

THE ROLE OF APPROXIMATION IN ANALYTICAL CONTINUOUS-TIME WIENER-MODEL PREDICTIVE CONTROL

Simon Oblak¹, Andrés García², Igor Škrjanc¹, Osvaldo Agamennoni²

¹University of Ljubljana, Faculty of Electrical Engineering
1000 Ljubljana, Tržaška 25, Slovenia

² Departamento de ingeniería eléctrica y de computadoras, Universidad Nacional del Sur
Av. Alem 1253, Bahía Blanca, Argentina
simon.oblak@fe.uni-lj.si (Simon Oblak)

Abstract

The paper investigates the role of the nonlinear-function approximation in the case of Wiener-model predictive control for nonlinear time-delayed systems. As the control law is derived in a closed analytical form, it is important that the open-loop prediction of the process output is as accurate as possible. In this sense we studied three different approximations of the static function in the Wiener model, the piecewise-linear (PWL), fuzzy-system (FS) and spline approximation. In the FS case we also considered the cases with triangular and exponential membership functions, and 1st- and 2nd-order consequent functions of the fuzzy system. The main scope of the study was to analyze how the optimizing the static-function approximation affects the derivative of the function, which plays the key role in the control law. The results show that the best results can be achieved with the FS approximations. The only problem can be seen in the possible discontinuity of the derivative function for a low number of approximation segments. In the PWL case we get consistent results in terms of the approximation for any number of the segments; however, the overall results are worse than in the FS case. In the spline case it can be clearly seen that for good performance one needs more segments than in the FS case. However, due to a continuous derivative function, good results are obtained in terms of the energy of the control signal.

Keywords: Wiener system, time-delayed systems, predictive control, function approximation, pH neutralization

Presenting Author's Biography

Simon Oblak received a B.Sc from the Faculty of Electrical Engineering, University of Ljubljana in 2003. Currently he is working in the same institution as junior researcher. His research interests primarily include applications of fuzzy systems, especially in the fields of nonlinear control and fault detection. For his work he received many awards, including Prešeren scientific student award in 2003 and the first prize in the Baltic olympiade in automatic control in 2006.



1 Introduction

Model-predictive control has played one of the key parts of automatic control for three decades [1]. The essence of the approaches is the mathematical model of the process we want to control. On the basis of the model the process-output prediction is calculated for a specific time in the future. With respect to the prediction horizon, we can distinguish between discrete-time and continuous-time methods [2, 3]. In this paper we will focus on a continuous-time nonlinear method, presented in [4]. The method is appropriate for the nonlinear processes that can be efficiently modelled by a Wiener model. This model structure facilitates the model-output prediction, so that the predictive control law can be derived in a closed analytical form. The resulting closed-loop system is open-loop optimal, as the calculation of the optimal control signal is based on an open-loop cost function, the model accuracy plays a key role. For this specific model, the accuracy of the nonlinear static output function is crucial. However, when the identification of the model is performed, we seldom focus on the derivative of the static function, which is in fact an inherent part of the control law. The majority of procedures, e.g. [5], focuses only on approximating the static curve. This paper, on the other hand, investigates the effect of using different types of approximation and compares the performance both in the derivative-approximation stage and in using the obtained models in control.

The structure of the paper is as follows. In the first part the continuous-time prediction of the model output is presented. The section consists of presenting the approximations in question (piecewise-linear (PWL) approximation, fuzzy-system (FS) approximation, and spline approximation), calculating the model output using a Maclaurin series expansion, and forming a closed analytical predictive control law. The second part gives the results of the investigation, first the approximation results and second the control results. Final section concludes the paper.

2 Using nonlinear approximations in continuous-time system-output prediction

We shall focus on a nonlinear time-delayed continuous-time system

$$\begin{aligned} \dot{x}_p(t) &= f(x_p(t), u(t - T_d)) \\ y_p(t) &= g(x_p(t)) \end{aligned} \quad (1)$$

where $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$ and $g : \mathbb{R}^n \rightarrow \mathbb{R}$ are smooth functions, $x_p \in \mathbb{R}^n$ is a vector of n state variables, T_d denotes the time delay, $u \in \mathbb{R}$ is a process input and $y_p \in \mathbb{R}$ is a process output.

Let us assume that we model the system with a Wiener time-delayed model

$$\begin{aligned} \dot{x}(t) &= Ax(t) + Bu(t) \\ v(t) &= Cx(t - T_d) \\ y(t) &= h(v(t)) \end{aligned} \quad (2)$$

where $A \in \mathbb{R}^n \times \mathbb{R}^n$, $B \in \mathbb{R}^n$ and $C \in \mathbb{R}^n$. The variable $v(t) \in \mathbb{R}$ represents the intermediate variable that when connected in series with a static nonlinearity $h : \mathbb{R} \rightarrow \mathbb{R}$ forms the model output $y(t)$. Note that in the real system v is not necessarily measured; hence, it has to be extracted from either the physical model or the identification data, obtained from the process. Furthermore, we assume the so-called undelayed linear system, the output of which forms the auxiliary model output containing no time delays:

$$\begin{aligned} \dot{x}(t) &= Ax(t) + Bu(t) \\ \bar{v}(t) &= Cx(t) \\ \bar{y}(t) &= h(\bar{v}(t)) \end{aligned} \quad (3)$$

As we are dealing with a methodology suitable for processes that can be accurately described by their first-principle continuous-time models, we will assume that the steady-state data for the intermediate and output variables is obtained from the model. The resulting curve is in general nonlinear and it has to be approximated by a universal nonlinear approximator, such as a fuzzy system, a piecewise-linear function or a spline curve. In the following subsections we will review the approximations that were included in the research.

2.1 Piecewise-linear functions

The process-model output using the PWL approximation is defined as

$$y_{mp}(t) = \hat{h}_{mp}(v(t)) = \Theta^T \Lambda(v(t)), \quad (4)$$

where $\Theta^T \in \mathbb{R}^{\sigma+1}$ and $\Lambda \in \mathbb{R}^{\sigma+1}$. Using the PWL approximation, any nonlinear function h can be uniquely represented by the segmentation of its input domain. Let us consider the segmentation into σ segments by the parameters α_i , with $\alpha_0 \leq \alpha_1 \leq \dots \leq \alpha_\sigma$. In addition, the elements of the basis functions can be expressed as

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

and the vector of the parameters is defined as

$$\Theta^T = [\theta_0, \theta_1, \dots, \theta_\sigma]. \quad (6)$$

The locations of the segments are chosen by clustering algorithms [6], and the vector of the parameters can be calculated using common least-square algorithms.

2.2 Fuzzy systems

A fuzzy TS-type system in affine form with one antecedent variable and a polynomial consequent part is assumed. It can be given as a set of rules in the form

$$\begin{aligned} \mathbf{R}_j : & \text{if } x_p \text{ is } \mathbf{A}_j, \\ & \text{then } y_{mf} = \theta_{j,0} + \theta_{j,1}x_c + \dots + \theta_{j,n}x_c^n, \end{aligned} \quad (7)$$

where $j = 1, \dots, \sigma$ is the number of fuzzy rules and n is the polynomial order. The variable x_p denotes the input or variable in premise, and the variable y is the output of the model. The antecedent

variable is connected with σ fuzzy sets \mathbf{A}_j , and each fuzzy set \mathbf{A}_j ($j = 1, \dots, \sigma$) is associated with a real-valued function $\mu_{A_j}(x_p) : \mathbb{R} \rightarrow [0, 1]$, that produces a membership grade of the variable x_p with respect to the fuzzy set \mathbf{A}_j . The consequent vector is denoted $X_c^T = [1, x_c, \dots, x_c^n]$, and it implicitly represents an additional input to the fuzzy system. The system output is a linear combination of the consequent states. The system in (7) can be described in closed form

$$y_{mf} = \beta^T(x_p)\Theta_f X_c, \quad (8)$$

where the membership vector $\beta^T(x_p) = [\beta_1(x_p), \dots, \beta_\sigma(x_p)]$ is composed of normalized degrees of fulfilment

$$\beta_j(x_p) = \frac{\mu_{A_j}(x_p)}{\sum_{j=1}^{\sigma} \mu_{A_j}(x_p)}, \quad j = 1, \dots, \sigma, \quad (9)$$

and the matrix of fuzzy-model parameters

$$\Theta_f^T = [\theta_1 \quad \dots \quad \theta_\sigma] \quad (10)$$

is composed of vectors of parameters in individual fuzzy domains:

$$\theta_j^T = [\theta_{j,0} \quad \theta_{j,1} \quad \dots \quad \theta_{j,n}], \quad j = 1, \dots, \sigma \quad (11)$$

It is obvious that $\sum_{j=1}^{\sigma} \beta_j(x_p) = 1$ irrespective of x_p as long as the denominator of $\beta_j(x_p)$ in Eq. (9) is not equal to zero (which can easily be prevented by stretching the membership functions over the whole potential area of x_p).

Using the intermediate variable $v(t)$ as the antecedent variable x_p , the nonlinear output mapping can be written in closed form as

$$y_{mf}(t) = \hat{h}_{mf}(v(t)) = \beta^T(v(t))\Theta_f X_c(v(t)), \quad (12)$$

where $\beta^T \in \mathbb{R}^\sigma$, $\Theta_f \in \mathbb{R}^\sigma \times \mathbb{R}^n$ and $X_c \in \mathbb{R}^n$.

2.3 Spline approximation

A cubic spline has $\sigma + 3$ degrees of freedom, and we can write it in the form

$$s(x) = \sum_{j=1}^{\sigma+3} c_j N_j(x), \quad x_0 \leq x \leq x_\sigma, \quad (13)$$

where the N_j are linearly independent, normalized cubic B-splines (or basis-splines). Let $x_{-2} \leq x_{-1} \leq x_0 < x_1 < \dots < x_\sigma \leq x_{\sigma+1} \leq x_{\sigma+2}$ be an augmented knot set. The $\{M_{r,i}(x)\}_{i=1}^{\sigma+r}$ defined by the recurrence

$$M_{0,i}(x) = \begin{cases} \frac{1}{(x_i - x_{i-1})} & \text{for } x_{i-1} < x < x_i \\ 0 & \text{otherwise} \end{cases} \quad (14)$$

$$M_{r+1,i}(x) = \frac{k_1(x)M_{r,i-1}(x) + k_2(x)M_{r,i}(x)}{x_i - x_{i-2-r}}, \quad (15)$$

$$k_1(x) = (x - x_{i-2-r}), \quad k_2(x) = (x_i - x),$$

for $r = 0, 1, 2$

are splines of degree r defined on $[x_0, x_\sigma]$. They satisfy $M_{r,i}(x) = 0$ for $x_0 \leq x < x_{i-1-r}$ and $x_i \leq x \leq x_n$, and $M_{r,i}(x) > 0$ for $x_{i-1-r} < x < x_i$, and their derivatives can be for $r = 0, 1, 2$ computed from

$$M'_{r+1,i}(x) = (r+1) \frac{M_{r,i-1}(x) - M_{r,i}(x)}{x_i - x_{i-2-r}}. \quad (16)$$

The normalized cubic B-splines are given by

$$N_i(x) = (x_i - x_{i-4})M_{3,i}(x). \quad (17)$$

They satisfy

$$\sum_{j=1}^{\sigma+3} N_j(x) = 1 \text{ for } x_0 \leq x \leq x_\sigma \quad (18)$$

This choice of representation for the splines has some advantages. Each $N_i(x)$ is nonzero only in four consecutive knot intervals, and in the typical interval $[x_{j-1}, x_j]$ only $N_j(x)$, $N_{j+1}(x)$, $N_{j+2}(x)$ and $N_{j+3}(x)$ are nonzero. Furthermore, the number of parameters equals the number of degrees of freedom, so that the size of the system of equations defining the actual spline is as small as possible. Also, it should be noted that all quantities in (14) and (15) are positive. This implies that the recurrence is numerically stable.

Using a segmentation into σ segments $v_0, v_1, \dots, v_\sigma$ and the coefficients c_j , obtained by a curve-fitting procedure, the system output in the spline-approximation case will be written as

$$y_{sp}(t) = \hat{h}_{sp}(v(t)) = \sum_{j=1}^{\sigma+3} c_j N_j(v(t)), \quad v_0 \leq x \leq v_\sigma. \quad (19)$$

2.4 How to calculate the model-output prediction

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. 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 as $w(t)$. In the moving time frame the model-output prediction at time τ can be approximated by a truncated Maclaurin series expansion

$$y(t + \tau|t) = \Gamma^T(\tau)Y(t) \quad (20)$$

where the vectors Γ and Y are given by

$$\Gamma(\tau) = \left[1 \quad \tau \quad \dots \quad \frac{\tau^i}{i!} \quad \dots \quad \frac{\tau^{n_y}}{n_y!} \right]^T, \quad (21)$$

$$Y(t) = \left[y(t) \quad y^{[1]}(t) \quad \dots \quad y^{[i]}(t) \quad \dots \quad y^{[n_y]}(t) \right]^T, \quad (22)$$

with $Y \in \mathbb{R}^{n_y}$, 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 $y_r(t + \tau|t) = \Gamma^T(\tau) \cdot r \cdot w(t)$ where the vector of the Markov parameters $r \in \mathbb{R}^{n_y+1}$ is defined as

$$r = [0 \ C_r B_r \ C_r A_r B_r \ \dots \ C_r A_r^{n_y-1} B_r]^T. \quad (23)$$

Let us first investigate the model-output prediction (20) in the PWL approximation case. The i th derivative of $y(t)$ is defined as

$$y_{mp}^{[i]}(t) = \Theta^T \frac{d\Lambda(v)}{dv} C A^i x(t) + \Theta^T \frac{d\Lambda(v)}{dv} [C A^{i-1} B \ \dots \ C B] U(t), \quad (24)$$

where $U(t)$ stands for

$$U(t) = [u(t) \ u^{[1]}(t) \ \dots \ u^{[i]}(t)]^T \quad (25)$$

and where

$$\frac{d\Lambda(v)}{dv} = \begin{bmatrix} 0 \\ \frac{1}{2} (1 + \text{sign}(v - \alpha_0)) \\ \vdots \\ \frac{1}{2} (1 + \text{sign}(v - \alpha_{\sigma-1})) \end{bmatrix}. \quad (26)$$

Because all of the higher derivatives of the PWL mapping with respect to v are equal to 0 ($\frac{d^2\Lambda(v)}{dv^2} = \dots = \frac{d^n\Lambda(v)}{dv^n} = 0$), all of the higher powers of $\dot{v}(t)$ are cancelled as well. This is, however, not the case when using the FS approximation and B-splines. Differentiating (12) or (19) with respect to time, the first two derivatives will be as follows:

$$\begin{aligned} \dot{y}_{mf} &= \frac{d\hat{h}_{mf}(v)}{dv} \cdot \dot{v}(t) \\ \dot{y}_{sp} &= \frac{d\hat{h}_{sp}(v)}{dv} \cdot \dot{v}(t) \end{aligned} \quad (27)$$

$$\begin{aligned} \ddot{y}_{mf} &= \frac{d^2\hat{h}_{mf}(v)}{dv^2} \cdot (\dot{v}(t))^2 + \frac{d\hat{h}_{mf}(v)}{dv} \cdot \ddot{v}(t) \\ \ddot{y}_{sp} &= \frac{d^2\hat{h}_{sp}(v)}{dv^2} \cdot (\dot{v}(t))^2 + \frac{d\hat{h}_{sp}(v)}{dv} \cdot \ddot{v}(t). \end{aligned} \quad (28)$$

It is obvious that the first term cannot be canceled, and hence the analytical definition of the output prediction becomes too complex for higher derivatives. For this reason, all the terms $(\dot{v}(t))^k$, $k \geq 2$ are assumed to be 0, and the prediction problem is reformulated to be very similar to the form in the PWL case:

$$\begin{aligned} y_{mf}^{[i]}(t) &= \frac{d\hat{h}_{mf}(v)}{dv} \cdot \frac{d^i v}{dt^i} = \\ &= \frac{d\hat{h}_{mf}}{dv} (C A^i x(t) + [C A^{i-1} B \ \dots \ C B] U(t)), \end{aligned} \quad (29)$$

where

$$\frac{d\hat{h}_{mf}}{dv} = \frac{d\beta^T}{dv} \Theta_f X_c + \beta^T \Theta_f \frac{dX_c}{dv} \quad (30)$$

for the FS case and

$$\begin{aligned} y_{sp}^{[i]}(t) &= \frac{d\hat{h}_{sp}(v)}{dv} \cdot \frac{d^i v}{dt^i} = \\ &= \frac{d\hat{h}_{sp}}{dv} (C A^i x(t) + [C A^{i-1} B \ \dots \ C B] U(t)), \end{aligned} \quad (31)$$

where

$$\frac{d\hat{h}_{sp}}{dv} = \sum_{j=1}^{n+3} c_j \frac{dN_j(v(t))}{dv} \quad (32)$$

for the B-spline case. For the sake of clarity we will assume the same notation of the model output y for all three cases of approximations. 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 τ . 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 $u(t + \tau)$.*

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

$$U(t) = [u(t) \ u^{[1]}(t) \ \dots \ u^{[n_u]}(t)]^T. \quad (33)$$

Combining equations (20)-(22) with (24), (29) or (31), the prediction of the model output $y(t + \tau|t)$ at time τ is defined as

$$y(t + \tau|t) = \Gamma^T [P y(t) + q(v) K_q x(t) + q(v) K_h U(t)], \quad (34)$$

where $P = [1 \ 0 \ \dots \ 0]^T \in \mathbb{R}^{n_y+1}$. The matrices $K_q \in \mathbb{R}^{n_y+1} \times \mathbb{R}^n$ and $K_h \in \mathbb{R}^{n_y+1} \times \mathbb{R}^{n_u+1}$ 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

$$q(v) = \Theta^T \frac{d\Lambda(v)}{dv} \quad (35)$$

for the PWL approximation,

$$q(v) = \frac{d\beta^T(v)}{dv} \Theta_f X_c(v) + \beta^T(v) \Theta_f \frac{dX_c(v)}{dv} \quad (36)$$

for the FS approximation, and

$$q(v) = \sum_{j=1}^{n+3} c_j \frac{dN_j(v(t))}{dv} \quad (37)$$

for the B-spline approximation. Matrices K_q and K_h are defined as

$$K_q = [0 \ (CA)^T \ (CA^2)^T \ \dots \ (CA^{n_y})^T]^T, \quad (38)$$

and

$$K_h = \begin{bmatrix} 0 & \cdots & \cdots & 0 \\ CB & 0 & \cdots & 0 \\ CAB & CB & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ CA^{n_y-1}B & CA^{n_y-2}B & \cdots & CA^{n_y-1-n_u}B \end{bmatrix}. \quad (39)$$

2.5 Continuous-time Wiener-model predictive control (CTWMP)

The future control error should decrease according to the dynamics defined by the reference model

$$e(t + \tau) = \Gamma^T r(w(t) - \bar{y}_p(t)), \quad (40)$$

where $\bar{y}_p(t)$ is the estimated undelayed process output. Since this signal is not available in the measurements, we have to estimate it from the actual process output and the process model. We assume that the difference between the actual and the undelayed process outputs is equal to the difference between the delayed and the undelayed process-model outputs:

$$y_p(t) - \bar{y}_p(t) = y(t) - \bar{y}(t). \quad (41)$$

In this sense the undelayed process output \bar{y}_p can be replaced by

$$\bar{y}_p(t) = y_p(t) - y(t) + \bar{y}(t). \quad (42)$$

The idea of the proposed continuous-time MPC, referring to the predictive functional control derivation [7], is based on a minimization of the difference between the future control error and the difference between the predicted model output at time horizon $\tau \in [0, T]$ and the current model output:

$$\epsilon(t, \tau) = e(t + \tau) - (\bar{y}(t + \tau|t) - \bar{y}(t)) \quad (43)$$

The control law will be obtained by minimizing the cost function

$$V = \int_0^T \|\epsilon(t, \tau)\|^2 d\tau. \quad (44)$$

Given the prediction of the process-model output in (34), the cost function $V(U, v, t)$ (44) is

$$V = \int_0^T \Psi(v)^T \Gamma \Gamma^T \Psi(v) d\tau, \quad (45)$$

where

$$\Psi(v) = r(w - \bar{y}_p) - q(v)K_h U - q(v)K_q x \quad (46)$$

denotes the term depending only on the values of u and v in time instant t . The minimization of the cost function results in the continuous-time model-predictive control law

$$\frac{\partial V}{\partial U} = -2q(v)K_h^T \int_0^T \Gamma \Gamma^T \Psi(v) d\tau = 0. \quad (47)$$

Let us define the matrix $\bar{\Gamma} \in \mathbb{R}^{n_y+1} \times \mathbb{R}^{n_y+1}$ as

$$\bar{\Gamma} = \int_0^T \Gamma \Gamma^T d\tau. \quad (48)$$

Given that the general term of the matrix $\Gamma \Gamma^T$ is $T^{i-1+j-1}/((i-1)!(j-1)!)$, equation (48) can be rewritten as

$$\bar{\Gamma} = \begin{bmatrix} \gamma_{(1,1)} & \cdots & \gamma_{(1,n_y+1)} \\ \vdots & \ddots & \vdots \\ \gamma_{(n_y+1,1)} & \cdots & \gamma_{(n_y+1,n_y+1)} \end{bmatrix}, \quad (49)$$

where

$$\gamma_{(i,j)} = \frac{1}{(i+j-1)(i-1)!(j-1)!} T^{i+j-1} \quad (50)$$

for every $i, j = 1, \dots, n_y + 1$. Equation (47) is then reformulated as

$$\frac{\partial V}{\partial U} = -2q(v)K_h^T \bar{\Gamma} \Psi(v) = 0 \quad (51)$$

and by inserting the estimation from (42) the control vector becomes

$$U = \frac{1}{q(v)} (K_h^T \bar{\Gamma} K_h)^{-1} K_h^T \bar{\Gamma} \times [r(w - y_p + y(t) - \bar{y}(t)) - q(v)K_q x]. \quad (52)$$

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 $(K_h^T \bar{\Gamma} K_h)^{-1} K_h^T \bar{\Gamma} \in \mathbb{R}^{n_u+1} \times \mathbb{R}^{n_y+1}$ as κ . Now the control law of the nonlinear Wiener-type model-predictive control is given by

$$u(t) = \frac{1}{q(v)} \kappa [r(w - y_p + y(t) - \bar{y}(t)) - q(v)K_q x]. \quad (53)$$

It is obvious that the term $q(v)$, presented in Eqs. (35), (36), and (37), plays the key role in the quality of control, as it eliminates the effect of the system nonlinearity in each time instant. This is why it is necessary that the approximation we are using be as accurate as possible.

3 Main results

3.1 Wiener model of a pH neutralization process

The proposed method was tested on a chemical process with marked nonlinearity. A mathematical model of a pH neutralization process was adopted from [8]. 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 behaviour with respect to different titration curves.

Figure 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

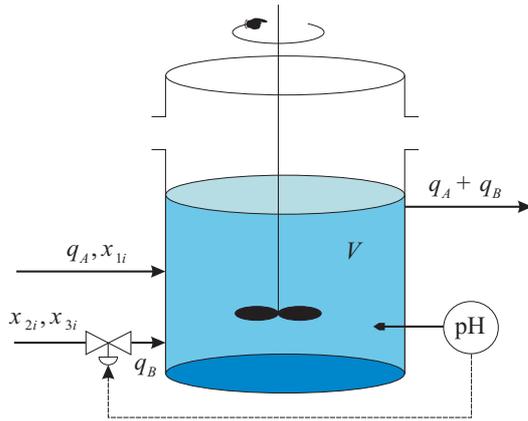


Fig. 1 pH-neutralization process

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 behaviour of the process can be described considering the state variables

$$\begin{aligned} x_1 &= [A^-]; \\ x_2 &= [B^+]; \\ x_3 &= [X^-]. \end{aligned} \quad (54)$$

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

$$\begin{aligned} \dot{x}_1 &= \frac{1}{\theta} \cdot (x_{1i} - x_1) - \frac{1}{V} \cdot x_1 \cdot u, \\ \dot{x}_2 &= -\frac{1}{\theta} \cdot x_2 + \frac{1}{V} \cdot (x_{2i} - x_2) u, \\ \dot{x}_3 &= -\frac{1}{\theta} \cdot x_3 + \frac{1}{V} \cdot (x_{3i} - x_3) u, \end{aligned} \quad (55)$$

$$g(x, \xi) = \xi + x_2 + x_3 - x_1 - \frac{K_w}{\xi} - \frac{x_3}{1 + \frac{K_x \xi}{K_w}} = 0, \quad (56)$$

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 (55)-(56) are $x_{2i} = 0.0020$ mol NaOH/L, $x_{3i} = 0.0025$ mol NaHCO₃/L, $K_x = 10^{-7}$ mol/L, $K_w = 10^{-14}$ mol²/L² and $V = 2.5$ L. Equation (56) 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:

$$\begin{aligned} g(x, \xi) &= \xi^3 + (K_w/K_x + x_2 + x_3 - x_1)\xi^2 + \\ &+ (x_2 - x_1 + K_x)\xi - K_w^2/K_x = 0. \end{aligned} \quad (57)$$

A Wiener model is derived directly from the first-principle model. The approach is particularly appealing in control of chemical processes because first principles give a straightforward way of obtaining nonlinear continuous-time models. Considering the system in (2), a model in the Wiener form can be obtained by linearization of the functions f and g around a given point, normalizing the model 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 (55)-(56) is given by

$$\begin{aligned} A &= \begin{bmatrix} -\frac{1}{\theta}(1 + u_s) & 0 & 0 \\ 0 & -\frac{1}{\theta}(1 + u_s) & 0 \\ 0 & 0 & -\frac{1}{\theta}(1 + u_s) \end{bmatrix}, \\ B &= \begin{bmatrix} -\frac{1}{\theta}x_{1,s} \\ \frac{1}{\theta}(x_{2i} - x_{2,s}) \\ \frac{1}{\theta}(x_{3i} - x_{3,s}) \end{bmatrix}, \quad C = \begin{bmatrix} \frac{\partial \eta}{\partial x_1} & \frac{\partial \eta}{\partial x_2} & \frac{\partial \eta}{\partial x_3} \end{bmatrix}, \end{aligned} \quad (58)$$

where

$$\frac{\partial \eta}{\partial x_k} = \frac{\partial h(x)/\partial k}{\xi \ln(10) \partial h(x)/\partial \xi}, \quad k = 1, 2, 3. \quad (59)$$

From the polynomial pH equation (56) the following terms are easily calculated:

$$\begin{aligned} \frac{\partial h(x)}{\partial \xi} &= 3K_x \xi^2 + 2[K_w + (x_3 + x_2 - x_1)K_x]\xi + \\ &+ (x_2 - x_1 - K_x)K_w, \\ \frac{\partial h(x)}{\partial x_1} &= -K_x \xi^2 - K_w \xi, \\ \frac{\partial h(x)}{\partial x_2} &= -K_x \xi^2 + K_w \xi, \\ \frac{\partial h(x)}{\partial x_3} &= K_x \xi^2. \end{aligned} \quad (60)$$

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

$$x_{k,s} = \frac{1}{1 + u_s} x_{k,i}, \quad k = 1, 2, 3 \quad (61)$$

$$\xi + x_{2,s} + x_{3,s} - x_{1,s} - \frac{K_w}{\xi} - \frac{x_{3,s}}{1 + \frac{K_x \xi}{K_w}} = 0, \quad (62)$$

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 $0 \leq u(t) \leq 1$; therefore, we used 200 equidistant steady-state points from the intermediate-variable range $v \in [0, 1]$ for the input

set. The optimized parameters of the approximations were then obtained by curve fitting to the steady-state points.

One can also note the diagonal structure of the matrix A . In [8] 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:

$$A = -0.5477, \quad B = 1, \quad C = 0.5477 \quad (63)$$

3.2 Tuning of the function parameters in the approximation procedures

We considered six different types of approximations. In the PWL case we chose PWL approximation of the static curve, which results in a piecewise-constant derivative approximation. In fuzzy-system approximation we explored the difference between triangular and exponential membership functions and 1st or 2nd-order polynomial in the consequent part. Spline approximation was a third-order piece-wise polynomial approximation with continuous first and second derivative.

To ensure fair comparison, all of the curve-fitting procedures were unified into the following algorithm:

1. Choose a number of segments and distribute them equidistantly over the complete input range of the input-output data set.
2. Calculate the values of the basis functions - PWL basis in $\Lambda(v)$, membership functions $\beta(v)$ for fuzzy approximations, and values of spline basis in $N(v)$.
3. Calculate the optimal parameters of the functions (Θ for PWL, Θ_f for FS and c_j for B-splines) so that the obtained approximations fit to the data in least-square sense.
4. Repeat steps 2 and 3 in an optimization procedure to find the optimal segmentation; in the research the Nelder-Mead unconstrained nonlinear minimization of the sum-square cost function was applied with end tolerance on the parameter and the cost function equal to 10^{-6} , and maximum number of iterations 5000.
5. Stop when tolerances or the maximum number of iterations have been exceeded.

In the experiment we used 5, 7, 9, and 11 segments, respectively. The measure of approximation quality was mean-square error of derivatives, and the calculations for corresponding approximations are given in Table 1. All of the optimizations were done on the data from the static curve, and the resulting approximations were checked for the derivative cases.

Tab. 1 Mean-square-error results for the approximations

Approximation	5 seg.	7 seg.	9 seg.	11 seg.
PWL stat.	57.13	46.53	41.1	42.94
FS triang. 1.	32.94	18.36	11.61	16.92
FS triang. 2.	78.88	12.21	8.21	10.01
FS exp. 1.	375.4	193.1	28.18	23.36
FS exp. 2.	105.2	13.13	8.691	28.42
Spline	51.62	51.21	9.596	7.325

Figures 2 to 4 show the results for the case where 5 segments were used, and 5 to 7 for the ones where 11 segments were used. The MSE calculations are presented in the corresponding figures.

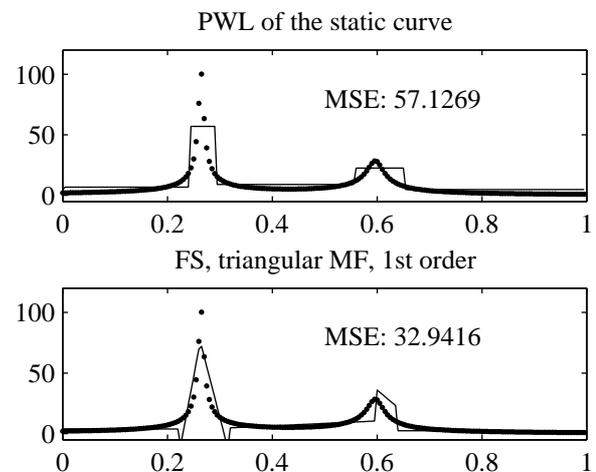


Fig. 2 5-segment approx., PWL - static (upper) and FS - triangular MF, 1st order (lower)

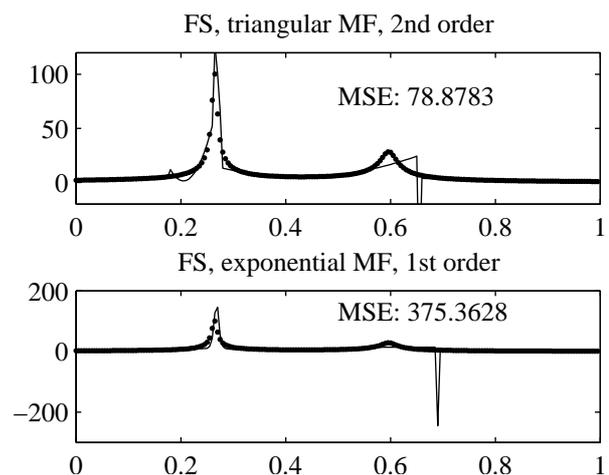


Fig. 3 5-segment approx., FS - triangular MF, 2nd order (upper), FS - exponential MF, 1st order (lower)

In the cases of the FS exp. 2nd order and spline methods, the quality of derivative approximation increases with the increase of the parameter number. In all the

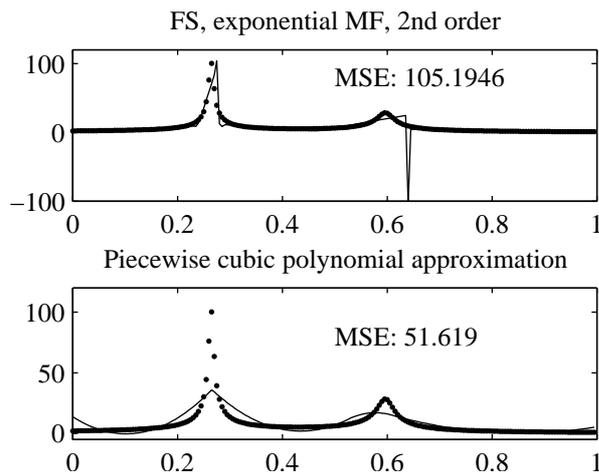


Fig. 4 5-segment approx., FS - exponential MF, 2nd order (upper) and spline approximation (lower)

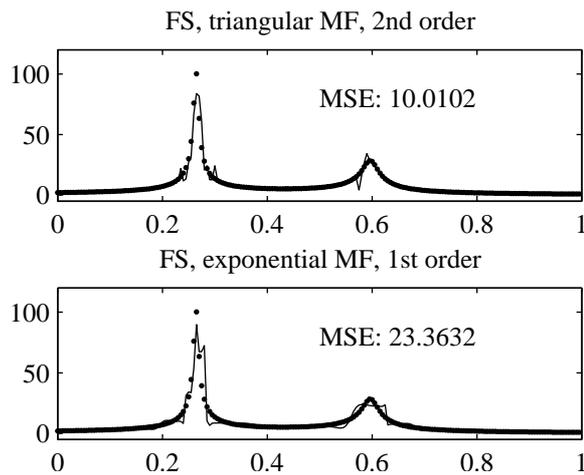


Fig. 6 11-segment approx., FS - triangular MF, 2nd order (upper), FS - exponential MF, 1st order (lower)

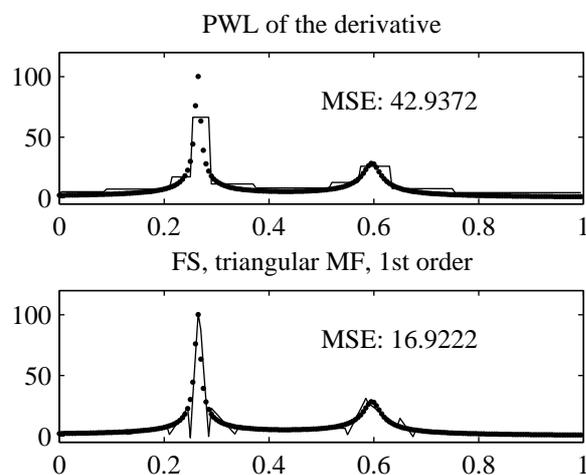


Fig. 5 11-segment approx., PWL - static (upper) and FS - triangular MF, 1st order (lower)

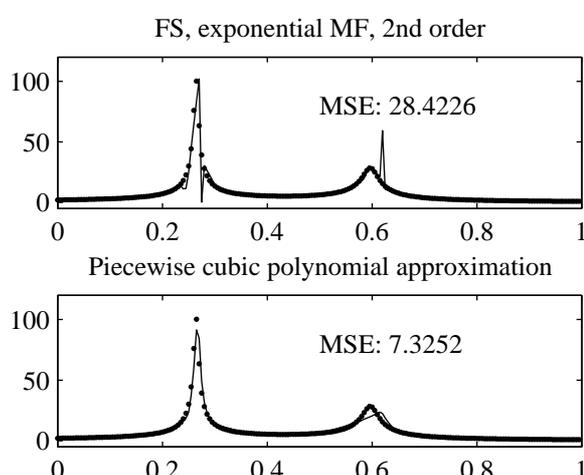


Fig. 7 11-segment approx., FS - exponential MF, 2nd order (upper) and spline approximation (lower)

other cases this does not hold. The quality of the derivative approximation increases to the cases with 9 segments when the best results are obtained; then in the 11-segment cases they deteriorate, even though the results in the static-function approximation improve. This is because more segments also bring more derivative discontinuities which contribute to the sum of square error. This shows that we have to be careful when we choose the number of segments - the effect of "over-parametrization" is here manifested in bigger number of discontinuities in the derivative approximation. The other problem is "under-parametrization" which manifests best in the cases of FS and Spline approximations. The poor results in the FS exp. 1st and 2nd order are the consequence of huge jumps of the derivative function in some discontinuity points. As we will see later, this does not necessarily affect the overall closed-loop performance; however, a designer should be careful when he is dealing with systems that can be destabilized by an excessive control action.

3.3 Control experiments

The control-design parameters for the proposed method were chosen as follows: $n_u = 1$, $n_y = 4$, $T = 0.3$ s, $A_r = -1/0.5$, $B_r = 1$, and $C_r = 1/0.5$. The choice of n_y and T is connected with the desired model-prediction accuracy, and it was discussed in [4]. Closed-loop experiments on a piecewise-constant reference signal and using the corresponding approximations were conducted. We used MSE measure for the control quality (output error) and the control energy (derivative of the control signal). The results are presented in Tables 2 and 3. The results show that the control quality increases with the increase of the number of segments. However, taking into consideration the minimum number of segments, the FS approximations in the case of second-order consequent functions gave the best results. The comparison with the PWL case being to some extent expected, it is surprising to see how they outperform the case with spline approxima-

Tab. 2 Mean-square-error results for the output error $w - y_p$

Approximation	5 seg.	7 seg.	9 seg.	11 seg.
PWL stat.	7.85	4.67	3.81	3.83
FS triang. 1	11.8	3.83	2.91	2.89
FS triang. 2.	3.98	3.45	2.79	2.39
FS exp. 1.	7.73	4.42	3.65	3.01
FS exp. 2.	3.53	2.71	2.42	2.16
Spline	28.3	14.9	2.64	2.52

Tab. 3 Mean-square-integral results for the control-signal changes $\dot{u} \doteq \Delta u$

Approximation	5 seg.	7 seg.	9 seg.	11 seg.
PWL stat.	2.06	2.08	2.77	2.09
FS triang. 1.	2.61	2.19	1.95	1.96
FS triang. 2.	1.95	1.81	2.05	1.95
FS exp. 1.	1.65	2	2.4	2.01
FS exp. 2.	2.02	2.04	2.2	1.8
Spline	1.13	1.58	1.89	1.74

tion for 5 and 7 segments. This shows that for a small number of segments one should consider using fuzzy systems. When the number of the segment increases, the values of the cost function become more even in all the cases. The only fact that encourages the designer to consider using the spline approximation is that it results in a smoother control signal, which demonstrates through a low value of the cost function regarding the control-signal change. This can be seen in the last row of table 3 where the values are minimal in all cases.

Figures 8 and 9 present the diagrams of the output and control signals in the cases of the worst and best results in the closed-loop test, respectively.

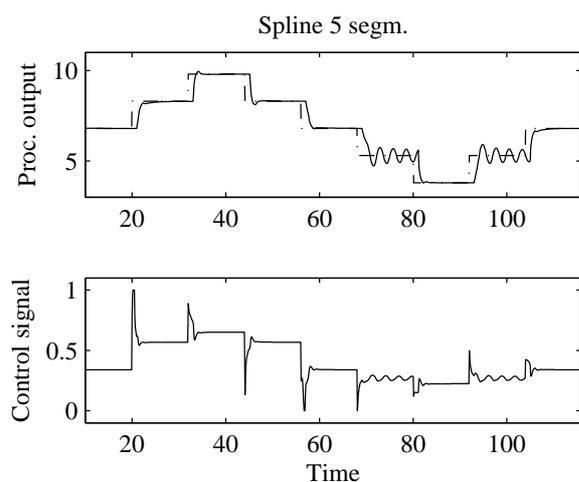


Fig. 8 Closed-loop experiment in the spline case, 5 segments, reference and the output (upper), control signal (lower)

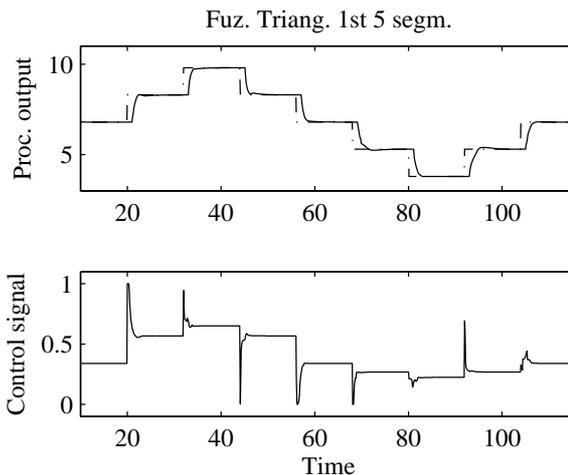


Fig. 9 Closed-loop experiment in the FS exp. 2nd-order case, 11 segments, reference and the output (upper), control signal (lower)

4 Conclusion

In the paper the role of the nonlinear-function approximation was studied in the case of Wiener-model predictive control for nonlinear time-delayed systems. As the control law is derived in a closed analytical form, it is important that the open-loop prediction of the process output is as accurate as possible. In this sense we studied three different approximations of the static function in the Wiener model, the piecewise-linear (PWL), fuzzy-system (FS) and spline approximation. In the FS case we also considered the cases with triangular and exponential membership functions, and 1st- and 2nd-order consequent functions of the fuzzy system. The main scope of the study was to analyze how the optimizing the static-function approximation affects the derivative of the function, which plays the key role in the control law. The results show that the best results can be achieved with the FS approximations. The only problem can be seen in the possible discontinuity of the derivative function for a low number of approximation segments. In the PWL case we get consistent results in terms of the approximation for any number of the segments; however, the overall results are worse than in the FS case. In the spline case it can be clearly seen that for good performance one needs more segments than in the FS case. However, due to a continuous derivative function, good results are obtained in terms of the energy of the control signal.

5 References

- [1] C. E. García, D. M. Prett, and M. Morari. Model predictive control: theory and practice - a survey. *Automatica*, 25(3), 1989.
- [2] H. Demircioğlu and P. J. Gawthrop. Continuous-time generalized predictive control. *Automatica*, 27(1):55-74, 1991.
- [3] Wen-Hua Chen, Donald J. Ballance, and Peter J. Gawthrop. Optimal control of nonlinear systems: a

- predictive control approach. *Automatica*, 39:633–641, 2003.
- [4] Simon Oblak and Igor Škrjanc. A comparison of fuzzy and cpwl approximations in the continuous-time nonlinear model-predictive control of time-delayed wiener-type systems. *Journal of intelligent and robotic systems*, 47:125–137, 2006.
 - [5] Su Whan Sung and Jitae Lee. Modeling and control of wiener-type processes. *Chemical Engineering Science*, 59:1515–1521, 2004.
 - [6] Nikhil R. Pal and James C. Bezdek. On cluster validity for the fuzzy c -means model. *IEEE Transactions on Fuzzy Systems*, 3(3):370–379, 1995.
 - [7] Igor Škrjanc and Drago Matko. Fuzzy predictive functional control in the state space domain. *Journal of Intelligent and Robotic Systems*, 31:283–297, 2001.
 - [8] Omar Galán, José A. Romagnoli, and Ahmet Palazoglu. Robust h_∞ control of nonlinear plants based on multi-linear models: an application to a bench-scale ph neutralization reactor. *Chemical Engineering Science*, 55:4435–4450, 2000.