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ADAPTIVE LINEARIZING CONTROL OF BIOREACTORS

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In this communication we shall present developments concerning the synthesis of Single-Input, Single-Output (SISO) and Multi-Input, Multi-Output (MIMO) adaptive linearizing algorithms for the operation of bioreactors. Results will be illustrated for the baker's yeast fermentation process.

The synthesis of these non-linear control laws is performed by employing differential geometry techniques with system linearization by state feedback. The controller design includes a step of order reduction of the process state model. The adaptive feature comes from the on-line estimation of the required process time varying parameters. The adaptive algorithm proposed enforces a desired and pre-set second order convergence dynamics as originally introduced by Oliveira *et al.* (1). Formulating the estimator on this basis leaves the user with the choice of two simple and intuitive tuning parameters with physical meaning - a damping coefficient and a natural period of oscillation.

PROCESS MODEL

The baker's yeast process is accepted as occurring in two possible metabolic regimes, *viz.* - i) a respiro-fermentative regime, corresponding to an ethanol production state, and ii) a respirative regime, corresponding to an ethanol consumption pathway as stated by Sonnleitner and Käpelli (2). The fermentation is carried out in semi-batch reactor with the controlled addition of substrate.

TABLE 1a - Model for respiro-fermentative regime

State Equations
$\dot{X} = -DX + \varphi_1 + \varphi_2$
$\dot{S} = -DS - k_1\varphi_1 - k_2\varphi_2 + DS_{in}$
$\dot{E} = -DE + k_3\varphi_2$
$\dot{O} = -DO - k_5\varphi_1 + OTR$
$\dot{C} = -DC + k_7\varphi_1 + k_8\varphi_2 - CTR$

TABLE 1b - Model for respirative regime

State equations
$\dot{X} = -DX + \varphi_1 + \varphi_3$
$\dot{S} = -DS - k_1\varphi_1 + Ds_{in}$
$\dot{E} = -DE - k_4\varphi_3$
$\dot{O} = -DO - k_5\varphi_1 - k_6\varphi_3 + OTR$
$\dot{C} = -DC + k_7\varphi_1 + k_9\varphi_3 - CTR$

Classical mathematical modelling leads to two partial models, as represented in Table 1a and Table 1b where *S*, *O*, *X*, *C* and *E* represent respectively glucose, oxygen, biomass, carbon dioxide and ethanol concentrations; φ_1, φ_2 and φ_3 represent growth rates, the k_i are yield coefficients, *OTR* is the oxygen transfer rate, *CTR* is the carbon dioxide transfer rate, S_{in} is the inlet concentration of glucose in the feed, and, finally, *D* is the dilution rate (ratio feed rate / volume).

The two partial models above may be described in a space-state matrix form by a *general dynamic model of biological reactors* as:

$$\frac{d\xi}{dt} = K\varphi(\xi, t) - D\xi + F - Q \qquad (1)$$

where ξ represents the state components; $K\varphi$ represents the kinetic structure, assumed unknown; the vectors F and Q represent respectively the process inputs and outputs, known from on-line measurements.

Model Order Reduction

Given that the kinetic structure is usually unknown, a procedure of on-line parameter estimation will have to be employed, which however will have to be based on a reformulated model free of the kinetic terms. In those cases where a number of fast dynamic state components are recognised, this number being equal to or larger than

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the number of unknown kinetic terms, it is possible to assume that such components are in pseudo steady-state and, through the single perturbation method, to reformulate the problem in terms of a reduced model.

Assuming that glucose and CO_2 exhibit *fast* dynamics relatively to the *slow* limiting dynamics of biomass, ethanol, and oxygen, and adopting the single perturbation procedure, it is possible to obtain, a reduced model representation of the process: i) recurring to the algebraic equations in glucose and CO_2, growth rates (φ_1, φ_2 and φ_3) are obtained as functions of the input and output vectors; ii) substituting in the dynamic equations for X, E and O leads to the following reduced representation of such dynamics:

$$\frac{d}{dt}\begin{bmatrix} O \\ E \\ X \end{bmatrix} = -\begin{bmatrix} \theta_1 \\ \theta_3 \\ \theta_5 \end{bmatrix} CTR + \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} OTR + \begin{bmatrix} \theta_2 S_{in} - O \\ \theta_4 S_{in} - E \\ \theta_6 S_{in} - X \end{bmatrix} D \quad (2)$$

where the parameters $\theta_1,\ldots, \theta_6$ are variable functions of the yield coefficients, depending at each moment on the prevalent metabolic regime.

ADAPTIVE CONTROL

The synthesis of the non-linear control laws is performed by employing differential geometry techniques with system linearization by state feedback, as proposed by Bastin and Dochain (3). The adaptive feature comes from the on-line estimation of the required process time varying parameters.

The feedback control objective is that a control variable y follows a reference value represented by $y^*(t)$. The linearizing control problem consists of deducing and implementing a non-linear law such that the controller convergence error $\tilde{y} = (y^* - y)$ be governed by a pre-specified stable linear differential equation, known as reference model.

The SISO Problem

In the single output problem, the objective will be to control a scalar y which will be taken as a linear combination of the state variables, of the form:

$$y = \sum_{i=1}^{n} L_i \xi_i = L^T \xi \quad (3)$$

where $L^T = [L_1, L_2, \ldots, L_n]$ is a vector of known constants. Combining the reduced model equations (which in the present case study correspond to eqns. (2)) with the transformation (eqn. (3)), leads to an input-output reduced model, which can be conveniently written (for the sake of error analysis) in the general form:

$$\frac{dy}{dt} = \Phi(\xi) + \theta^T \phi(F, Q) + u(t)\Psi(\xi) \quad (4)$$

where: Φ, Ψ and ϕ are known functions of ξ, F and Q; θ represents the matrix of unknown parameters which characterise the kinetics; and, $u(t)$ is the manipulated input (the dilution rate, for this SISO case). The kinetics has been taken as unknown, but even if this were not the case, the fact that model (eqn. (4)) is the result of some simplifying hypotheses means that θ is always a matrix of unknown parameters, which necessarily will have to be adapted on-line. From this point of view, ϕ represents the corresponding regression vector associated to θ.

The control objective will consist of imposing a stable first order closed-loop dynamics of the trajectory for the control error system, of the form:

$$\frac{d}{dt}(y^* - y) + \lambda(y^* - y) = 0 \quad (5)$$

characterised by a positive time constant corresponding to the inverse of the characteristic time of the control error trajectory.

Combining the input-output reduced model (eqn. (4)) with the reference model (eqn. (5)), will easily lead to the following linearizing control law:

$$u(t) = \Psi(\xi)^{-1}\left\{\lambda(y^* - y) + \frac{dy^*}{dt} - \Phi(\xi) - \hat{\theta}^T \phi(\xi)\right\} \quad (6)$$

Employing the reduced model, will lead to concentrate all the unknowns in the parameter matrix θ, which will be estimated on-line. Hence, in eqn. (6) the estimates $\hat{\theta}$ will be employed rather than the true values θ.

The dynamics of the control error $\tilde{y} = (y^* - y)$, for the situation where estimated $\hat{\theta}$ are employed, is modelled by substituting eqn. (6) in eqn. (4), giving:

$$\frac{d\tilde{y}}{dt} \equiv \frac{dy^*}{dt} - \frac{dy}{dt} = -\lambda\tilde{y} - \tilde{\theta}^T \phi \quad (7)$$

where $\tilde{\theta}$ represents the error in the parameters θ, defined by $\tilde{\theta} \equiv \theta - \hat{\theta}$.

Baker's yeast case study. Axelsson (4), Dairaku *et al.* (5) and Pomerleau (6) have shown that the regulation of ethanol concentration is an effective means for achieving a good compromise between yield (ratio of biomass produced to sugar added) and productivity (biomass production by volume and time). The accumulation of ethanol affects negatively both yield and productivity. It is however known that a low level of

ethanol will have the desirable effect of inducing the enzymatic system of the fermentative catabolic pathway, in this way avoiding a long adaptation period when using the yeast (6).

The objective for the SISO control scheme consists of regulating ethanol concentration ($y = E$, i.e. $L^T=[0\ 1\ 0]$), employing the feed rate (or dilution rate) as control variable. It is assumed that ethanol measurements are available. Yield coefficients and reaction rates are taken as unknowns.

The reduced input-output model can be seen to correspond to eqn. (4) where: $\phi^T= [-CTR\ \ DS_{in}]$, $\Phi = 0$ and $\Psi = -E$. Substituting such values in eqn. (6) will lead to the following linearizing adaptive control law:

$$D = \frac{\lambda\left(E^* - E\right) + \hat{\theta}_3 CTR}{\hat{\theta}_4 S_{in} - E} \tag{8}$$

The adaptive control algorithm corresponds to implementing an algorithm for the on-line estimation of parameters θ_3 and θ_4 prior, at every step, to calculating and implementing the control law. This adaptive methodology has the significant advantages of compensating for model mismatches and of not requiring the identification of the metabolic regime.

Estimation Laws

The basis for the method adopted is the so-called Lyaponov design. For the single output problem, it is assumed that each parameter θ_i is estimated by the following adaptive law:

$$\frac{d\hat{\theta}_i}{dt} = -\Gamma_i \phi_i\left(F,Q\right)\left(y^* - y\right) \tag{9}$$

where $\phi_i(F,Q)$ is the regressor associated to θ_i, function of F and Q, and Γ_i the positive definite estimator gain.

The dynamic model for the error system, composed by the control error $\tilde{y}$ and by the parameter error $\tilde{\theta}_i$, can be deduced from eqns. (9) and (7) and written as

$$\frac{d}{dt}\begin{bmatrix}\tilde{y}\\ \tilde{\theta}_i\end{bmatrix} = \begin{bmatrix}-\lambda & -\phi_i\\ \Gamma_i\phi_i & 0\end{bmatrix}\begin{bmatrix}\tilde{y}\\ \tilde{\theta}_i\end{bmatrix} + \begin{bmatrix}0\\ 1\end{bmatrix}\frac{d\theta_i}{dt} \tag{10}$$

whose characteristic equation presents the roots

$$-0.5\lambda \pm \sqrt{0.25\lambda^2 - \Gamma_i\phi_i^2} \tag{11}$$

The criterion chosen for the error dynamics determines the parameter convergence and as such the quality and even the feasibility of the proposed adaptive scheme.

Choice of a real double pole. Perrier and Dochain (**7**) proposed to fixing the closed loop dynamics by choosing a real double pole, which leads to the following relationship between controller and estimator parameters:

$$\Gamma_i = 0.25\lambda^2\phi_i^{-2} \tag{12}$$

Substituting eqn. (12) in eqn. (9), gives:

$$\frac{d\hat{\theta}_i}{dt} = -\gamma\phi_i^{-1}\left(y^* - y\right) \tag{13}$$

with $\gamma \equiv 0.25\lambda^2$.

Generalising for 2nd order convergence. The θ estimator (eqn. (13)) will be employed, with a constant but undefined γ. Differentiating, leads to:

$$\frac{d^2\hat{\theta}_i}{dt^2} = -\frac{\gamma}{\phi_i}\frac{d\tilde{y}}{dt} + \frac{\gamma}{\phi_i^2}\frac{d\phi_i}{dt}\tilde{y} \tag{14}$$

Combining with eqn. (10), leads to the following 2nd order equation:

$$\frac{1}{\gamma}\frac{d^2\hat{\theta}_i}{dt^2} + \frac{1}{\gamma}\left(\lambda + \frac{1}{\phi_i}\frac{d\phi_i}{dt}\right)\frac{d\hat{\theta}_i}{dt} + \hat{\theta}_i = \theta_i \tag{15}$$

Defining the characteristic adaptive and control parameters as:

$$\lambda \equiv \frac{2\zeta}{\tau} - \frac{1}{\phi_i}\frac{d\phi_i}{dt} \tag{16}$$

$$\gamma \equiv \frac{1}{\tau^2} \tag{17}$$

equation (14) can be rewritten as -

$$\tau^2\frac{d^2\hat{\theta}_i}{dt^2} + 2\zeta\tau\frac{d\hat{\theta}_i}{dt} + \hat{\theta}_i = \theta_i \tag{18}$$

which has the meaning that each $\hat{\theta}_i$ converges for the true θ_i through a 2nd order dynamic trajectory, with a natural period of oscillation τ and a damping coefficient ζ.

In the specific case of the choice of a double pole (i.e. $\gamma \equiv 0.25\lambda^2$) the controller gain is inversely proportional to the corresponding periods of oscillation, as follows:

$$\lambda = 2/\tau \tag{19}$$

and, in fact, parameters ζ and τ will not be independent, rather being related by:

$$\zeta = 1 + \frac{\tau}{2\phi_i}\frac{d\phi_i}{dt} \quad (20)$$

This problem formulation based on the 2nd order convergence dynamics has the advantages of linking the controller tuning to the estimator tuning through two parameters (or one in the case of the real double pole criterion) which have a simple and well established physical meaning. In the case where the choice is the tuning of both 2nd order convergence parameters, the controller gain will be a function of the regressor $\phi_i(t)$, hence being time varying.

Baker's yeast case study. The on-line estimation of $\hat{\theta}_3$ and $\hat{\theta}_4$ (noting that the related regressors are, respectively–*CTR* and DS_{in}) is performed by using a discrete time implementation as follows:

$$\hat{\theta}_{3,k+1} = \hat{\theta}_{3,k} + T(E^* - E_k)/(CTR_k\tau^2) \quad (21)$$

$$\hat{\theta}_{4,k+1} = \hat{\theta}_{4,k} - T(E^* - E_k)/(D_kS_{in}\tau^2) \quad (22)$$

with the controller gain computed as:

$$\lambda = 2\zeta/\tau - (CTR_k - CTR_{k-1})/T/CTR_k \quad (23)$$

in which the index *k* is the time index and *T* is the sampling period. The 2nd order parameters have been set to the following values: $\zeta = 2.0$, $\tau = 0.10$ h.

The MIMO Problem

In the MIMO problem, the objective will be to control a vector *y* with each element taken as a linear combination of the state variables. In eqn. (3) *L* is now a matrix of known constants.

Dochain (8) introduced an extension of SISO adaptive linearizing control laws for bioreactors, leading to a MIMO scheme.

The development presented in this work follows the line of Dochain's publication, distinguishing itself mainly in the step of process identification and its implications in the tuning of the adaptive control law.

Baker's yeast case study. Williams *et al*. (9) demonstrated that for this particular biological system, one SISO control loop is insufficient to maximise simultaneously yield and productivity. These authors proposed a linear adaptive controller composed of two SISO loops to regulate respiratory quotient and dissolved oxygen, by manipulating the sugar feed rate and stirrer speed respectively. The approach suffers from the limitations related to employing an approximated linear model for the process.

For the present work the goal is still to maximise both yield and productivity through the MIMO control problem of regulating both the ethanol (*E*) and dissolved oxygen (*O*) concentrations, by manipulating the feed and the aeration rates. It is assumed that *CTR* can be measured on-line. Similarly to the SISO problem, yield coefficients and reaction rates are taken as unknowns.

The control strategy will consist of imposing a stable first order closed-loop dynamics for the control error system as:

$$\frac{d}{dt}\begin{bmatrix}(O^* - O)\\(E^* - E)\end{bmatrix} + \begin{bmatrix}\lambda_1 & \lambda_2\end{bmatrix}\begin{bmatrix}(O^* - O)\\(E^* - E)\end{bmatrix} = 0 \quad (24)$$

with λ_1 and λ_2 corresponding to the inverse of the characteristic time constants of the control error trajectories.

The linearizing adaptive control laws can be shown to be obtained from the MIMO counterpart of the general control eqn. (6), or, in more simple terms, by substituting the equations for ethanol and dissolved oxygen from the reduced model (eqn. (2)) in the reference model (eqn. (24)), leading to:

$$\begin{bmatrix}OTR\\D\end{bmatrix} = \begin{bmatrix}1 & -\frac{(\theta_2 S_{in} - O)}{(\theta_4 S_{in} - E)}\\0 & \frac{1}{(\theta_4 S_{in} - E)}\end{bmatrix}\left\{\begin{bmatrix}\lambda_1(O^* - O)\\\lambda_2(E^* - E)\end{bmatrix} + \begin{bmatrix}\hat{\theta}_1\\\hat{\theta}_3\end{bmatrix}CTR\right\} \quad (25)$$

Similarly to the method employed for the SISO problem, this control law was implemented together with an on-line estimator of the model parameters θ. The simultaneous adaptation of these 4 parameters has proved to constitute an ill-conditioned problem of convergence, the system exhibiting strong sensitivity to the tuning parameters involved in the procedure. Hence, it was decided to freeze parameters θ_2 and θ_4 and carry out the estimation for θ_1 and θ_3. Following the same 2nd order approach and using a discrete time implementation, has led to:

$$\hat{\theta}_{1,k+1} = \hat{\theta}_{1,k} + T(O^* - O_k)/(CTR_k\tau_1^2) \quad (26)$$

$$\hat{\theta}_{3,k+1} = \hat{\theta}_{3,k} + T(E^* - E_k)/(CTR_k\tau_2^2) \quad (27)$$

with the controller gains computed as:

$$\lambda_1 = 2\zeta_1/\tau_1 - (CTR_k - CTR_{k-1})/CTR_k/T \quad (28)$$

$$\lambda_2 = 2\zeta_2/\tau_2 - (CTR_k - CTR_{k-1})/CTR_k/T \quad (29)$$

The 2nd order parameters have been set to the following values: $\zeta_1 = \zeta_2 = 2.0$, $\tau_1 = \tau_2 = 0.10$ h.

RESULTS

Figure 1 shows concentration profiles of ethanol and of the manipulated variable, for the SISO problem. A set-point change of ±10% to the initial set-point of 0.5 gL^{-1} of ethanol is shown. After 8 hours of operation, a typical exponential profile for *D* is observed, corresponding to

the maintenance of the respiro-fermentative regime.

In this problem the 'second order convergence' law for the estimator has lead to the best Integral of Time weighted Absolute Error (ITAE) convergence indices as compared to those obtained with other Lyapunov techniques and with recursive least squares methods. Furthermore, robustness analysis for the control and adaptation laws has demonstrated that the reduced model was adequate for the control design.

Results for the MIMO problem are presented in Figure 2. It shows concentration profiles for ethanol (a) and dissolved oxygen (b) which are significantly kept very close to the reference values (E^*=0.5 g.L-1 and O^*=2 mg.L^{-1}). Also, frames (c) and (d) show adequate smooth profile for the manipulated variables.

The MIMO control configuration has led to average values of 0.54 g.L^{-1}.h^{-1} for productivity and of 0.46 g.g^{-1} for yield. These indices compare most favourably with those observed when employing the SISO approach, respectively 0.34 g.L^{-1}.h^{-1} and 0.43 g.g^{-1}.

CONCLUSIONS

Algorithms were presented for the adaptive control of fermentation processes. The synthesis of the non-linear control laws was performed by applying a model-based procedure which ensures linear behaviour of the closed loop feedback system. A new scheme was proposed for the required on-line parameter identification, which guarantees second-order convergence for the dynamics of the error system.

A case-study consisting of the regulation of ethanol concentration in fed-batch of baker's yeast production was employed for tests by simulation. Two alternative identification methods were also employed for comparison purposes.

The control and adaptive laws based on the reduced model representation of the key component dynamics proved to be adequate for process operation. The scheme based on the second order estimation procedure showed better performance, albeit small, as assessed by the ITAE and by the mean error criteria.

Comparing the SISO and the MIMO schemes, the operation was not carried out under optimal (or optimum) trajectories, hence it is clear that these are not definite results on the advantages of the latter configuration. Yet, one would expect that the additional degree of freedom of the MIMO configuration should lead to some improvement in the operation. The present work supports this indication and furthermore shows the feasibility of its implementation.

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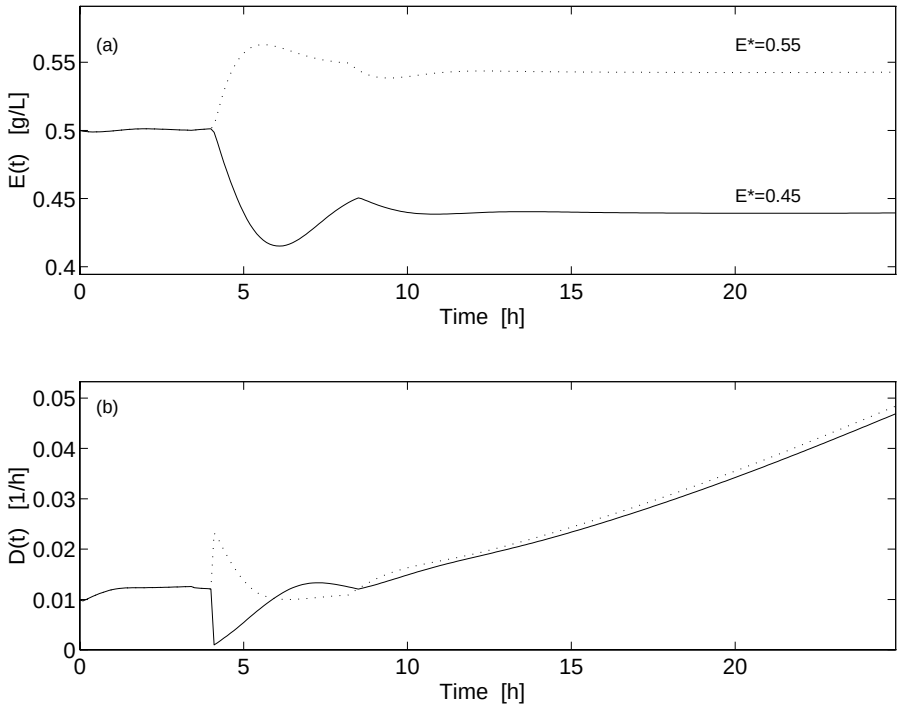

Figure 1 SISO control of ethanol: 10% set-point change

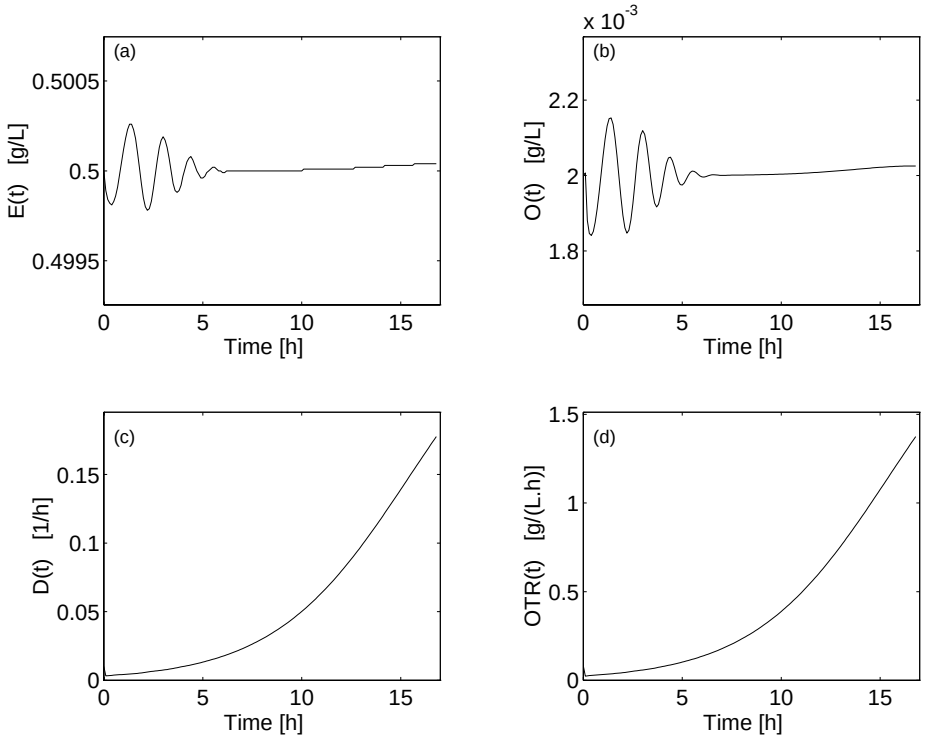

Figure. 2 MIMO control of ethanol and dissolved oxygen