

Adaptive Receding Horizon Control of Tubular Bioreactors

J.M. Igreja, J. M. Lemos* and R. N. Silva

Abstract—This paper presents a case study of application of an adaptive nonlinear predictive control algorithm to tubular bioreactors. According to the control strategy proposed, the system of PDEs describing the reactor is approximated by a lumped parameter model obtained using the Orthogonal Collocation Method. An adaptive receding horizon controller is then designed using Control Lyapunov Function methods. The design procedure and the resulting performance is illustrated by simulations in a two reactions model with Contois kinetics .

I. INTRODUCTION

Nonlinear Predictive Control is receiving a strong attention in recent years, both for applications and basic research [1], [2]. Although the incorporation of adaptation mechanisms is a quite natural idea, the literature on the subject is scarce. A significant exception is [3] in which a solution to this problem is proposed on the basis of Control Lyapunov Functions (CLF), extending the work of [4] to incorporate adaptation.

In this paper, the aim is to apply the methods of [3], [4] to distributed parameter systems of hyperbolic type, using as a prototype problem the control of tubular bioreactors. The approach followed consists in approximating the hyperbolic PDE describing the plant by the Method of Orthogonal Collocation [10], and then designing an adaptive RHC using CLF methods.

Several works deal with the problem of tubular bioreactor control. The monograph [5] provides a comprehensive view of methods for nonlinear and robust control of both hyperbolic and parabolic PDE systems. The paper [6] applies MPC with active constraints to a parabolic PDE model of autoclave composite processing. The paper [7] applies DMC (Dynamic Matrix Control) to a linearized version of a tubular reactor in which a toluen hydro-dealkylation process takes process. None of the previous papers considers parameter adaptation or state estimation. Instead, paper [10] describes the adaptive control of a tubular bioreactor of hyperbolic type in which the distributed model is reduced to a system of ODEs by orthogonal collocation (as in here) the control being based in output feedback linearization assuming complete access to the state of the lumped model. The estimates are done by recursive least squares.

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The main contribution of this paper consists in the application of adaptive RHC to a case study in tubular bioreactors, thereby applying to distributed parameter plants this control strategy.

The paper is organized as follows: After this introduction, section 2 considers how to obtain a lumped parameter approximation for the class of plants considered using the Orthogonal Collocation Method. Section 3 tackles the adaptation law and sections 4 and 5 the design of RHC. The case study is developed in sections 6. Section 7 draws conclusions.

II. REACTOR MODELS

A. Distributed parameter model

Consider the following general model for fixed bed tubular reactors with m biochemical reactions and n components:

$$\frac{\partial b(z,t)}{\partial t} = k_b r(b,s) \quad (1)$$

$$\frac{\partial s(z,t)}{\partial t} + \frac{u(t)}{L} \frac{\partial s(z,t)}{\partial z} = k_s r(b,s) \quad (2)$$

where $b(z,t)$ is a $(n_b \times 1)$ vector of biomass concentrations, with initial condition $b(z,0)$, $s(z,t)$ is a $(n_s \times 1)$ vector of substrate concentrations flowing at velocity $u(t)$ with initial condition $s(z,0)$ and boundary condition $s(0,t) = s_{in}(t)$ (inlet concentration), $r(b,s)$ ($m \times 1$) is the kinetics of the bio-reaction which, associated to the yield coefficient matrices k_b ($n_b \times m$), k_s ($n_s \times m$) form the kinetic model, and L is the length of the tubular bioreactor. The variables z and t denote, respectively, normalized space and time: $z \in [0, 1]$, $t \in [0, +\infty[$.

Equations (1)-(2) form a set of matrix hyperbolic nonlinear PDEs. These equations are obtained by making mass balances and assuming that diffusion phenomena can be neglected.

B. Orthogonal Collocation

In the approach followed, the plant PDE model is approximated by the Orthogonal Collocation Method.

Consider the approximation for N collocation points expressed by:

$$b(z,t) = \sum_{i=0}^{N+1} \varphi_i(z) b_i(t) \quad (3)$$

$$s(z,t) = \sum_{i=0}^{N+1} \varphi_i(z) s_i(t) \quad (4)$$

The functions $\varphi_i(z)$ are usually selected as Lagrange interpolation polynomials verifying:

$$\varphi_i(z_j) = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

The z_i for $i, j=0, \dots, N+1$ are the collocation points, z_0 and z_{N+1} are the boundary collocation points, respectively for $z = 0$ and $z = 1$, and the interior collocation points $(1, \dots, N)$ are selected as the zeros of a Jacobi polynomial ($P_N^{\alpha, \beta}$). Replacing (3) and (4) in the model (1)-(2) one gets at the collocation points:

$$\dot{b}_j = k_b r(b_j, s_j) \quad (5)$$

$$\dot{s}_j + \frac{u}{L} \sum_{i=0}^{N+1} \varphi'_i(z_j) s_i(t) = k_s r(b_j, s_j) \quad (6)$$

with: $\varphi'_i(z_j) \equiv \frac{d\varphi_i(z)}{dz} \Big|_{z=z_j}$ and $j = 0, \dots, N+1$. Including the boundary condition at $z = 0$, $s_0(t) = s(0, t) = s_{in}(t)$ it is written in matrix form:

$$\dot{b} = K_b(b, s) \quad (7)$$

$$\dot{s} + \frac{u}{L} A s(t) + \frac{u}{L} B s_0(t) = K_s(b, s) \quad (8)$$

with

$$A = \begin{bmatrix} \varphi'_1(z_1) & \varphi'_2(z_1) & \cdots & \varphi'_{N+1}(z_1) \\ \varphi_1(z_2) & \varphi_2(z_2) & \cdots & \varphi_{N+1}(z_2) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi'_1(z_{N+1}) & \varphi'_2(z_{N+1}) & \cdots & \varphi'_{N+1}(z_{N+1}) \end{bmatrix} \quad (9)$$

$$B = \begin{bmatrix} \varphi'_0(z_1) \\ \varphi'_0(z_2) \\ \vdots \\ \varphi'_0(z_{N+1}) \end{bmatrix} \quad (10)$$

and in which

$$b(t) = [b_1(t) \quad b_2(t) \quad \cdots \quad b_{N+1}(t)]^T$$

$$s(t) = [s_1(t) \quad s_2(t) \quad \cdots \quad s_{N+1}(t)]^T$$

the vectors $K_b(b, s)$ and $K_s(b, s)$, of adequate dimensions, being build from the matrices k_b, k_s , respectively, and from the vectors $r(b_j, s_j)$.

Equations (7)-(8) may be written as the affine state-space model:

$$\dot{x} = K_\theta(x, \theta) + P(x, x_0)u \quad (11)$$

where $x(t) = [b(t) \quad s(t)]^T$ represents the state and $u(t)$ is the fluid velocity.

III. ADAPTATION LAW

Consider model (11) in which the parameter uncertainty is described by the term $W(x)\theta$:

$$\dot{x} = K(x) + W(x)\theta + P(x, x_0)u \quad (12)$$

It is possible in this way to tackle ill-understood kinetics, typical of bio-processes [10]. The vector θ ($p \times 1$) contains the parameters to estimate, in practice possibly slowly time varying.

Assume that the state x is estimated by x_p , yielded by the observer:

$$\dot{x}_p = K(x) + W(x)\hat{\theta} + P(x, x_0)u + K_p(x - x_p) \quad (13)$$

in which $\hat{\theta}$ is the estimate of the parameter vector θ and K_p ($n \times n$) is a symmetric positive definite matrix. The error dynamics $e = x - x_p$ satisfies:

$$\dot{e} = W(x)\tilde{\theta} - K_p e \quad (14)$$

where $\tilde{\theta} = \theta - \hat{\theta}$. In order to obtain a parameter estimation law consider the candidate Lyapunov function:

$$V(e, \tilde{\theta}) = \frac{1}{2} (e^T e + \tilde{\theta}^T \Gamma^{-1} \tilde{\theta}) \quad (15)$$

with Γ symmetric positive definite. Differentiating yields:

$$\dot{V} = -e^T K_p e + \frac{1}{2} \tilde{\theta}^T (W^T(x)e + \Gamma^{-1} \dot{\tilde{\theta}}) + \frac{1}{2} (e^T W(x) + \dot{\tilde{\theta}}^T \Gamma^{-1}) \tilde{\theta} \quad (16)$$

By choosing

$$\dot{\tilde{\theta}} = -\Gamma W^T(x) e \quad (17)$$

it is ensured that $\dot{V} < 0$ for $e \neq 0$ if $W(x) \neq 0 \forall x > 0$. Invoking LaSalle's invariance theorem it is concluded that when $t \rightarrow \infty$ then $e \rightarrow 0$. Assuming that $\hat{\theta} \approx 0$, i. e. that the parameters are constant, the following estimation law is obtained:

$$\dot{\hat{\theta}} = \Gamma W^T(x) e \quad (18)$$

IV. RECEDING HORIZON CONTROL

Consider the affine model (12) with output equation

$$\dot{x} = K(x) + W(x)\theta(t) + P(x, x_0)u \quad (19)$$

$$y = h(x) \quad (20)$$

in which $y(t)$ is the output to control and $u(t)$ is the manipulated input. Define the following general formulation of nonlinear receding horizon control [11], [2] to apply to this model:

$$\min_u J = \int_t^{t+T} [l(\tilde{y}(\tau)) + \tilde{u}(\tau)^T \rho \tilde{u}(\tau)] d\tau \quad (21)$$

subject to

$$\dot{x} = K(x) + W(x)\theta(t) + P(x, x_0)u \quad (22)$$

$$C(x, u, t) \leq 0 \quad (23)$$

with

$$\tilde{y}(t) = r(t) - y(t) \quad (24)$$

$$\tilde{u} = u - u_* \quad (25)$$

Here, J is the cost functional to minimize, $l(\tilde{y}(t))$ is a function weighting the error $\tilde{y}(t)$, $r(t)$ being the reference to track, ρ is the quadratic deviation of $u(t)$ with respect to the equilibrium u_* (associated to $r(t)$) and $C(x, u, t)$ represents the constraints (both operational and other).

A computationally efficient form of solving the above non-linear programming problem, which is of infinite dimension, consists in using a finite parameterization for the control signal $\{u(\tau), \tau \in [t, t+T]\}$, in which N_u sections of constant value u_1, \dots, u_{N_u} and duration $\frac{T}{N_u}$ are used. Thus,

the infinite dimensional non-linear programming problem is approximated by:

$$\min_{u_1, \dots, u_{N_u}} J = \int_t^{t+T} [l(\tilde{y}(\tau)) + \tilde{u}(\tau)^T \rho \tilde{u}(\tau)] d\tau$$

subject to

$$\begin{aligned} \dot{x} &= K(x) + W(x)\hat{\theta}(t) + P(x, x_0)u \\ x(t) &= \hat{x}(t) \\ C(x(\bar{t}), u(\bar{t}), t) &\leq 0 \\ u(\bar{t}) &= \text{seq}\{u_1, \dots, u_{N_u}\} \end{aligned}$$

in which $u(\bar{t})$ is a sequence of steps of amplitude u_i ($i = 1, \dots, N_u$) and duration $\frac{T}{N_u}$. The variable \bar{t} represents time during the minimization $\bar{t} \in [0, T]$.

Once the minimization result $u(\bar{t})$ obtained, only u_1 is applied to the plant at $t+\delta$ and the whole process is repeated. Here δ denotes the time needed to obtain the solution, being assumed that δ is assumed much smaller than the sampling interval. Since θ is not available, it is replaced by its estimate. Furthermore, when u_* is uncertain, it is common to replace \tilde{u} by $\Delta u = u_i - u_{i-1}$ with $u_0 = u(t)$.

V. STABILITY ISSUES

One way of ensuring stability of the adaptive RHC with accessible state consists in enforcing a constraint that implies a performance that is equal or greater to a control law that is stabilizing. Such a law is obtained on the basis of the existence of a positive definite function, $V(\tilde{x}) : \mathbb{R}^n \rightarrow \mathbb{R}_+$, called ISS-CLF (Input to State Stabilizing Control Lyapunov Function), satisfying [15]:

$$\begin{aligned} \inf_{\tilde{u}} \sup_{\theta} \dot{V} &= \inf_{\tilde{u}} \sup_{\theta} \{L_{K_*} V + \\ &+ L_{W_*} V \theta + L_{P_*} V \tilde{u}\} < 0 \quad \forall x \neq 0 \end{aligned} \quad (26)$$

or equivalently:

$$\begin{aligned} \inf_{\tilde{u}} \dot{V} &= \inf_{\tilde{u}} \{L_{K_*} V + \\ &+ L_{P_*} V \tilde{u} + \sum_{i=1}^{i=p} |L_{W_{*i}} V| \bar{\theta}_i\} < 0 \quad \forall x \neq 0 \end{aligned} \quad (27)$$

where $L_{(\cdot)} V$ is the Lie derivative of $V(\tilde{x})$ along the argument vector and $\bar{\theta}_i$ is an upper bound of $\hat{\theta}_i(t)$, *i. e.* $\bar{\theta}_i \geq |\hat{\theta}_i(t)|$ and \tilde{x} is the state deviation with respect to equilibrium, verifying:

$$\dot{\tilde{x}} = K_*(\tilde{x}) + W_*(\tilde{x})\tilde{\theta} + P_*(\tilde{x})\tilde{u} \quad (28)$$

with $K_*(0) = 0$. Remark that $\tilde{\theta}$ is bounded if a gradient projection method is used in the adaptation law (18), thereby constraining the estimate to the interior of a bounded convex set in the space of parameters [12]:

$$\mathcal{G}(\tilde{\theta}) = \{ \tilde{\theta} | \tilde{\theta}^2 \leq \bar{\theta}^2 \} \quad (29)$$

Furthermore, remark that the adaptation law (18) does not depend on $u(t)$ and implies that $\tilde{\theta} \rightarrow 0$, thereby ensuring the existence of a well defined equilibrium point. The universal feedback formula (Sontag's controller) [9] ensures, in a constructive way, the existence of a function $\tilde{u}(t) = k(\tilde{x})$, with

$k(0) = 0$, that verifies (27) and guarantees thus asymptotic stability, where $V(x)$ is a Lyapunov function for the closed-loop system:

$$\dot{V} < -\sqrt{a^2 + b^4} < 0 \quad (30)$$

where

$$\begin{aligned} a &:= L_{K_*} V + \sum_{i=1}^{i=p} |L_{W_{*i}} V| \bar{\theta}_i \\ b &:= L_{P_*} V \end{aligned}$$

In these conditions, the RHC+ISS-CLF can be formulated as:

$$\min_u J = \int_t^{t+T} l(\tilde{y}(\tau)) + \tilde{u}(\tau)^T \rho \tilde{u}(\tau) d\tau \quad (31)$$

subject to

$$\dot{x} = K(x) + W(x)\hat{\theta}(t) + P(x, x_0)u \quad (32)$$

$$C_1(x, u, t) \leq 0 \quad (33)$$

$$V(x_{rhc}(t+T)) \leq V(x_{iss}(t+T)) \quad (34)$$

where the condition (34) forces to attain a level curve, $V(x_{rhc})$, in the interior or at the boundary of the level curve which is attained when Sontag's formula is applied, $V(x_{iss})$, during the same time T . In other words, the stability condition imposes that the RHC controller has a performance equal or higher to the one yielded by Sontag's controller when applied in the same conditions for T seconds.

A detailed proof of stability of the RHC+CLF may be found in [12] and, for RHC+ISS-CLF, adaptive case, in [3].

VI. BIOREACTOR WITH CONTOIS KINETICS

Consider now the application of the above techniques to the specific case of a fixed bed tubular bioreactor with two reactions, where the specific growth rate is given by a Contois kinetics model [10].

A. Finite dimensional model

Consider the distributed parameter model of the reactor: with Contois kinetics with parameters $\bar{\mu}$, k_c . This model may be written in the general form (1)-(2) by making:

$$\begin{aligned} b(z, t) &= X(z, t) \\ s(z, t) &= [S(z, t) \quad X_d(t)]^T \\ s_{in}(t) &= [S_{in}(t) \quad 0]^T \\ r(b, s) &= [\mu X \quad k_d X]^T \\ k_b &= [1 \quad -1]^T \\ k_s &= [-k_1 \quad 0]^T \\ &= [0 \quad 1]^T \end{aligned}$$

Performing the reduction by OCM yields:

$$\begin{aligned} \dot{X}_j &= \left(\frac{\bar{\mu} S_j}{k_c X_j + S_j} \right) X_j - k_d X_j \\ \dot{S}_j &+ \frac{u}{L} \sum_{i=1}^{N+1} \varphi'_i(z_j) S_i(t) + \end{aligned} \quad (35)$$

TABLE I
BIOREACTOR PARAMETERS.

Parameter	Value	Units
L	1	m
k_1	0.4	-
k_c	0.4	-
k_d	0.05	h^{-1}
$\bar{\mu}$	0.35	h^{-1}

$$+\frac{u}{L} \varphi'_0(z_j) S_0(t) = -k_1 \left(\frac{\bar{\mu} S_j}{k_c X_j + S_j} \right) X_j \quad (36)$$

In matrix form (7)-(8) is written:

$$\dot{X} = K_x(X, S) \quad (37)$$

$$\dot{S} = -\frac{u}{L} (A S + B S_0) + K_s(X, S) \quad (38)$$

with $X(t) = [X_1 \cdots X_{N+1}]^T$, $S(t) = [S_1 \cdots S_{N+1}]^T$. The output is in this case the substrate concentration measure at the outlet, that is:

$$y(t) = S(t, 1) = S_{N+1}(t) \quad (39)$$

Table (I) shows the nominal values of the system "physical" parameters.

B. Adaptation

The adaptation laws for parameters $\theta_1 = k_d$ and $\theta_2 = k_1$ (consumption rate and yield rate – assumed uncertain) are now obtained. The coefficients associated to the kinetics, $\bar{\mu}$ and k_c are assumed to be known. According to the theory explained above, the adaptation law is given by

$$\dot{X}_p = M(X, S)X - \hat{\theta}_1 X + k_{px}(X - X_p) \quad (40)$$

$$\begin{aligned} \dot{S}_p = & -\frac{u}{L} (A S + B S_0) - \\ & -\hat{\theta}_2 M(X, S)X + k_{ps}(S - S_p) \end{aligned} \quad (41)$$

$$\dot{\hat{\theta}}_1 = -\gamma_x X^T (X - X_p) \quad (42)$$

$$\dot{\hat{\theta}}_2 = -\gamma_s X^T M^T(X, S)(S - S_p) \quad (43)$$

with $M(X, S) = \left[\frac{\bar{\mu} S_1}{K_c X_1 + S_1} \cdots \frac{\bar{\mu} S_{N+1}}{K_c X_{N+1} + S_{N+1}} \right]^T$ and where k_{px} and k_{ps} are the estimation gains and γ_x and γ_s are convergence coefficients of the adaptation law. It is assumed that the state is available at the collocation points, where the system coincides with the reduced model. Furthermore, remark that $M(X, S) > 0, \forall X, S > 0$.

C. Adaptive RHC control with the nominal model

Assuming that the state is accessible, the adaptive RHC for the bioreactor is defined by:

$$\min_u J = \int_t^{t+T} \tilde{y}^2(\tau) + \rho \Delta u^2(\tau) d\tau \quad (44)$$

TABLE II
RHC PARAMETERS.

Parameter	Value
T	8 h
N_u	8
ρ	250

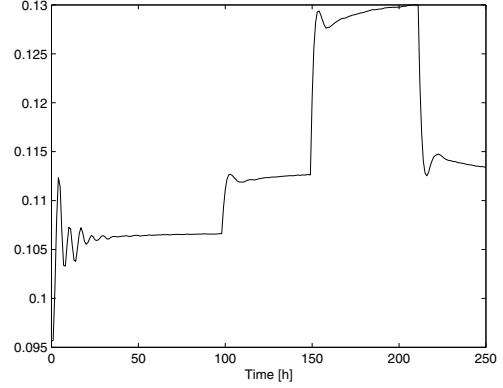


Fig. 1. Velocity: $u(t)$ [ms^{-1}].

subject to

$$\dot{X} = M(X, S)X - \hat{\theta}_1(t)X \quad (45)$$

$$\dot{S} = -\frac{u}{L} (A S + B S_0) - \hat{\theta}_2(t)M(X, S)X \quad (46)$$

$$M(X, S) = \left[\frac{\bar{\mu} S_1}{K_c X_1 + S_1} \cdots \frac{\bar{\mu} S_{N+1}}{K_c X_{N+1} + S_{N+1}} \right]^T \quad (47)$$

$$0.01 < u < 0.5 \quad (48)$$

Figures (1)-(3) show respectively the velocity (manipulated variable) $u(t)$, the output $y(t) = S_{N+1}(t) = s(1, t)$ (together with the correspondent reference) and the parameter estimates for the adaptive RHC controller of table (II). It is remarked that the parameter estimates converge in the first 30 h thereby not degrading the controller performance (fig. 3). The response to a sudden change in reference has a settling time smaller than 12.5 h and an overshoot of about 4%, fig. (2).

Figure (3) shows the estimate of the parameters, as a function of time, for an initial value of $\hat{\theta}_1(0) = 0.1$, $\hat{\theta}_2(0) = 0.3$. The estimates converge to $\hat{\theta}_1(\infty) = k_d = 0.05$ and $\hat{\theta}_2(\infty) = k_1 = 0.4$ which are coincident with the values of table (I). The estimation gains and the convergence coefficients are given in table (III).

TABLE III
ESTIMATION AND CONVERGENCE PARAMETERS.

Parameter	Value
k_{px}	$0.1 I_{N+1}$
k_{ps}	$0.1 I_{N+1}$
γ_x	0.1
γ_s	1.0×10^{-3}

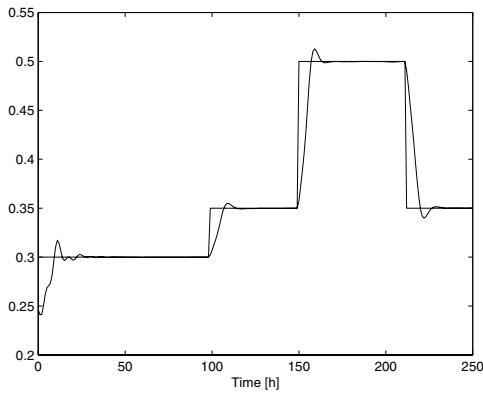


Fig. 2. Output: $s(1, t)$ [$gCODl^{-1}$].

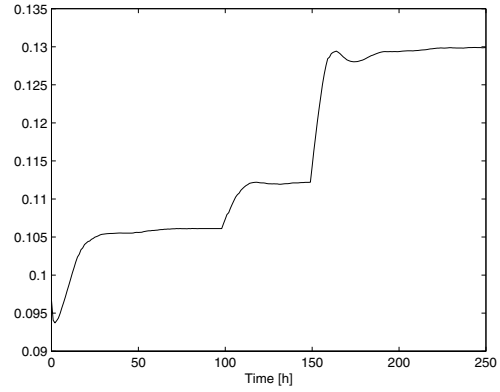


Fig. 4. Velocity: $u(t)$ [ms^{-1}].

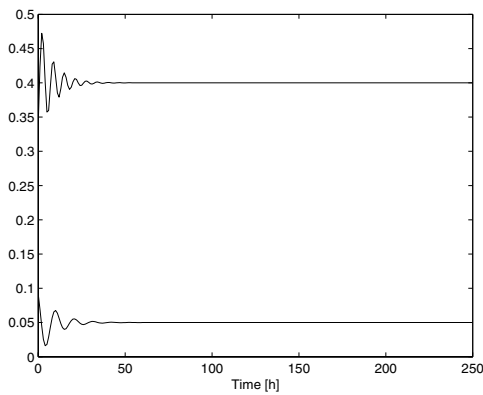


Fig. 3. Parameter estimates.

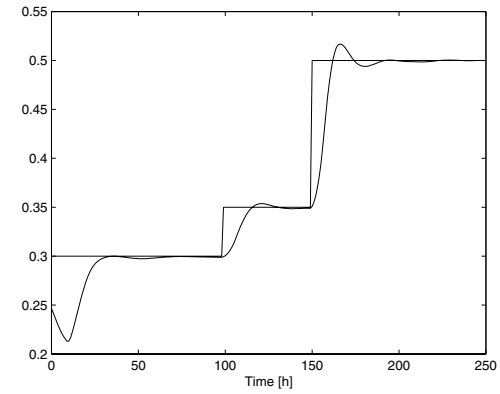


Fig. 5. Output: $s(1, t)$ [$gCODl^{-1}$].

D. Adaptive RHC with non-nominal model

Consider now the situation in which adaptive RHC is tested in a model obtained by finite differences (FD) with 500 elements, while the controller is still based on the reduced model obtained by OCM. It is assumed that the state is not accessible for measure, except at the outlet. In this situation, in addition to estimating the parameters, the unaccessible states ought to be estimated as well. This may be done by using an Adaptive Luenberger Observer [12], [13] and corresponds to modify the adaptation dynamics (40)-(43) such as to estimate also the states. This study mimics in a closer way a real situation in which there is model uncertainty and the states are not accessible. It is remarked that stability is no longer ensured.

Figures (4)-(6) show the results for the controller of (IV). In order to get an overshoot below 5% the value of ρ must be decreased, see table (IV). It is observed that the steady-state is attained with no static error. Finally, remark that the estimate of the parameters depends now on the velocity $u(t)$ thereby implying the existence of deviations in relation to the nominal value during transients. However, the estimates converge to the correct values in the first 50 h, as seen in the simulation performed with initial values $\hat{\theta}_1(0) = 0.1$, $\hat{\theta}_2(0) = 0.2$.

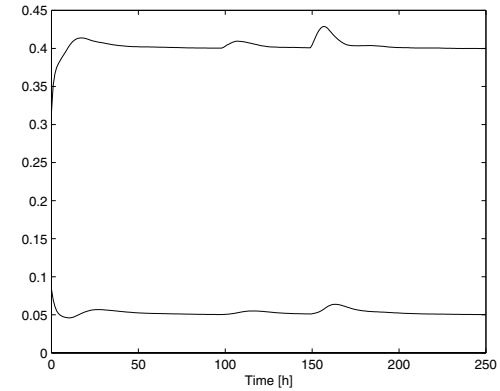


Fig. 6. Parameter estimates.

TABLE IV
RHC PARAMETERS.

Parameters	Value
T	6 h
N_u	6
γ	1250

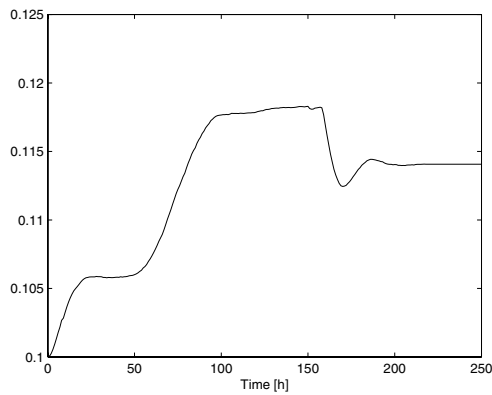


Fig. 7. Velocity: $u(t)$ [ms^{-1}].

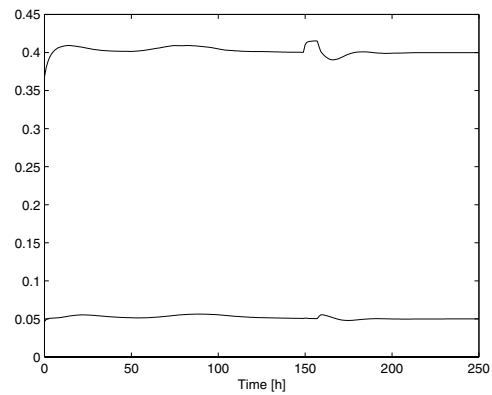


Fig. 9. Parameter estimates.

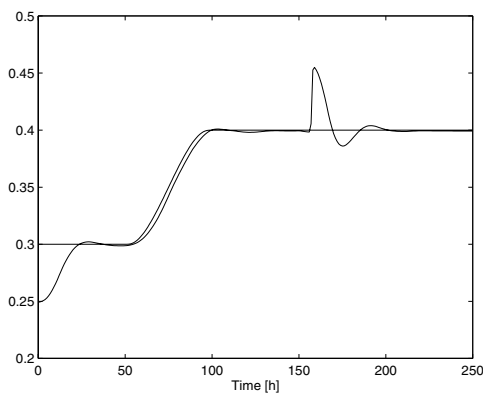


Fig. 8. Output: $s(1, t)$ [$gCODl^{-1}$].

Figs. (7)-(9) show the behaviour of the reactor when the inlet substrate suddenly raises 10% at 150 h. After the transient the output returns to the reference value, as well as the estimates.

VII. CONCLUSIONS

The paper extends to distributed parameter hyperbolic models an adaptive receding horizon control strategy based on Orthogonal Collocation and Lyapunov functions. The proposed method is illustrated in simulation through its application to a fixed bed tubular bioreactor with two reactions.

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