1}{\theta}(x_{3i}-x_{3,s}) \end{bmatrix}, \quad C=\begin{bmatrix} \frac{\partial\eta}{\partial x_1} & \frac{\partial\eta}{\partial x_2} & \frac{\partial\eta}{\partial x_3} \end{bmatrix}, \tag{37}$$

where

$$\frac{\partial\eta}{\partial x_k}=\frac{\partial h(x)/\partial k}{\xi\ln(10)\partial h(x)/\partial\xi}, \quad k=1,2,3. \tag{38}$$

From the polynomial pH equation (35) the following terms are easily calculated:

$$\frac{\partial h(x)}{\partial\xi}=3K_x\xi^2+2[K_w+(x_3+x_2-x_1)K_x]\xi+(x_2-x_1-K_x)K_w,$$

$$\frac{\partial h(x)}{\partial x_1}=-K_x\xi^2-K_w\xi, \quad \frac{\partial h(x)}{\partial x_2}=-K_x\xi^2+K_w\xi, \quad \frac{\partial h(x)}{\partial x_3}=K_x\xi^2. \tag{39}$$

The nonlinear functionality for the input–output map is given by

$$x_{k,s}=\frac{1}{1+u_s}x_{k,i}, \quad k=1,2,3, \tag{40}$$

$$\xi+x_{2,s}+x_{3,s}-x_{1,s}-\frac{K_w}{\xi}-\frac{x_{3,s}}{1+\frac{K_x\xi}{K_w}}=0, \tag{41}$$

where $u_s$ and $x_{k,s}$ represent the input and the states in the linearization point. The process input was assumed to be bounded by the interval $0\le u(t)\le 1$; therefore, we used 200 equidistant steady-state points from the intermediate-variable range $v\in[0,1]$ for the input set. A PWL approximation of the static output curve was then obtained by optimizing the PWL parameters using the steady-state points.

One should also note the diagonal structure of the matrix $A$. In Galán et al. (2000), it was shown that the dynamics can be successfully approximated by a first-order model. In terms of a system-transfer function it would mean that two zeros and two poles lie in the same position and can be cancelled. Therefore, linearization around the steady-state point $u_s=0.3692$ (pH = 7) gave the following values:

$$A=-0.5477, \quad B=1, \quad C=0.5477. \tag{42}$$

For the approximation we assumed eight PWL simplices. The positions of the simplex border points $\alpha_i$, $i=1,2,\ldots,8$ and the PWL gains in $\Theta\in\mathbb{R}^9$ were calculated using a least-squares optimization. The optimization yielded

$$\alpha=[0 \;\; 0.1879 \;\; 0.2526 \;\; 0.2805 \;\; 0.3233 \;\; 0.5586 \;\; 0.6337 \;\; 0.7373],$$

$$\Theta^T=[2.8842 \;\; 3.0618 \;\; 7.6707 \;\; 58.8349 \;\; -55.2754 \;\; -8.4142 \;\; 15.7595 \;\; -16.4792 \;\; -3.7013].$$

The resulting approximation $\hat{h}(v)$ is compared to the identified mapping $h(v)$ in the upper diagram of Fig. 3. In Fig. 4 the input and output signals of the process and the model in the case of open-loop simulation experiment are shown. To show the accuracy of the described Wiener model also the relative modelling error is presented in Fig. 5. The relative modelling error $e_m$ is described by the following equation:

$$e_m(t)=\frac{y_p(t)-y(t)}{y_p(t)}. \tag{43}$$

It is shown that the corresponding Wiener model gives accurate model of pH process in a wide operating regime.

The proposed method was compared to the method described in Biagiola et al. (2004). In this paper a robust $H_\infty$ compensator for controlling an SISO Wiener system was developed. The controller also took the form of a Wiener model. The design approach

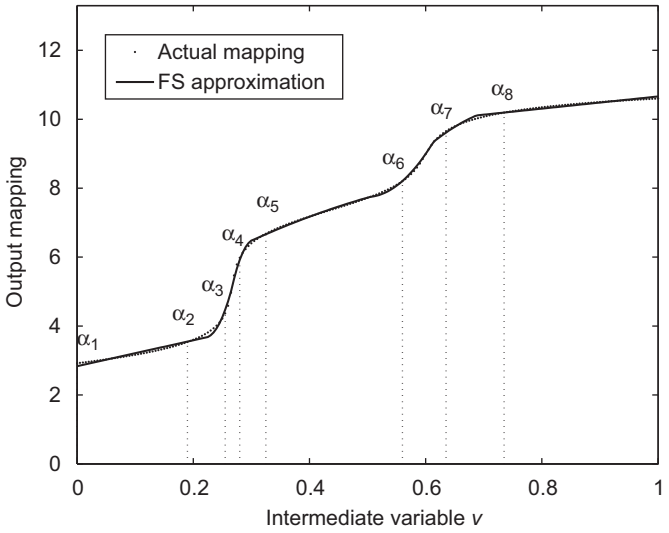


**Fig. 3.** Comparison of the PWL approximation and the actual mapping.

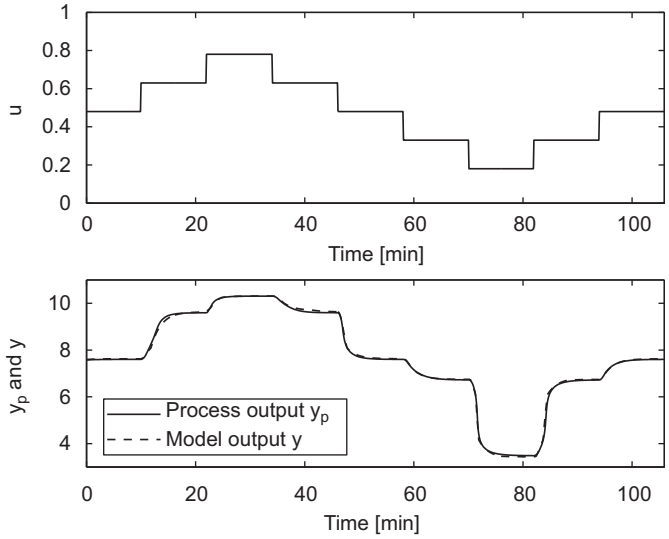


**Fig. 4.** Comparison between open-loop process output and process model (lower) and the open-loop input to the process (upper).

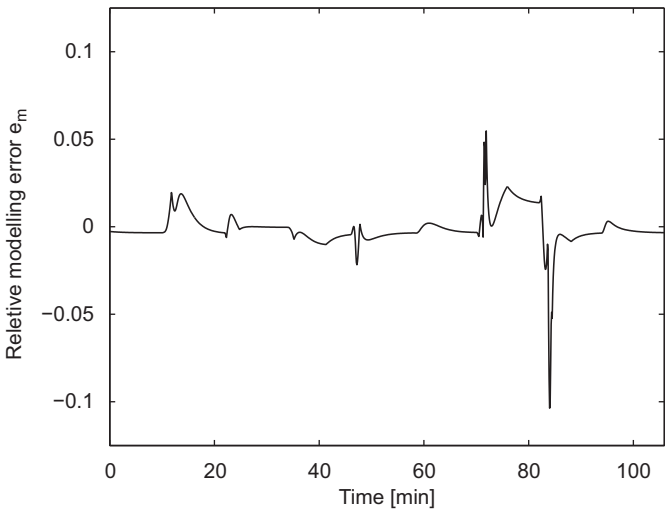


**Fig. 5.** Relative modelling error $e_m(t)$.

consisted of an approximation of the nonlinear gain using a piecewise linear (PWL) function and of using a linear controller for each sector obtained from this approximation. Therefore, the general controller structure can be stated as a linear dynamic compensator in series with a PWL static gain.

The control-design parameters for the proposed method were chosen as follows: $n_u = 1$, $n_y = 4$, $T = 0.3$ min, $A_r = -1/0.9$, $B_r = 1$, and $C_r = 1/0.9$. The choice of $n_y$ and $T$ is connected with the desired model-prediction accuracy, as was discussed in Oblak and Škrjanc (2006). The time constant of the reference model was chosen such that the closed-loop response would be approximately as fast as in Biagiola et al. (2004).

A closed-loop experiment with a piecewise-constant reference signal was conducted. The results, presented in Fig. 6, imply that the process output successfully follows the reference in the whole operating region in both cases. However, it is clear that in the case of the proposed method the overall performance is better. The overshoot is significantly lower in the CTWMPC case, and is not dependent on the region of the process output. In terms of the quadratic-integral cost function, we achieved a 30% decrease in the tracking error. The corresponding input variables are shown in Fig. 7. Note the impulse-like behavior of the CTWMPC control signal in the time after the step reference changes—for practical applications with slow actuators this can be avoided by using a reference model with higher time constant.

To test the method in a more practical environment, a white noise with a variance of 0.01, filtered through a first-order filter with a time constant $T_f = 0.1$ min, was added to the process output. Figs. 8 and 9 present the results.

The disturbance rejection mode of the proposed algorithm was tested by adding the unmeasured input disturbance as proposed on Figs. 10 and 11. By the means of simulation it has been proven that also the disturbance rejection properties of the proposed control algorithm are suitable.

At the end the simulation experiment is given, where the value of the control signal is constrained as follows: $0 \le u(t) \le 1$ and $-0.15/\text{min}^{-1} \le du(t)/dt \le 0.15\,\text{min}^{-1}$. The simulation results are given in Figs. 12 and 13.

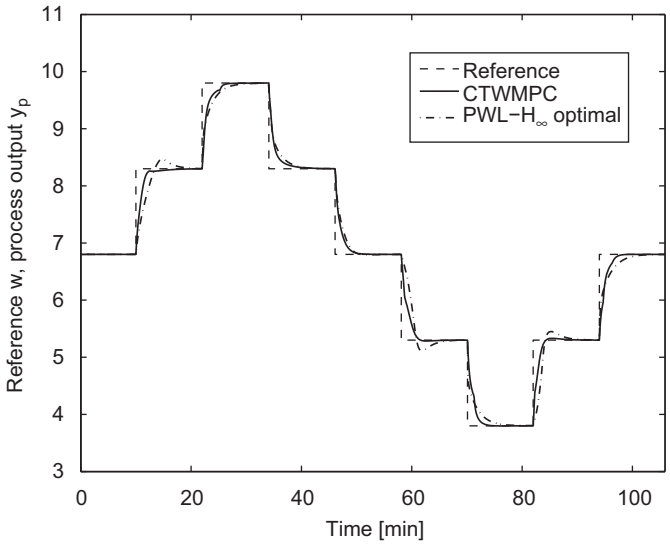


**Fig. 6.** Comparison of the closed-loop-experiment results for both methods.

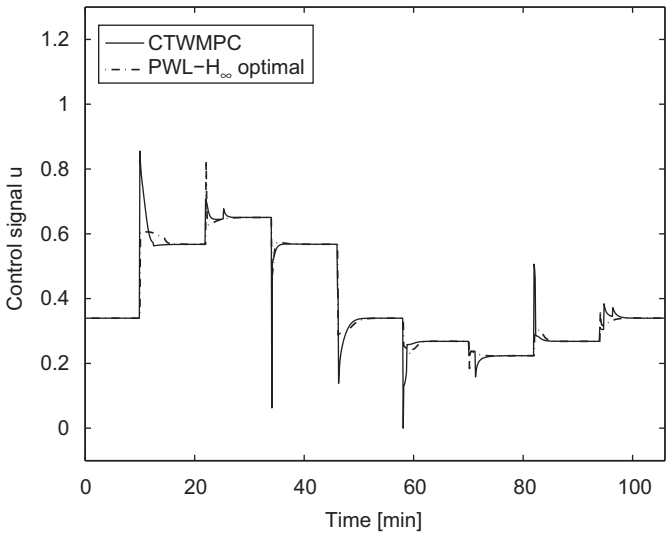


**Fig. 7.** Control signals in the experiment.

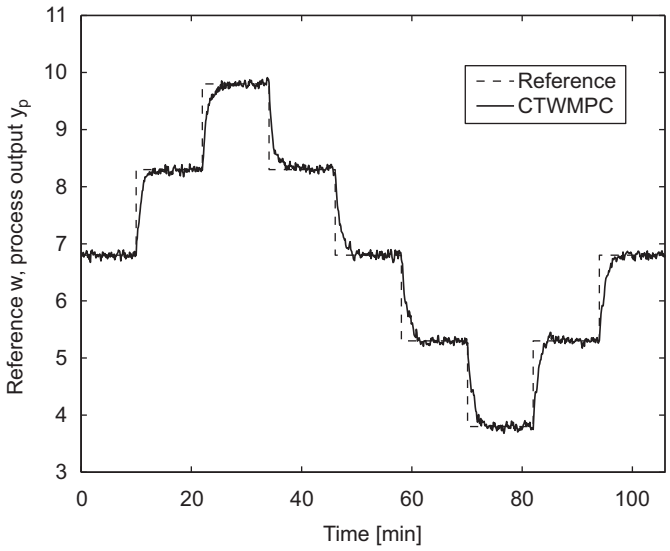


**Fig. 8.** Comparison of the closed-loop-experiment results for both methods, output noise added.

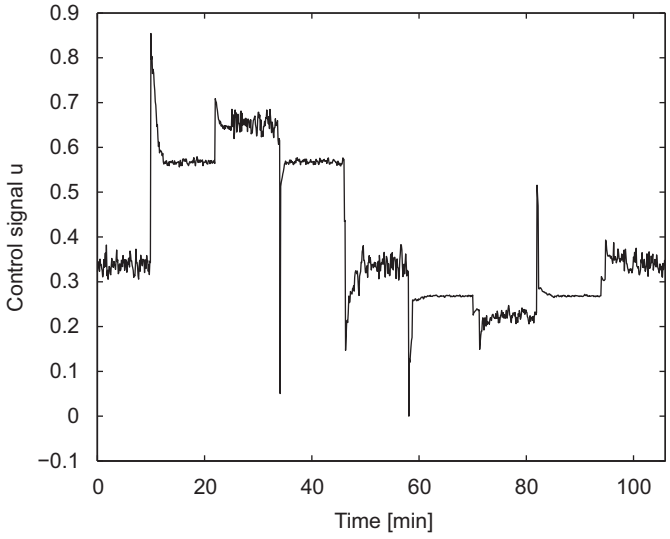


**Fig. 9.** Control signals in the experiment, output noise added.

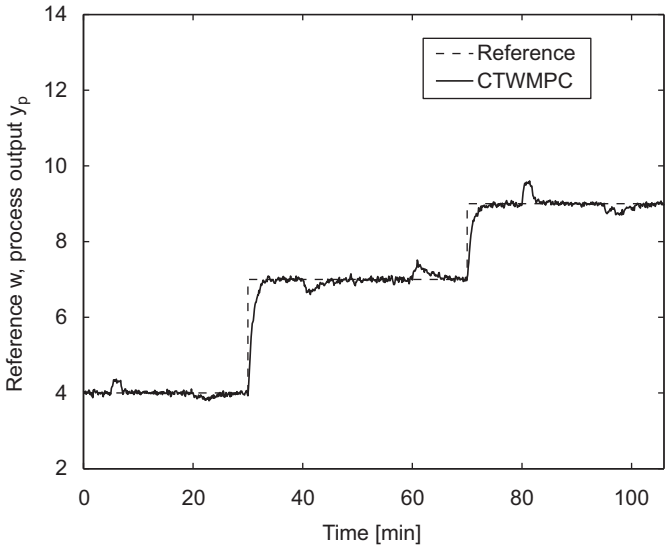


**Fig. 10.** Output and reference signals in the case of input disturbance.

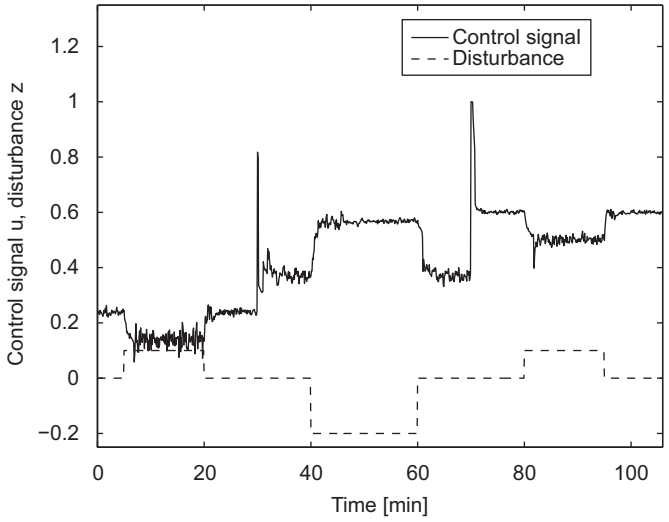


**Fig. 11.** Control and disturbance signals in the case of input disturbance.

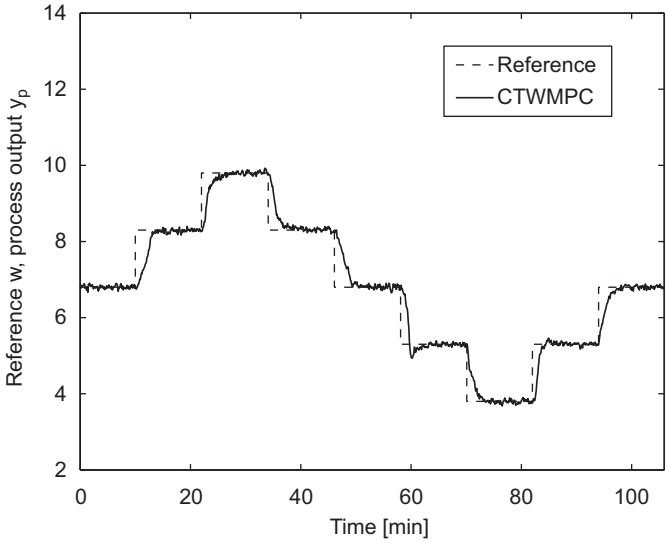


**Fig. 12.** Output and reference signals in the case of control input constraints.

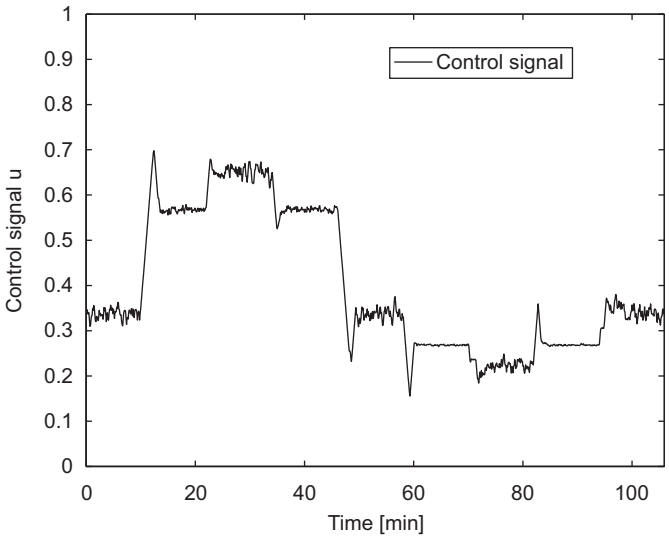


**Fig. 13.** Control signal in the case of control input constraints.

## 5. Conclusion

A method of nonlinear continuous-time model-predictive control was presented. In the derivation procedure the method inherently incorporates a PWL static nonlinear-mapping approximation. The control law is in compact analytical form; furthermore, adaptation of the control parameters as a response to the nonlinear behavior of the process is only a matter of scalar-product computation. As a consequence, the computational burden is low and the proposed method is suitable for real-time applications where high-quality control is desired. Being based on a first-principles model, the method is particularly suitable for nonlinear chemical processes that can be described in the form of a Wiener-type system. It was shown for the case of a pH-neutralization process that our proposed method exhibits a level of quality control that outperforms the robust nonlinear $H_\infty$ method.

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