LYAPUNOV STABILITY CONSTRAINED ADAPTIVE NMPC FOR TUBULAR BIOREACTORS [*]

J. M. Igreja [*] **J. M. Lemos** [**] **S. J. Costa** [***]

[*] *INESC-ID and ISEL, Rua Alves Redol, 9, 1000-029 Lisboa, Portugal.*
jigreja@deea.isel.ipl.pt
[**] *INESC-ID/IST, Rua Alves Redol, 9, 1000-029 Lisboa, Portugal.*
jlml@inesc.pt
[***] *ISEL, Rua Cons. Emdio Navarro, 1, 1959-007 Lisboa, Portugal.*
sjcosta@deq.isel.ipl.pt

Abstract: An adaptive NMPC for a given class of uncertain (bio)systems with transport phenomena in which the manipulated variable is the velocity is formulated and developed. A stable distributed parameter estimator is derived, in the Lyapunov sense, and combined with the NMPC algorithm using the certainty equivalence principle. Stability, for the combined NMPC with the adaptive law, is guaranteed without increasing significatively the computational burden through a pointwise constraint that ensures outperforming a robust control stabilizing law. The design procedure and the resulting performance is illustrated by simulations in a bioreactor with a Contois kinetics. *Copyright ©Controlo 2012.*

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1. INTRODUCTION

Nonlinear Model Predictive Control [6, 17, 18] has important advantages for advanced process control. This is due to the fact that it allows an easy incorporation of constraints, making it a decisive advantage for industrial applications when compared to other methods. It can also be very easily extended to (and well understood in) the multivariable case. However, from a implementation standpoint, a major issue consists in ensuring stability for a short finite horizon in an uncertain environment without dramatically increasing the computational effort. From a practical perspective guaranteed closed-loop stability is convenient but not decisive and many MPC techniques applied in process industries do not meet this feature. In this paper a stabilizing NMPC for a given class of uncertain biosystems with transport phenomena, associated with fluid flow in pipes, is formulated. NMPC robust closed-loop stability is guaranteed with the inclusion of a stabilizing condition based in a robust Lyapunov control function (RLCF) also known as pointwise min-norm control (PWMNC) [14, 15, 16]. A stable distributed parameter estimator, in the Lyapunov sense, is also combined with the NMPC algorithm, using the certainty equivalence principle for adaptation proposes.

Albeit Nonlinear Predictive Control continue to receive a strong attention in recent years, both in basic research and in applications, the incorporation of adaptation mechanisms, as the natural idea to tackle parametric uncertainty at a low computational cost, is quite new. The literature on the subject is gaining now some meaning, see for instance [1, 2]. Early results for distributed systems can be found in [8]. Predictive control of hyperbolic PDE systems, namely transport-reaction processes, was studied in [5, 20] for SISO cases. In the former the controller is based on a predictive model developed using the method of characteristics and does not consider constraints. In the latter finite differences for space discretization and a space distributed actuator were used with success.

In [7] adaptive predictive control was obtained via Orthogonal Collocation (OC) [19] reduced modelling, also for SISO hyperbolic tubular transport-bioreaction processes, that demonstrated to achieve the control objectives. Stability conditions are also derived and discussed. Pioneer research for adaptive control of tubular bioreactors with OC reduced models and Feedback Linearizing can be found in [4].

The main contribution of this paper consists in the formulation of a Lyapunov stable efficient adaptive NMPC for a broad class of parametric uncertain nonlinear partial differential equation systems, that exhibits (bio)mass and energy transport. Therein adaptation is achieved by a stable distributed law, suitable for the entire system class, which requires a low computational effort. Stability is ensured online by a constraint justified via a RCLF condition that arises from the relation between PWMNC and RHC (Receding Horizon Control).

The paper is organized as follows: after this introduction, the prototype model of the tubular biosystem class is considered and described by a set of partial differential equations (PDE), section 2. Section 3 introduces the general stabilizing formulation of a NMPC for the infinite dimension system class. Stability condition is derived in section 4. In section 5 a distributed adaptive law in the sense of Lyapunov (LAL) is obtained and the adaptive NMPC is stated combining RH+LAL. Application to Contois kinetics tubular bioreactor is described in section 6. Section 7 draws conclusions.

2. CLASS OF PDE MODELS

Considered the dynamical model

$$\frac{\partial x(z,t)}{\partial t} + \mathcal{L}(x(z,t),u(t);\theta) = s(x(z,t),u(t);\theta) \quad (1)$$

$$\mathcal{M}(x(z,t),u;\theta) = 0 \qquad (2)$$

$$y_k(t) = \int_0^1 b_k(z)\, h_k(x(z,t))\, dz \quad (k=1,...,p), \quad (3)$$

where $(z,t) \in [0,1] \times \mathbb{R}^+$, the state trajectories $x(.,t) \in X \subset [0,1] \times \mathbb{R}^n$, the manipulated input $u(t) \in U \subset \mathbb{R}^m$ is bounded and the output $y(t) \in Y \subset \mathbb{R}^p$ is also bounded. Operator $\mathcal{L}(.,u;\theta)$ is a quasi-linear matrix space operator. Boundary conditions are given by the nonlinear space operator $\mathcal{M}(.,u;\theta)$. Vectors functions $s(x,u), h(x)$ are smooth vectors of nonlinear functions, $s(x,u) : \mathbb{R}^n \times \mathbb{R}^m \mapsto \mathbb{R}^n$, $h(x) : \mathbb{R}^n \mapsto \mathbb{R}$. The space weight $b_k(z) > 0 : [0,1] \to \mathbb{R}^+$ satisfies $\int_0^1 b_k(z)\, dz = 1$. The column vector $\theta \in \Theta \subset \mathbb{R}^q$ denotes the uncertain parameters or additive disturbances that lies within a known open convex set $\Theta = \{\theta : \underline{\theta} < \theta < \overline{\theta}\}$. The $\mathcal{L}$ operator must include convection terms $v\frac{\partial(.)}{\partial z}$ and will depend on the manipulated variable(s) when $u \equiv v$ (v is the fluid velocity). If the manipulated variable is space weighted additive in the production

term then $s(x,u;\theta) = s_x(x;\theta) + s_u(x;\theta)\, w(z)\, u$, in both cases the manipulated variable(s) is explicit on equation (1) and it will be implicit when it only appears in the boundary condition (2). These prototype class allows the study of a wide variety of processes with transport phenomena and define the class of systems under study. Remark that this set of equations models a process that occurs in a tubular or cylindrical domain. The state variables $x_k(z,t)$ $(k=1,\ldots,n)$ represent the (bio)chemical species and the mixture temperature along normalized space ($z \in [0,1]$) and time ($t \in [0,+\infty[$), being v the transport velocity. The system is thus modelled by n quasi-linear PDEs in the state variables $x_k(x,t)$, that result from applying conservation principles (mass or biomass and energy balances) [3, 13].

3. PROPOSED NMPC GENERAL FORMULATION

The aim is to control the output $y(t)$, eq. (3), a state nonlinear function weighted in the space domain, by manipulating the input $u(t)$, solving an open loop optimization problem and applying a receding horizon (RH) strategy according to the NMPC approach [17, 18]. Therefore, define the basic optimal control problem with quadratic cost functional:

$$\min_u J = \int_t^{t+T} \left(\|\tilde{y}(\tau)\|_Q^2 + \|\tilde{u}(\tau)\|_R^2 \right) d\tau, \qquad (4)$$

where $Q \geq 0$ and $R > 0$ are weighting matrices, subject to the model (1)-(3) with operational constraints of the general form

$$O(\dot{\xi}(x(t)), \dot{y}(t), \dot{u}(t), \xi(x(t)), y(t), u(t), t) \leq 0 \quad (5)$$

and with a specific stability constraint, discussed in the sequel:

$$\max_{\theta \in \Theta} \{\dot{V}(\tilde{x};\theta)\} + \alpha V(\tilde{x}) < 0. \qquad (6)$$

In (4) to (6)

$$V(\tilde{x}) = \frac{1}{2} \int_0^1 \tilde{x}^T q(z) \tilde{x}\, dz$$

$$\xi(x(t)) = \int_0^1 B(z)\zeta(x)\, dz, \quad \int_0^1 B(z)\, dz = I,$$

$$\tilde{y} = y_r - y, \quad \tilde{u} = u_r - u \text{ and } \tilde{x} = x_r - x, \qquad (7)$$

where y_r, x_r and u_r define the reference trajectory to track, $\xi(t)$ is broad set of state functions and $q(z)$ is a space weighting matrix. The stability condition forces the RHC to have a performance that is equal or higher to a stabilizing control law when applied in the same conditions [7]. One approximated computationally efficient procedure for solving the stated nonlinear, infinite dimension, non-convex programming problem is to use a finite parametrization for the control signal $u(t) \in [t, t+T[$, where N_u segments of constant value $u_1, \ldots, u_{N_u}$ and duration $\frac{T}{N_u}$, as decision variables. Thus the suboptimal, finite dimension, constrained programming problem amounts to solve:

$$\min_{u(\bar{t})} J = \int_t^{t+\mathcal{T}} \left(\left(\|\tilde{y}\|_Q^2 + \|\tilde{u}\|_R^2 \right) \right) d\tau \qquad (8)$$

$$s.\,t. \quad O(\dot{\xi}(x(\bar{t})), \dot{y}(\bar{t}), \dot{u}(\bar{t}), \xi(x(\bar{t})), y(\bar{t}), u(\bar{t}), \bar{t}) \le 0$$

$$\max_{\theta \in \Theta} \{\dot{V}(\tilde{x}(t); \theta)\} + \alpha V(\tilde{x}(t)) < 0$$

$$u(\bar{t}) = seq\{u_1, \dots, u_{N_u}\}$$

and also subject to the proper space semi-discrete model obtained from the original distributed one [7], where $u(\bar{t})$ is the sequence of steps of amplitude u_i and the variable $\bar{t}$ represents virtual time during the minimization computation, $\bar{t} \in [0, \mathcal{T}[$. Once the minimization result $u(\bar{t})$ is obtained, the first sample u_1 is applied at $t + \delta$ and the whole procedure is repeated. The interval δ corresponds to the time needed to obtain a solution, being assumed that δ is much smaller than the sampling interval. Remark that, if θ is uncertain, an estimate $\hat{\theta}$ of it is needed to perform the minimization, see [9]. As stated in [17] the MPC solution (8) "*is best regarded as a practical means of implementing the Dynamic Programming solution (control law)*" of (4-7).

4. STABILITY

In this section a PWMN [14] control based in a RCLF [16] is developed for the stated class of systems. The relation with NMPC problem is explained suggesting at the same time how the stability condition could be included as a constraint in the optimization problem statement.

An implicit stabilizing controller may be design using the following optimization statement [16]: *if $V(\tilde{x}) > \phi$ then*

$$\min_{u \in U} \quad u^T u \qquad (9)$$

$$s.\,t.\,(1) \textit{ and } \max_{\theta \in \Theta}\{\dot{V}(\tilde{x}; \theta)\} + \alpha V(\tilde{x}) < 0$$

where $V(\tilde{x}) : X \to \mathbb{R}_{\ge 0}$ is a continuously differentiable, positive definite and radially unbounded function in respect to the L_2 norm of $\tilde{x}$, and $\tilde{x}(z,t) = x(z,t) - x_r(z; \theta_0)$ is the difference between the actual state and a steady state profile along space length, where $x_r \in X_r$, obtained for parameter nominal value θ_0. In other words, $V(\tilde{x})$ is simply a robust CLF candidate whose derivative maximum can be made less than $-\alpha V(\tilde{x})$ pointwise by the choice of control values outside a small region around the origin. This region can be made arbitrarily small by picking ϕ sufficiently small. Small control property, see [21], and numerical issues can be avoided in this way. The parameter α relax convergence.

The most obvious choice for the CLF candidate is:

$$V(\tilde{x}) = \frac{1}{2} \int_0^1 \tilde{x}^T q(z) \tilde{x} \, dz \qquad (10)$$

where $\int_0^1 q(z) \, dz = 1$, with $q(z)$ positive definite. Using Lyapunov stability arguments [12]: any $\tilde{x}(z,t)$ solution, originating in a bounded region, will asymptotically tend to the included invariant region parameterized by ϕ as $t \to \infty$, if $\dot{V} < 0$ ($\forall \tilde{x} \ne 0$). In this case, the time derivative of (10) yields:

$$\dot{V} = \frac{1}{2} \int_0^1 \frac{\partial}{\partial t} \left(\tilde{x}^T(z,t) \, q(z) \, \tilde{x}(z,t) \right) dz \qquad (11)$$

using (1):

$$\dot{V} = \int_0^1 (s(x,u;\theta) - \mathcal{L}(x,u;\theta)^T q(z) \tilde{x}(z,t) \, dz \qquad (12)$$

and the robust optimization condition, for the class of systems under study, is given by:

$$\max_{\theta} \left\{ \int_0^1 (s(x,u;\theta) - \mathcal{L}(x,u;\theta))^T q(z) \tilde{x}(z,t) \, dz \right\}$$
$$+ \frac{\alpha}{2} \int_1^0 \tilde{x}^T q(z) \tilde{x} \, dz < 0 \quad (13)$$

Remark that one of the following conditions must hold *a priori* in relation to the manner how the inputs appear in eq. (1). Condition $\int_0^1 (\frac{\partial x}{\partial z})^T A_v \, q(z) \tilde{x} \, dz \ne 0$, where A_v is a diagonal matrix with one or zero in the main diagonal, must hold if the corresponding state is related with the manipulated velocity. Or $\int_0^1 (s_u(x;\theta) \, w(z) \, u)^T q(z) \tilde{x} \, dz \ne 0$ *iff* $u \ne 0$ if u is related with the production term. Finally $\mathcal{M}(x,u,\theta) \ne 0$ *iff* $u \ne 0$ if u is implicit through boundary conditions. If these conditions do not hold then controllability from u to the 'output' $\equiv V$ is lost. Remark also that these conditions depend on $q(z)$ for finding V and if the corrected condition does not hold then the candidate V is not a RCLF and a different candidate or method must be used.

An important PWMN control feature is the fact that it corresponds to a NMPC limit stabilizing solution when the horizon value goes to zero. Consider the following NMPC formulation:

$$\min_{u \in U} \int_0^{\mathcal{T}} (V(\tilde{x}(z,\tau)) + \|\tilde{u}\|_R^2) d\tau \qquad (14)$$

$$s.\,t.\,(1) \textit{ and } \max_{\theta \in \Theta}\{\dot{V}(\tilde{x}; \theta)\} + \alpha V(\tilde{x}) < 0,$$

when the horizon $\mathcal{T}$ tends to zero:

$$\min_u \lim_{\mathcal{T} \to 0} \frac{1}{\mathcal{T}} \int_0^{\mathcal{T}} (V(\tilde{x}(z,\tau)) + \|\tilde{u}\|_R^2) d\tau$$
$$= \min_u \{V(\tilde{x}(z,t)) + \|\tilde{u}\|_R^2\} \Leftrightarrow \min_u \|\tilde{u}\|_R^2 \qquad (15)$$

showing the equivalency to the PWMN control. Remark that dividing (14) by $\mathcal{T}$ has no effect on the optimization problem and also that when $\mathcal{T}$ goes to zero there is no need to include the term $V(\tilde{x})$ because it is not affected by u and so forth constant. Hence this simple observation, stated in [14], indicates that as $\mathcal{T}$ goes to zero, RH controllers loses the ability to maintain acceptable performance by just minimizing

input energy. Performance degradation can lead in general to closed-loop instability if the robust PWMN condition or some other equivalent mechanism is not included to assure stability. Remark also that the constraint requires V to be a Robust Control Lyapunov Function (RCLF) for any receding horizon value and by that closed-loop stability is guaranteed. More details about the robust stability condition can be found in [10].

5. ADAPTIVE CONTROL

One way to tackle parameter uncertainty is to use an observer for estimating parameters since the state is considered accessible [1, 8]. Consider the model (1) in pug-flow conditions and that the manipulated variable is the fluid velocity:

$$\mathcal{L}_x = \mathcal{L}(x(z,t),u(t);\theta) = \frac{u}{L}A_v\frac{\partial x(z,t)}{\partial z} \qquad (16)$$

where A_v is a diagonal matrix with one or zero main diagonal elements, depending if there is a related transport term or not. Considering that typical process production terms are in many cases linear affine in θ it's assumed that:

$$s(x;\theta) = s_0(x) + \sum_{i=1}^{q}\theta_i s_i(x) = s_0(x) + S(x)\theta \qquad (17)$$

where $s_0(x)$ is a vector of smooth nonlinear functions $(n \times 1)$, $S(x)$ is a matrix of smooth nonlinear functions $(n \times q)$ and $\theta = [\theta_1 \cdots \theta_q]^T$ is an uncertain parameters vector assumed time constant or very slowly varying, the observer filter dynamics in the form [22, 1]

$$\frac{\partial x_a(z,t)}{\partial t} + \frac{u}{L}A_v\frac{\partial x(z,t)}{\partial z} = s(x;\hat{\theta}) + \mathcal{K}(x-x_a) \quad (18)$$

where $\mathcal{K} > 0$, the observation error dynamics ($e_a = x - x_a$) is given by

$$\frac{\partial e_a}{\partial t} = S(x)\tilde{\theta} - \mathcal{K}e_a$$

with $\tilde{\theta} = \theta - \hat{\theta}$. Finally introducing the Lyapunov candidate function [12]:

$$V(e_a,\tilde{\theta}) = \frac{1}{2}\left(\int_0^1 e_a^T e_a\, dz + \tilde{\theta}^T\Gamma^{-1}\tilde{\theta}\right), \qquad (19)$$

where Γ is a weighting matrix, differentiating V with respect to time, using the error dynamics and choosing:

$$\dot{\hat{\theta}} = -\Gamma\int_0^1 S(x)^T e_a\, dz \qquad (20)$$

it guarantees $\dot{V}(e_a) < 0$ when $e_a \neq 0$.

By this way the errors go to zero ($e_a(t)$ and $\tilde{\theta} \to 0$ as $t \to \infty$), after initial conditions transient ($w(0)$, $x(0)$ and $\hat{\theta}(0)$), if the nonlinear functions $S(x) \neq 0$ locally. Remark that $\tilde{\theta}$ can be bounded by the use of the projection method [11], thereby constraining the estimated to the interior of a bounded convex parameters space.

Combining NMPC with LAL dynamics, the RHC+LAL solution is formulated, like in [9], using (4) subject to the predictive model (1), in which θ is made equal to $\hat{\theta}(t)$, operational constraints (5) and the stability constraint (6). Additionally, parameters estimate and distributed observer dynamics are computed in parallel, for each sampling period, by:

$$\frac{\partial x_a}{\partial t} = -\mathcal{L}_x + s_0(x) + S(x)\hat{\theta} - \mathcal{K}(x-x_a) \qquad (21)$$

$$\dot{\hat{\theta}} = \text{Proj}\left\{\Gamma\int_0^1 S^T(x)(x-x_a)\, dz, (\overline{\theta},\underline{\theta},\varepsilon)\right\} \qquad (22)$$

where x and x_a are the system and observer state respectively and $\overline{\theta} + \varepsilon \geq \hat{\theta} \geq \underline{\theta} - \varepsilon$.

6. 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 is given by a Contois kinetics model [4]:

$$\frac{\partial x_b}{\partial t} = \mu x_b - k_d x_b \qquad (23)$$

$$\frac{\partial s}{\partial t} + \frac{u}{L}\frac{\partial s}{\partial z} = -k_1\mu x_b \qquad (24)$$

$$\frac{\partial x_d}{\partial t} + \frac{u}{L}\frac{\partial x_d}{\partial t} = k_d x_b \qquad (25)$$

$$\mu = \frac{\bar{\mu}s}{k_c x_b + s}, \qquad (26)$$

where $x_b(z,t)$ is the biomass concentration, $s(z,t)$ and x_d are the substrate and non-active biomass concentration flowing at velocity $u(t)$, k_1 is the yield coefficient, k_d is the consumption rate. The coefficients associated to the kinetics, $\bar{\mu}$ and k_c are assumed known. Nominal parameter values are given in table 1, consumption and yield rates are assumed uncertain $\theta = [k_d \ k_1]^T$.

The NMPC algorithm proposed uses a space semi-discrete model obtained by the OC Method in $N = 6$ space collocation points, for details see [7]. The velocity satisfies $0.01 < u < 0.5$. The state is considered available at the collocation points. It can be shown that using OC with $N = 6$ corresponds to more than 500 finite difference for semi-discretized space in the numerical PDE model solution.

Figures 1-3 show respectively the velocity (manipulated variable) $u(t)$, the output $y(t) = s(1,t)$ and the parameters estimates for the *tuned* adaptive NMPC controller of table 2 (where ρ is the control effort). Remark that the parameter estimates converge in the first $30h$ thereby not degrading the controller performance. The response to a sudden change in set-point has a settling time smaller than $12.5h$ and an approximately 20% overshoot. Figure 3 shows the estimated parameters, for initial values $\hat{\theta}_1(0) = 0.1$, $\hat{\theta}_2(0) = 0.3$. The estimates converge to the nominal values given in table 1. The estimation gains and the convergence

Table 1. Bioreactor parameters.

Parameters	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}

Table 2. Tuned RHC parameters.

Parameters	Value
$\mathcal{T}$	$6\,h$
N_u	6
ρ	250
α	0.001

Table 3. Estimation and convergence parameters.

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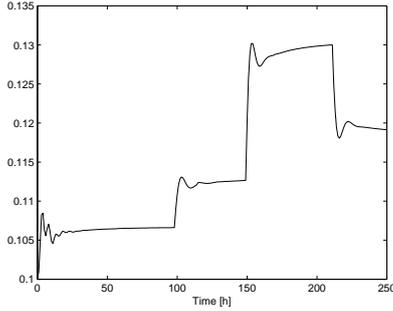
Fig. 1. Velocity: $u(t)$ $[ms^{-1}]$.
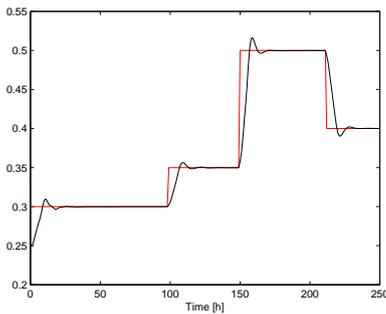
Fig. 2. Output: $s(1,t)$ $[gCODl^{-1}]$.

coefficients are given in table 3. Figure 4 shows the Lyapunov function decreasing for each step set-point change. Because the control law is well tuned the stability condition is not active during all simulation. Figures 5-7 show the behavior for a *detuned* control law with minimum prediction horizon $\mathcal{T} = 1\,h$ and very small input weight $\rho = 0.01$. In this case the stability condition is active during some periods preventing closed-loop instability. Figures also compare results with and without including the stability condition. Figure 8 shows that the adaptation converges even when closed-loop stability is in risk.
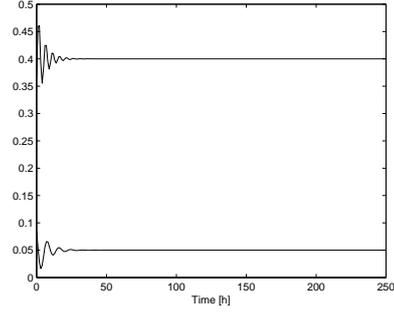

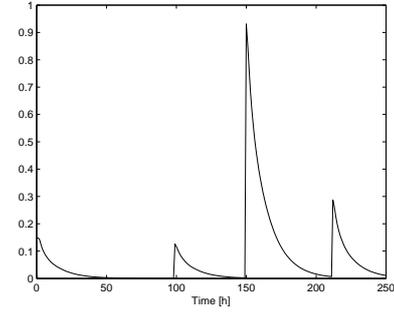Fig. 3. Parameters estimation: $\hat{k}_d$, $\hat{k}_1$.
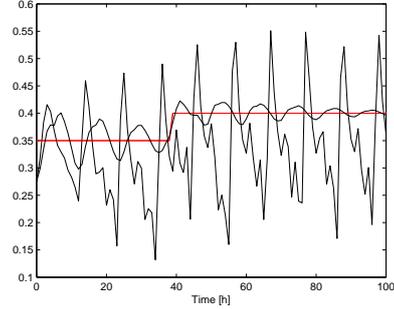

Fig. 4. Lyapunov function: $V(t)$.
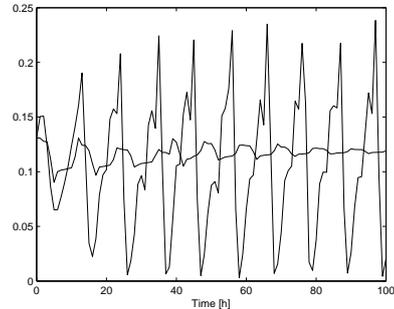

Fig. 5. Output: $s(1,t)$ $[gCODl^{-1}]$.

Fig. 6. Velocity: $u(t)$ $[ms^{-1}]$.

7. CONCLUSIONS

An stable adaptive NMPC formulation for an uncertain class of distributed parameter biosystems is introduced and exemplified. A general stability condition for the combined NMPC nominal formulation with a stable parameter observer is developed. Low com-
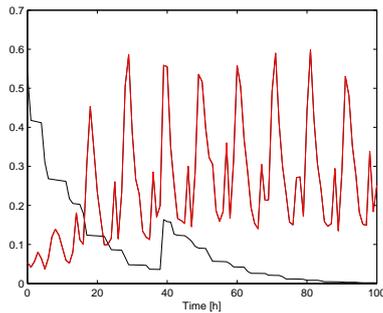
Fig. 7. Lyapunov function: $V(t)$ decreasing, $V(t)/10$ without stability condition oscillating.
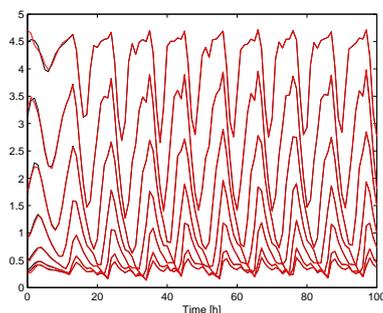

Fig. 8. Substrate and Subtract estimation: $S(t)$, $S_a(t)$ $[gCODl^{-1}]$.

putational effort for closed-loop stability and on-line parameter estimation as a way to deal with uncertainty can justified this type of approach. Application of a stabilizing NMPC+LAL was successful for tubular bioreactor.

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