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Model Predictive Control of a pH Maintaining System

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Abstract*. In this paper the problem of optimal regulation of a pH maintaining system is considered, where the outputs are the pH value and the liquid level in the system and the control inputs are the flow rates of the base input flow and the output flow. The optimal regulation problem is formulated as a nonlinear model predictive control problem in the presence of constraints. Two cases are considered: 1) presence of box constraints only on the control inputs and 2) considering also constraints on the rate of change of the inputs.*

Introduction

Model Predictive Control (MPC) has become the accepted methodology to solve complex control problems related to process industries [1-9]. It allows the design of multi-input multi-output (MIMO) control systems that minimize a certain performance index in the presence of input and output constraints imposed on the system. It is an optimization-based method of control which involves the solution of a finite horizon constrained optimal control problem at each sampling instant.

The main reasons for successful application of MPC are the following [6]:

- MPC handles multivariable control problems naturally.
- MPC is a control method, which allows strict satisfaction of the constraints, imposed on the control inputs, state variables and output variables of the plant.
- MPC allows the use of complex analytical models, which are obtained from the understanding of the physical and chemical transformations occurring inside a process. The analytical models can be used for significantly more accurate prediction of the future plant behaviour in comparison to the black-box linear input-output models, obtained from simple plant tests or by applying system identification methods to plant data.
- MPC allows operation closer to constraints (compared with conventional control), which

The conceptual structure of MPC is given in *figure 1* [4]. The name MPC stems from the idea of employing an explicit model of the plant to be controlled which is used to predict the future output behaviour. This prediction capability allows solving optimal control problems on line, where the tracking error, namely the difference between the predicted output and the desired reference, is minimized over a future horizon [4].

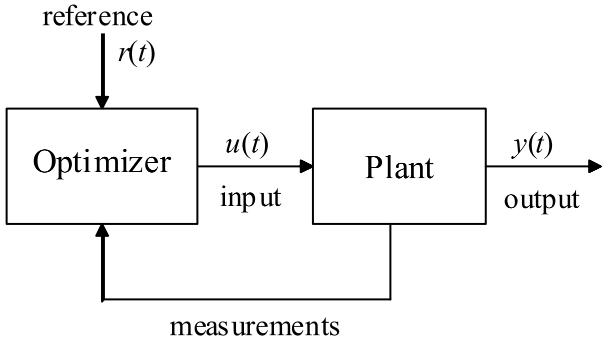

Figure 1. Basic MPC structure [4]

The result of the optimization is applied according to a receding or moving horizon philosophy [4]: At time t only the first input of the optimal command sequence is actually applied to the plant. The remaining optimal inputs are discarded, and a new optimal control problem is solved at time $t + 1$. This idea is illustrated in *figure 2.*

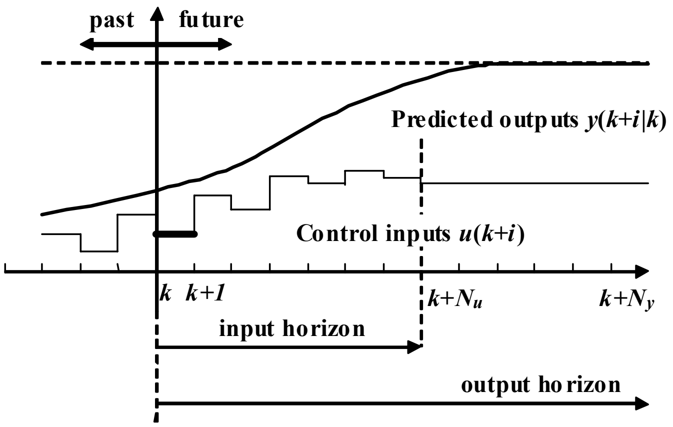

Figure 2. Receding horizon strategy: only the first input of the computed optimal input sequence is implemented [4]

NMPC Problem Formulation of Continuous-Time Systems

Consider the nonlinear continuous-time system, whose dynamics is described by the ordinary differential equation (ODE):

(1) $$\frac{d}{dt}x(t) = f(x(t), u(t))$$

where $x(t) \in \Re^n$ is the state vector, $u(t) \in \Re^m$ is the control input vector, $f: \Re^n \times \Re^m \to \Re^n$ is a nonlinear vector-function, and t is the continuous time. It is assumed that all state variables are measurable. We consider the optimal regulation problem where the control objective is to steer the system state to the origin by minimizing a certain performance index. Let the measured values of the state variables at the current discrete time k be x_k, i.e. $x(kT_s) = x_k$, where T_s is the sampling interval. For system (1) the regulation *nonlinear* MPC (NMPC) problem at the current time instant k includes the solution of the following optimal control problem:

(2) $$J^*(x_k) = \min_{u[kT_s, kT_s+T]} J(u[kT_s, kT_s+T], x_k)$$

subject to the input and state constraints

(3) $$u_{\min} \le u(kT_s + t) \le u_{\max},\ t \in [0,T]$$

(4) $$g(x(kT_s+t), u(kT_s+t)) \le 0,\ t \in [0,T]$$

where the evolution of the state vector is determined by solving the ODE

(5) $$\frac{d}{dt} x(kT_s+t) = f(x(kT_s+t), u(kT_s+t)),\ x(kT_s) = x_k,\ t \in [0,T].$$

In (4) $g: \Re^n \times \Re^m \to \Re^q$ is the constraints vector-function and in (2) $J(u[kT_s, kT_s+T], x_k)$ is the cost function defined by

(6) $$J(u[kT_s, kT_s+T], x_k) = \int_0^T l(x(kT_s+t), u(kT_s+t))dt + S(x(kT_s+T))$$

where the function $l: \Re^n \times \Re^m \to \Re$ is known as the stage cost, the function $S: \Re^n \to \Re$ is the terminal cost, and T is the horizon. The constraints (4) may result from both physical and operational constraints of the control system and stability-preserving terminal sets (see [9], chapters 2, 5). The properties of l and S have consequences for the control performance, including stability, and must be carefully tuned [5].

The above formulation defines an infinite-dimensional optimal control problem whose solution can be characterized using classical tools like Pontryagin's maximum principle [10] and dynamic programming [11]. As mentioned in [9], in these indirect methods such characterizations of the solution can help us only in a very limited number of special cases to find an analytic exact representation of the solution. Although numerical solutions can be found based on the indirect methods, in the context of NMPC the so-called direct methods seem to be most promising and popular. They are characterized by discretization and finite parameterization being introduced in the optimal control problem formulation, which is then directly solved by numerical methods [9, chapter 2].

In order to reformulate the problem into a finite-dimensional and practical setting, the following assumptions are made that will allow the integral and differentiation operators to be approximated by numerical integration methods [9, chapter 2]:

- The horizon T is finite and given.
- The input signal $u[kT_s, kT_s+T]$ is assumed to be piecewise constant with a regular sampling interval t_u, such that T is an integer multiple of t_u, and parameterized by a vector $U \in \Re^p$, such that $u(kT_s+t) = \mu(kT_s+t, U) \in \Re^m$ is piecewise continuous.
- An (approximate) solution to (5) is assumed to be defined in the form $x(kT_s+t) = \varphi(kT_s+t, U, x_k)$ at N discrete time instants $T_d = \{kT_s+t_1, kT_s+t_2, \dots kT_s+t_N\} \subset [kT_s, Kt_s+T]$ for some ODE solution function $\varphi(\cdot)$. The discrete set T_d results from discretization of the ODEs and its time instants may not be equidistant. In general, the time instants need not coincide with the sampling instants.

As classified in [12], [9, chapter 2] there are two main approaches to direct numerical optimal control:

- **The sequential approach.** The ODE constraint (5) is solved via numeric simulation when evaluating the cost and constraint functions. This means that the intermediate states $x(kT_s+t_1), \dots x(kT_s+t_N)$ disappear from the problem formulation by substitution into the cost and constraint functions, while the control trajectory parameters U are treated as unknowns. This leads to a sequence of simulate-optimize iterations, often known as *Direct Single Shooting* (e.g. [13]).
- **The simultaneous approach.** The ODE constraints (5) are discretized in time and the resulting finite set of nonlinear algebraic equations are treated as nonlinear equality constraints. The intermediate states $x(kT_s+t_1), \dots x(kT_s+t_N)$ are treated as unknown variables together with the control trajectory parameters , and the cost function is evaluated simply by replacing the integral (6) by a finite sum. This leads to simultaneous solution of the ODEs and the optimization problem with a larger number of constraints and variables. The most well known methods of this type are *Direct Multiple Shooting* (e.g. [14]), and *Collocation methods* (e.g. [15]).

Mathematical Model of the pH Maintaining System

In this paper, the design of NMPC controllers for regulation of a pH maintaining system is considered. It is based on the analytical model of the system, described in [16].

A simplified schematic diagram of the pH maintaining system with the NMPC controller is shown in *figure 3*. The system consists of an acid stream (Q_1), buffer stream (Q_2) and base stream (Q_3), that are mixed in a tank T_1. The acid and buffer flow rates are assumed to be constant. The effluent pH and the liquid level h_1 are the measured variables, which are controlled by manipulating the base flow rate Q_3 and the exit flow rate Q_4.

The dynamic model of the pH maintaining system is derived using conservation equations and equilibrium relations [16]. Modeling assumptions include perfect mixing, constant density, and complete solubility of the ions involved. The model is presented briefly below according to [16].

The chemical reactions for the system are:

(7) $$H_2CO_3 \leftrightarrow HCO_3^- + H^+$$

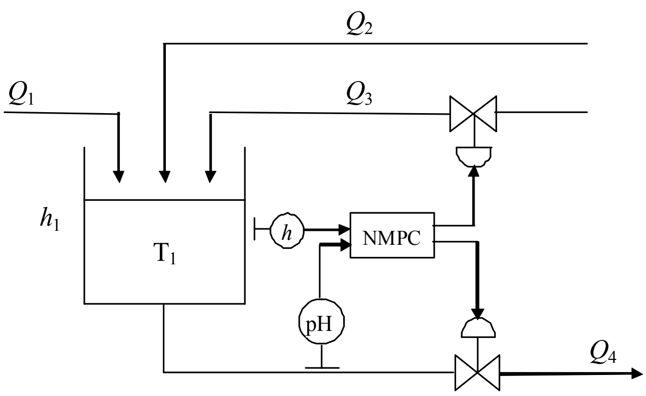

Figure 3. Scheme of the pH maintaining system with the NMPC controller

(8) $$HCO_3^- \leftrightarrow CO_3^= + H^+$$

(9) $$H_2O \leftrightarrow OH^- + H^+$$

The corresponding equilibrium constants are

(10) $$K_{a1} = \frac{[HCO_3^-][H^+]}{[H_2CO_3]},\ K_{a2} = \frac{[CO_3^=][H^+]}{[HCO_3^-]},\ K_w = [H^+][OH^-]$$

The chemical equilibria are modeled by defining two reaction invariants W_{ai} and W_{bi} for each of the streams Q_i, $i = 1,2,3,4$ [16]: [16]:

(11) $$W_{ai} = [H^+]_i - [OH^-]_i - [HCO_3^-]_i - 2[CO_3^=]_i$$

(12) $$W_{bi} = [H_2CO_3]_i + [HCO_3^-]_i + [CO_3^=]_i$$

The invariant W_a is a charge related quantity, while W_b represents the concentration of the $CO_3^=$ ion. The pH can be determined from W_a and W_b using the following relations [16]:

(13) $$W_b \frac{\frac{K_{a1}}{[H^+]} + \frac{2K_{a1}K_{a2}}{[H^+]^2}}{1 + \frac{K_{a1}}{[H^+]} + \frac{K_{a1}K_{a2}}{[H^+]^2}} + W_a + \frac{K_w}{[H^+]} - [H^+] = 0$$

(14) $$pH = -\log([H^+]).$$

In [16] a simplified model of the pH maintaining system is developed, where the dynamics of the pH transmitter is neglected. The mass balance on tank T_1 yields

(15) $$A_1 \frac{dh_1}{dt} = Q_1 + Q_2 + Q_3 - Q_4$$

where h_1 is the liquid level and A_1 is the cross-sectional area of the tank T_1. By combining mass balances on each of the ionic species in the system, the following differential equations for the effluent reaction invariants W_{a4} and W_{b4} are derived [16]

(16) $$A_1 h_1 \frac{dW_{a4}}{dt} = Q_1(W_{a1} - W_{a4}) + Q_2(W_{a2} - W_{a4}) + Q_3(W_{a3} - W_{a4})$$

(17) $$A_1 h_1 \frac{dW_{b4}}{dt} = Q_1(W_{b1} - W_{b4}) + Q_2(W_{b2} - W_{b4}) + Q_3(W_{b3} - W_{b4}).$$

Based on the above relations, a state space model of the pH maintaining system is obtained by defining the following state, input and output variables (x, u, y)

(18) $$x = [x_1\ x_2\ x_3] = [W_{a4}\ W_{b4}\ h_1],\ u = [u_1\ u_2] = [Q_3\ Q_4]$$
$$y = [y_1\ y_2] = [pH\ h_1]$$

The model has the form [16]

(19) $$\frac{dx}{dt} = f(x,u)$$

(20) $$c(x,y) = 0$$

where

(21) $$f(x,u) = \begin{bmatrix} \frac{Q_1(W_{a1} - x_1) + Q_2(W_{a2} - x_1) + u_1(W_{a3} - x_1)}{A_1 x_3} \\ \frac{Q_1(W_{b1} - x_2) + Q_2(W_{b2} - x_2) + u_1(W_{b3} - x_2)}{A_1 x_3} \\ \frac{Q_1 + Q_2 + u_1 - u_2}{A_1} \end{bmatrix}$$

(22) $$c(x,y) = x_1 + 10^{y_1 - 14} - 10^{-y_1} + \frac{x_2(1 + 2 \times 10^{y_1 - pK_2})}{1 + 10^{pK_1 - y_1} + 10^{y_1 - pK_2}}.$$

The relation between the constants K_{a1}, K_{a2} in (13) and the constants K_1, K_2 in (22) is

(23) $$K_{a1} = 10^{-pK_1},\ K_{a2} = 10^{-pK_2},\ p > 0.$$

The parameters of the model (19)-(23) are given in *table 1* [16].

Table 1. Nominal operating conditions for the pH maintaining system [16]

Q_1 = 16.6 [ml/s]	$K_{a1} = 4.47 \times 10^{-7}$
Q_2 = 0.55 [ml/s]	$K_{a2} = 5.62 \times 10^{-11}$
Q_3 = 15.6 [ml/s]	$K_w = 1 \times 10^{-14}$
Q_4 = 32.75 [ml/s]	$W_{a1} = 3 \times 10^{-3}$ [M]
Q_{1e} = 16.6 [ml/s]	W_{b1} = 0 [M]
A_1 = 207 [cm^2]	W_{a2} = – 0.03 [M]
A_2 = 42 [cm^2]	W_{b2} = 0.03 [M]
h_1 = 14 [cm]	$W_{a3} = -3.05 \times 10^{-3}$ [M]
H_2 = 3 [cm]	$W_{b3} = 5 \times 10^{-5}$ [M]
$\lceil Q_1 \rceil$ = 0.003 [M] HNO_3	$W_{a4} = -4.32 \times 10^{-4}$ [M]
$\lceil Q_2 \rceil$ = 0.03 [M] $NaHCO_3$	$W_{b4} = 5.28 \times 10^{-4}$ [M]
$\lceil Q_3 \rceil$ = 0.003 [M] NaOH, 0.0005 $NaHCO_3$	pH = 7

Nonlinear Model Predictive Control of the pH Maintaining System

In [16] a nonlinear output-feedback controller for the pH maintaining system is designed which combines an input-output linearizing controller with an open-loop observer. Here, the design and performance of two NMPC controllers for the pH maintaining system are considered, based on its analytical model.

NMPC Design with Box Constraints on the Control Inputs

At the current discrete time k the regulation NMPC solves the following optimal control problem:

(24) $$J^*(x_k) = \min_{u[kT_s, kT_s+T]} J(u[kT_s, kT_s+T], x_k)$$

given the current measured state x_k, satisfying the constraints on the two control inputs

(25) $10.6\ [\text{ml/s}] \le u_1(kT_s + t) \le 20.6\ [\text{ml/s}],\ t \in [0, T]$

(26) $22.75\ [\text{ml/s}] \le u_2(kT_s + t) \le 42.75\ [\text{ml/s}],\ t \in [0, T]$

and the terminal constraints

(27) $(y_1(kT_s + T) - y_1^*)^2 \le \delta_1$

(28) $(y_2(kT_s + T) - y_2^*)^2 \le \delta_2$.

In (27-28) $y_1(kT_s+T) = \text{pH}(kT_s+T)$, $y_2(kT_s+T) = h_1(kT_s+T)$ are the predicted values of the two outputs at the end of the prediction horizon (determined by solving the ODE (19) and the algebraic equation (20)), $y_1^* = 7$, $y_2^* = 14$ [cm] are the set-point values for pH and h_1, and $\delta_1 = \delta_2 = 0.01$. The cost function is defined by

(29) $$J(u[kT_s, kT_s+T], x_k) = \int_0^T \left[y^{\mathrm{T}}(kT_s+t)\Phi y(kT_s+t) + u^{\mathrm{T}}(kT_s+t)\Lambda u(kT_s+t) \right] dt + y^{\mathrm{T}}(kT_s+T)\Phi y(kT_s+T)$$

where $T = 140$ [s] is the prediction horizon, and $\Phi = \text{diag}\{150,100\}$ and $\Lambda = I$ are weighting matrices. In (29) $u_1^* = 15.6$ [ml/s] and $u_2^* = 32.75$ [ml/s] are the nominal values of the two control inputs. It should be noted that since the set-point value for the pH is 7, we have a pH neutralization system. However, the above NMPC problem can be easily reformulated to consider any other set-point value for the pH maintaining system.

The continuous pH maintaining process is discretized with a sampling interval $T_s = 7$ [s]. The trajectories of the two control inputs are parameterized with piecewise constant functions, such that the time horizon T is divided into $N = 20$ equal sized intervals. The infinite-dimensional optimal control problem (24-29) is transformed into a finite-dimensional optimization problem by applying the sequential approach (the single shooting method). The optimization variables are the values of the two control inputs at the N discrete times of the prediction horizon

(30) $U_1 = [u_{1,0}, u_{1,1}, \dots, u_{1,N-1}]$, $U_2 = [u_{2,0}, u_{2,1}, \dots, u_{2,N-1}]$.

The Euler's method with a step size $\Delta t = T_s/50 = 0.14$ [s] is applied to numerically integrate the ODE (19).

The following algorithm can be used for NMPC of the pH maintaining system:

Algorithm 1 (NMPC by on-line optimization)

1. Let the measured values of pH and the liquid level in the tank T_1 at the current discrete time k be $y_1(k) = \text{pH}(k)$ and $y_2(k) = h_1(k)$. The estimated values $\hat{W}_{a4}(k)$ and $\hat{W}_{b4}(k)$ of the two chemical invariants are obtained by using a state observer, as in [16]. The initial state vector for the optimal control problem (24-29) is $x_k = [\hat{W}_{a4}(k)\ \hat{W}_{b4}(k)\ h_1(k)]$.

2. The optimal control problem (24-29) is solved with an initial state vector x_k and the optimal trajectories $U_1^* = [u_{1,0}^*, u_{1,1}^*, \dots, u_{1,N-1}^*]$ and $U_2^* = [u_{2,0}^*, u_{2,1}^*, \dots, u_{2,N-1}^*]$ of the two control inputs are obtained.

3. The control input values applied to the pH maintaining system at the current time k are $u_1(k) := u^*_{1,0}$ and $u_2(k) := u^*_{2,0}$.

4. $k := k + 1$ and go to Step 1.

The performance of the NMPC controller is studied by simulations for different initial conditions of the pH maintaining system. In this case the values of the chemical invariants W_{a4} and W_{b4} are determined by numerical integration of the ODE (19) (not by using a state observer). The optimal trajectories of the two control inputs and the two outputs corresponding to the initial condition $h_1(0) = 14$ [cm], pH = 10.06 are shown in *figure 4* and *figure 5*.

It can be seen from *figure 4* that the control input takes the minimal allowed value at the initial part of its trajectory. From *figure 5* it is observed that the NMPC controller regulates pH to the set-point value.

NMPC Design with both Box Constraints and Rate of Change Constraints on the Control Inputs

In this case, at the current discrete time the regulation NMPC solves the following optimal control problem:

(31) $$J^*(x_k) = \min_{u[kT_s, kT_s+T]} J(u[kT_s, kT_s+T], x_k)$$

given the current measured state x_k, satisfying the constraints (25-28) and the additional constraints on the rate of change of the two control inputs

(32) $$-0.3\ [\text{ml/s}] \le T_s \frac{du_1(kT_s+t)}{dt} \le 0.3\ [\text{ml/s}],\ t \in [0, T]$$

(33) $$-0.3\ [\text{ml/s}] \le T_s \frac{du_2(kT_s+t)}{dt} \le 0.3\ [\text{ml/s}],\ t \in [0, T].$$

The cost function $J(u[kT_s, kT_s+T], x_k)$ is defined by (29). The optimal trajectories of the control inputs and outputs, corresponding to the initial condition $h_1(0) = 14$ [cm], pH(0) = 10.06 of the pH maintaining system are given in *figure 6* and *figure 7*.

It can be seen from *figure 6* and *figure 7* that the constraints on the rate of change of the two control inputs are active at the initial parts of their trajectories. From *figure 7* it can be observed that the pH transient is slower in comparison to the pH transient obtained with only box constraints on the control inputs (*figure 5*).

In *table 2* the CPU time required for the computation of the optimal control inputs with both NMPC controllers is given. The computations are performed on a PC with 3 GHz Intel Core 2 Duo processor.

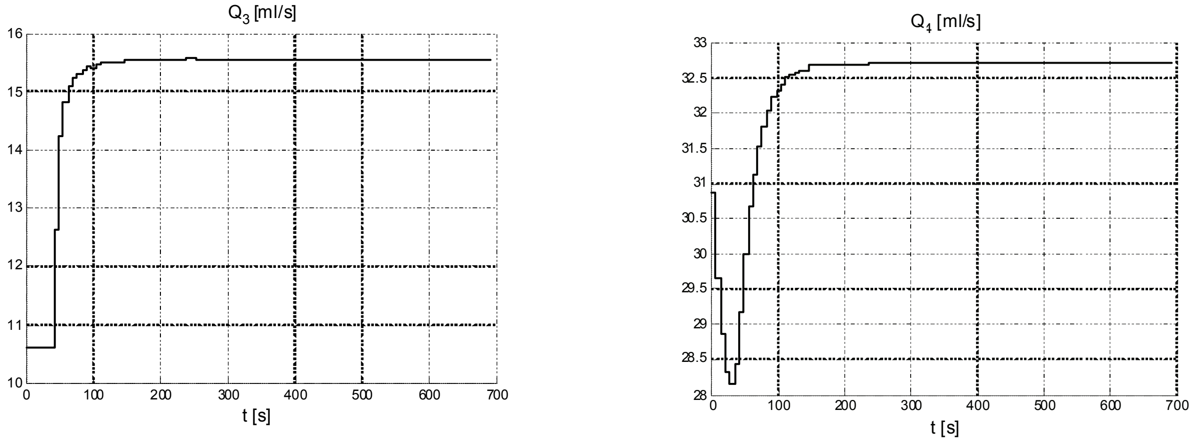

Figure 4. Optimal trajectories of the control inputs $u_1 = Q_3$ and $u_2 = Q_4$

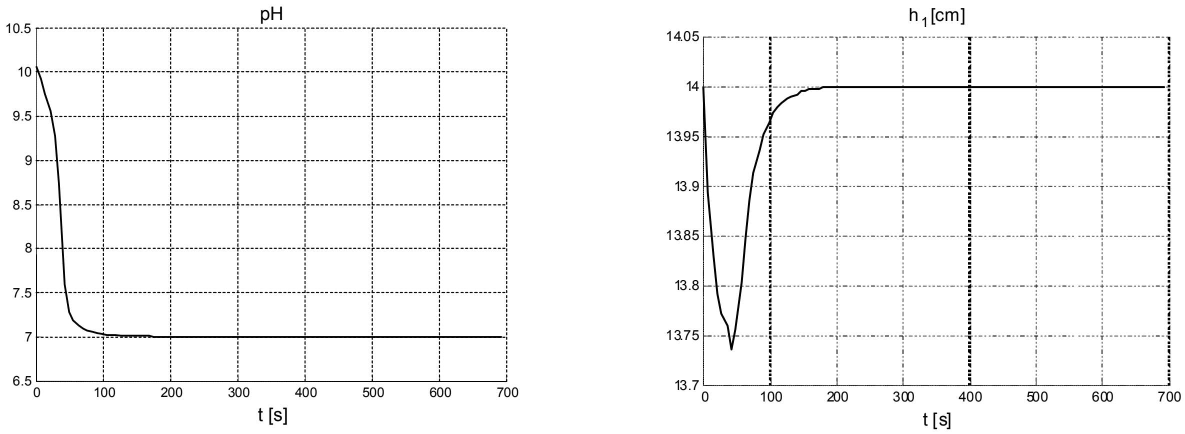

Figure 5. Optimal trajectories of the outputs y_1 = pH and $y_2 = h_1$

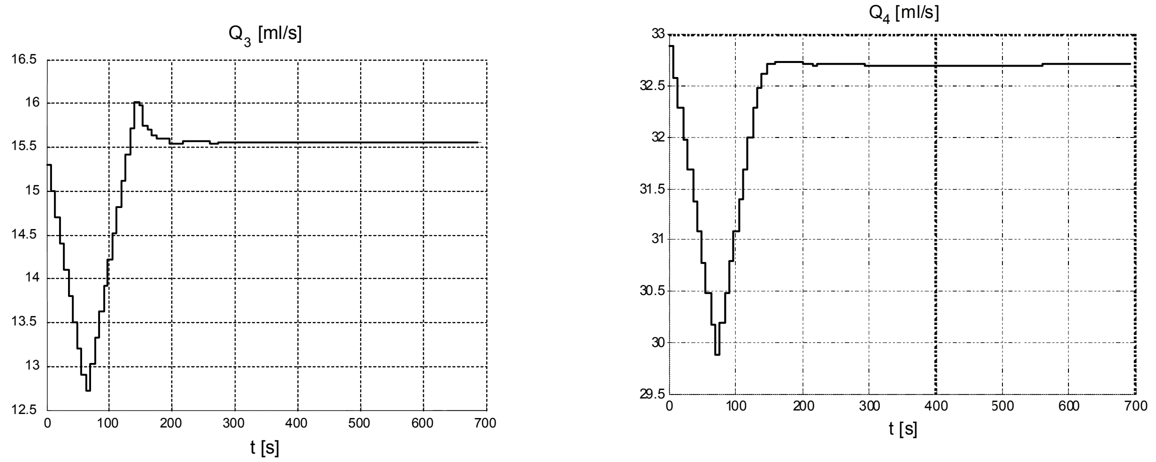

Figure 6. Optimal trajectories of the control inputs $u_1 = Q_3$ and $u_2 = Q_4$

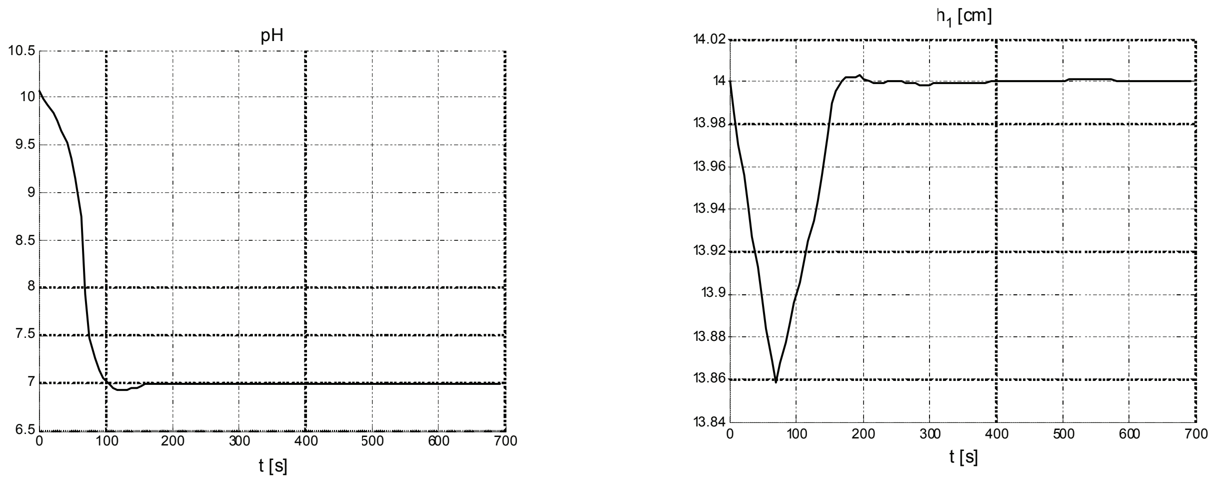

Figure 7. Optimal trajectories of the outputs y_1 = pH and $y_2 = h_1$

Table 2. CPU time for computation of the optimal control inputs

CPU time / NMPC controller	Average	Maximal
NMPC with only box constraints on the inputs	0.60 [s]	6.28 [s]
NMPC with both box and rate of change constraints on the inputs	0.72 [s]	5.17 [s]

Conclusions

In this paper the problem of optimal regulation of a pH maintaining system is considered, which is formulated as a NMPC problem in the presence of constraints. At each discrete time the optimal control inputs are computed by solving on-line a nonlinear programming (NLP) problem. It is shown that the NMPC controllers regulate the pH maintaining system to the specified set-point while satisfying all imposed constraints.

It should be noted that the on-line solution of a NLP problem is often computationally complex and time consuming. The on-line computational complexity can be circumvented with an explicit approach to NMPC, where an explicit approximate representation of the solution is computed using multi-parametric NLP (see [9,17]).

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