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A Study on the Convergence of Observer-Based Kinetics Estimators in Stirred Tank Bioreactors

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ABSTRACT

This paper is devoted to the tuning problem of the "observer-based kinetics estimator" in stirred tank bioreactors. This algorithm estimates the reaction kinetics from the on-line knowledge of the state variables (either from measurement or by means of state observer), when the yield coefficients are known. The relation between the dynamics of convergence and the tuning procedure is explored. The method proposed imposes a second-order dynamics to the convergence of the estimator. This approach will be shown to compare favourably with a pole placement based technique, in an application to a baker's yeast fed-batch fermentation.

INTRODUCTION

Two of the major problems limiting the use of modern control techniques to bioprocesses are the difficulty of modelling the growth kinetics of microorganisms and the lack of cheap and reliable sensors of biological variables. Model-based state observers and observer-based parameter estimation represent recent developments which may overcome such difficulties. Bastin and Dochain (1990) proposed a methodology for state and parameter estimation based upon the concept of a "general dynamical model for bioreactors":

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

For the on-line estimation of reaction rates when the yield coefficients are known and constant, the proposed observer-based estimator is expressed by

$$\frac{d\hat{\xi}}{dt} = KH(\xi)\hat{\rho} - D\xi + F - Q - \Omega(\xi - \hat{\xi}) \qquad (2a)$$

$$\frac{d\hat{\rho}}{dt} = \left[KH(\xi)\right]^T \Gamma(\xi - \hat{\xi}) \qquad (2b)$$

The reaction rates are defined as $\varphi(\xi)=H(\xi)\rho(t)$ to take advantage on any possible knowledge of the kinetics model, where $H(\xi)$ is an m×r known matrix (function of the state) while $\rho(t)$ is a vector of r unknown functions of the state which are considered as completely unknown time varying parameters.

A difficulty related with the application of this methodology is the tuning of the gain matrices Ω and Γ which are design parameters at the disposal of the user for the control of the stability and the tracking properties of the algorithm. This problem is discussed by Pomerleau and Perrier (1990) which proposed a pole placement based tuning for the estimation of the three specific growth rates involved in a Baker's yeast fed-batch fermentation.

This paper is devoted to the tuning problem of this estimator. An alternative approach is presented which is based on the concept of imposing that the estimated kinetics follow a second order dynamic response to the true reaction kinetics changes, leaving free to the user the setting of the natural period of oscillation and of the damping coefficient. The matrices of gains are presented as functions of those settings and of the system state. Hence, they are time variant but automatically adapted.

SECOND-ORDER DYNAMICS BASED TUNING

It is assumed that it is sufficient to base the kinetics estimator on a subset of r equations of the full state space model, provided that they involve all the r parameters that need to be estimated (this subset of equations is denoted by

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the index s). In this case the gain matrices are square with dimension r. In what follows, a reformulated dynamical model is adopted by considering the transformation $\psi = K_s^{-1}\xi_s$, which gives:

$$\frac{d\psi}{dt} = \varphi(\xi) - D\psi + K_s^{-1}(F - Q(\xi)) \quad (3)$$

The estimator can then be rewritten as:

$$\frac{d\hat{\psi}}{dt} = H\hat{\rho} - D\psi + K_s^{-1}(F_s - Q_s) - \Omega(\psi - \hat{\psi}) \quad (4a)$$

$$\frac{d\hat{\rho}}{dt} = H^T\Gamma(\psi - \hat{\psi}) \quad (4b)$$

The dynamics of the observation error is obtained by subtracting eqn (4a) from eqn (2):

$$\frac{d(\psi - \hat{\psi})}{dt} = H(\rho - \hat{\rho}) + \Omega(\psi - \hat{\psi}) \quad (5)$$

If the matrix Γ is such that $[H(\xi)]^T\Gamma$ is a constant matrix, then differentiating equation (4b) gives

$$\frac{d^2\hat{\rho}}{dt^2} = H^T\Gamma\frac{d(\psi - \hat{\psi})}{dt} \quad (6)$$

Moreover, if $H(\xi)$ is a diagonal matrix, then combining equations (4b), (5), and (6), and setting $\Omega=\text{diag}\{-\omega_i\}$ and $\Gamma=H(\xi)^{-1}\text{diag}\{\gamma_j\}$. (where $\gamma_j, \omega_i \in \Re^+$) the following result is obtained:

$$\tau_i^2\frac{d^2\hat{\rho}_i}{dt^2} + 2\zeta_i\tau_i\frac{d\hat{\rho}_i}{dt} + \hat{\rho}_i = \rho_i \quad i=1,...r \quad (7)$$

$$\tau_i = (\gamma_i h_i)^{-0.5} \quad (8)$$

$$\zeta_i = 0.5\omega_i(\gamma_i h_i)^{-0.5} \quad (9)$$

where h_i refers to the diagonal elements of matrix $H(\xi)$.

Eqns. (7), (8) and (9) show that each parameter follows a second order dynamic response to the true parameter changes with a natural period of oscillation of τ_i and a damping coefficient of ζ_i. Nevertheless they are functions of the system state, and hence, they are time variant.

The application of this methodology to the estimation problems of completely unknown reaction rates, specific reaction rates and specific growth rates is as follows:

i) completely unknown reaction rates

In this case we have:

r=M
$\rho(\xi)=\varphi(\xi)$
$H(\xi)=I_M$

Which gives:

$\tau_i = \gamma_j^{-0.5}$

$\zeta_i = 0.5\omega_j\gamma_j^{-0.5}$

ii) specific reaction rates

In this case we have:

r=M
$\rho(\xi)=\alpha(\xi)$
$H(\xi)=G(\xi)=\text{diag}\{g_j\}$

where $g_j = \prod_{n\sim j}\xi_n$ means multiplication over the components with index n which are reactants in the reaction j.

The result is:

$\tau_i = (\gamma_i g_i)^{-0.5}$
$\zeta_i = 0.5\omega_i(\gamma_i g_i)^{-0.5}$

iii) specific growth rates

In this case we have:

r=M
$\rho(\xi)=\mu(\xi)$
$H(\xi)=XI_M$

where X means biomass concentration.

The result is:

$\tau_i = (\gamma_i X)^{-0.5}$
$\zeta_i = 0.5\omega_i(\gamma_i X)^{-0.5}$

CASE STUDY - BAKERS YEAST FED-BATCH FERMENTATION

The process model

Yeast growth is characterised by three metabolic pathways:

$$S + C \xrightarrow{\mu_s^o} X + G \quad (10a)$$

$$S \xrightarrow{\mu_s^r} X + E + G \quad (10b)$$

$$E + C \xrightarrow{\mu_e^o} X + G \quad (10c)$$

with S: glucose; C: oxygen; X: biomass; E: ethanol; G: carbon dioxide and μ_s^o, μ_s^r, μ_e^o: specific growth rates for the three pathways.

Pathways (10a), (10b), and (10c) refer respectively to the respiratory growth on glucose (oxydative pathway), fermentative growth on glucose (redutive pathway) and the respiratory growth on ethanol (oxydative pathway).

The dynamic model for the fed-batch fermentor is obtained from a mass balance on the components, considering that the reactor is well mixed, the yield coefficients are constant and the dynamics of the gas phase can be neglected. The mass balances, in terms of

concentration, take the matrix form of the general dynamical model (eqn. 1):

$$\frac{d}{dt}\begin{bmatrix} X \\ S \\ E \\ C \\ G \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ -k_1 & -k_2 & 0 \\ 0 & k_3 & -k_4 \\ -k_5 & 0 & -k_6 \\ k_7 & k_8 & k_9 \end{bmatrix} \begin{bmatrix} \mu_s^o \\ \mu_s^r \\ \mu_e^o \end{bmatrix} X - D \begin{bmatrix} X \\ S \\ E \\ C \\ G \end{bmatrix} + \begin{bmatrix} 0 \\ DS_{in} \\ 0 \\ OTR \\ 0 \end{bmatrix} - \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ CTR \end{bmatrix} \quad (11)$$

where D is the dilution rate and the k_i are yield coefficients; S_{in} is the substrate concentration in the feed; OTR is the oxygen transfer rate and CTR is the carbon dioxide transfer rate.

This dynamic model and the kinetic model proposed by Sonnleitner and Käppeli (1986) with modifications made by Pomerleau and Perrier (1990) were used for simulation purpose. It is assumed that the baker's yeast fed-batch process can only be in an ethanol production state or in an ethanol consumption state, meaning that the yeast can only grow by two pathways simultaneously: pathways 10a and 10b corresponding to ethanol production, and pathways 10a and 10c corresponding to ethanol consumption.

The kinetics estimator

The "observer-based kinetics estimator" (eqns. 4) is applied to two partial models reflecting the two process states mentioned above, taking the form:

$$\frac{d\hat{\psi}}{dt} = X\hat{\mu} - D\psi + K_s^{-1}(F_s - Q_s) - \Omega(\psi - \hat{\psi}) \quad (12a)$$

$$\frac{d\hat{\mu}}{dt} = X\Gamma(\psi - \hat{\psi}) \quad (12b)$$

with:

$$\psi = K_s^{-1}\xi_s,\ \xi_s = \begin{bmatrix} C & G \end{bmatrix}^T,\ (F_s - Q_s) = \begin{bmatrix} OTR & -CTR \end{bmatrix}^T$$

and with the estimated specific growth rates $\hat{\mu}$ switching between ($[\mu_s^o\ \mu_s^r]^T$ and $[\mu_s^o\ \mu_e^o]^T$).

The use of eqns 12 requires the on-line knowledge of biomass concentration. This is achieved by means of a "Luenberger-type asymptotic observer" (Luenberger, 1971) which enables the on-line estimation of X, S and E from measurement of C and G:

$$\frac{d\hat{Z}}{dt} = -D\hat{Z} + (F_2 - Q_2) - K_2K_1^{-1}(F_1 - Q_1) \quad (13a)$$

$$\hat{\xi}_2 = \hat{Z} + K_2K_1^{-1}\xi_1 \quad (13b)$$

with

$$\xi_1 = \begin{bmatrix} C & G \end{bmatrix}^T\ \hat{\xi}_2 = \begin{bmatrix} X & S & E \end{bmatrix}^T$$

$$(F_1 - Q_1) = \begin{bmatrix} OTR & -CTR \end{bmatrix}^T\ (F_2 - Q_2) = \begin{bmatrix} 0 & DS_{in} & 0 \end{bmatrix}^T$$

As such, the estimation procedure consists of two steps, viz.- *i)* state estimation from available process measurements and *ii)* specific growth rates estimation.

The process model and the kinetic model adopted were implemented in a process simulator (Feyo de Azevedo et al., 1992; Pimenta and Feyo de Azevedo, 1993) which supplied this two-step estimation algorithm with the simulated measured variables - C, G, CTR, OTR, Sin and F – at sampling times of 6 minutes.

Second-order-dynamics based tuning

The gain matrices for the case of specific growth rates are given by:

$$\gamma_i = \frac{1}{\tau_i^2 X_m} \qquad \omega_i = \frac{2\zeta_i}{\tau_i} \quad (14)$$

where τ_i and ζ_i are the desired natural period of oscillation and damping coefficient, and X_m is a mean value of biomass estimates over the time interval. As given by eqns. 14, the γ_i parameters are piecewise functions of biomass, i.e., γ_i remains constant between measurements, being adjusted at each sampling period.

The kinetics estimator equations (eqns. 12 and 13) were integrated with a robust variable-step numerical integration algorithm (4th/5th order Runge-Kutta type embedded scheme due to Butcher) employing along the integration linear estimates of the relevant sampled variables.

Pole placement based tuning

The overall estimation procedure was also carried out, employing the Euler's discretization approach and tuning method proposed by Pomerleau and Perrier (1990). Basically, this method consists on defining time trajectories for the gain parameters in order to maintain constant the position of poles (on the discrete complex plan) of the discrete error system throughout the fermentation. The gain parameters are given by:

$$\gamma_i = \frac{(p_i - 1)^2}{\tau^2 X^2} \qquad \omega_i = \frac{2(p_i - 1)}{\tau} \quad (15)$$

where p_i is the desired double pole of the error system ($0<p_i<1$), X is biomass estimate, and τ the sampling period (and also the integration step).

Results and Discussion

Figures 1, 2 and 3 illustrate the tuning procedure proposed in this work. The results in fig. 1 are obtained with similar natural periods of oscillation (τ_i=0.01) and damping coefficients (ζ_i=0.5) for the three components. The influence of τ_i and ζ_i on the dynamics of convergence can be assessed from the plots in Figs. 2 and 3. This influence is in agreement with the characteristics of a typical second-order dynamics response: decreasing τ_i the response becomes faster and decreasing ζ_i the response becomes more oscillatory.

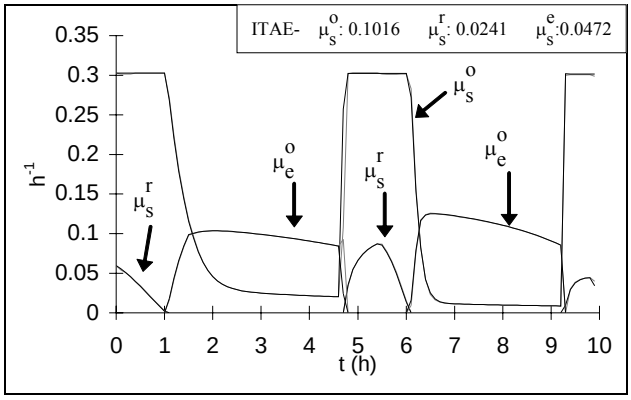

Figure 1-Specific growth rates (full lines-true; doted lines-estimates) using the 2nd order dynamics based tuning (τ=0.01, ζ=0.5)

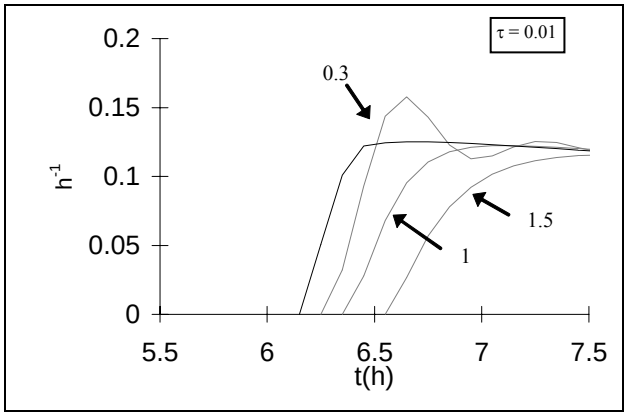

Figure 2 -μ_e^o estimates for different damping coefficients (ζ)

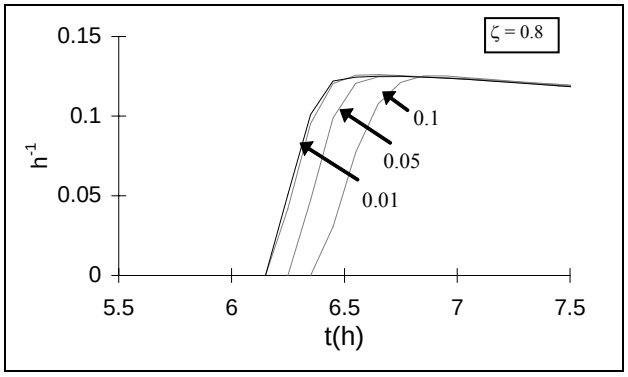

Figure 3 -μ_e^o estimates for different for different natural periods of oscillation (τ)

Figs. 4 and 5 illustrate the same application with the pole placement technique.

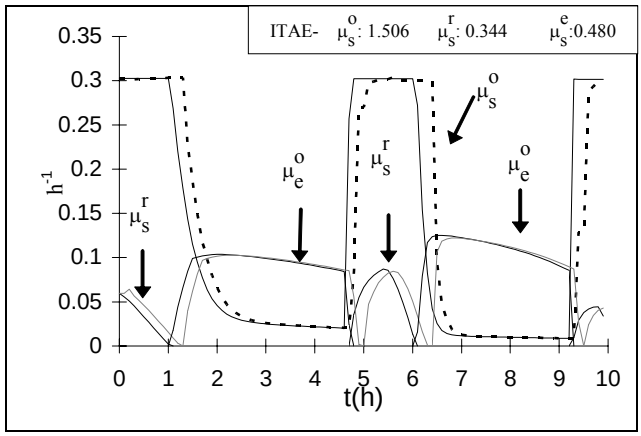

Figure 4 -Specific growth rates estimates (full lines-true; doted lines-estimated) using the pole placement based tuning

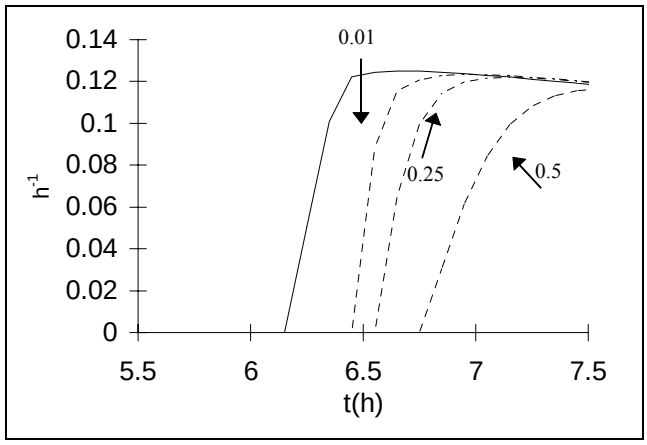

Figure 5 -μ_e^o estimates for different poles (p)

The best results are obtained when the double poles are close to zero (no significant improvement is obtained when p<0.01). In fig. 4 the three specific growth rates (estimated vs. 'true') are represented for p=0.01.

The information from Figs. 1 and 4 suggest that the 'second order dynamics' approach produces better results than the pole placement method. This is confirmed by the error indexes employed (ITAE – integral of time-weighted absolute errors) which are, for the former, an order of magnitude lower than those observed for the latter. The other possible advantage of the second order tuning is that the choice of parameters has an intuitive basis since this type of response is widely observed in natural phenomena and its theoretical study well disseminated.

Further theoretical analysis is out of scope of this paper. Work is in progress which aims in particular at establishing the domains of validity of the procedure proposed.

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NOMENCLATURE

C	dissolved oxygen concentration
CTR	carbon dioxide transfer rate
D	dilution rate
E	dissolved ethanol concentration
F	feed rate vector
G	dissolved carbon dioxide concentration
g_i	product of reactants concentration in reaction i
$H(\xi)$	(m×r) matrix of functions of the state
k_i	yield coefficients
K	yield coefficients matrix
m	number of reaction rates
n	number of state space variables
OTR	oxygen transfer rate
p_i	double pole of the discrete error system
Q	gas removal rate vector
r	number of parameters to estimate
S	glucose concentration
S_{in}	glucose feed concentration
T	sampling period
X	biomass concentration
X_m	average value of biomass concentration over the sampling period
α	specific reaction rates vector
φ	reaction rates vector
μ	specific growth rates vector
$\hat{\mu}$	vector of estimated specific growth rates
μ_s^r	specific growth rate for the fermentative growth on glucose pathway
μ_e^o	specific growth rate for the respiratory growth on ethanol pathway
μ_s^o	specific growth rate for the respiratory growth on glucose pathway
$\rho(t)$	vector of unknown time-varying parameters
$\hat{\rho}$	vector of estimated parameters
τ_i	natural period of oscillation
ω_i, γ_i	diagonal elements of Ω and Γ
Ω, Γ	gain matrices
$\hat{\xi}$	predicted state vector of concentrations
ξ_1	vector of measured concentrations
ξ_2	vector of non-measured concentrations
$\hat{\xi}_2$	estimated state vector of nonmeasured concentrations
ζ_i	damping coefficient