A study on the convergence of observer-based kinetics estimators in stirred tank bioreactors

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This paper is devoted to the tuning problem of an observer-based algorithm for the on-line estimation of reaction rates in stirred tank bioreactors. The relation between the dynamics of convergence and the tuning procedure is explored. The method proposed imposes a variable second-order dynamics on the convergence of the estimator. This approach is shown to compare favourably with a pole placement based technique, in an application to a baker’s yeast fed-batch fermentation. Copyright ©1996 Published by Elsevier Science Ltd.

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Two of the major problems limiting the use of modern control techniques in bioprocess operation are the difficulty of modelling the growth kinetics of microorganisms and the lack of cheap and reliable sensors of biological variables. Extended Kalman filters represent a possible solution for state and parameter estimation. However, it is known that this methodology is often difficult to apply to problems involving non-linear systems with time varying parameters, particularly when in the presence of noisy measurements. Model-based state observers and observer-based parameter estimators represent recent developments which may overcome these difficulties of lack of information and/or appropriate sensor technology. Bastin and Dochain proposed a methodology for state and parameter estimation based upon the concepts of a ‘general dynamical model for bioreactors’ and of ‘minimal kinetic modelling’. The system is represented by:

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

(1)

where $\hat{\xi}$ is the state vector (the set of $n$ component concentrations), $K$ is an $(n \times m)$ yield coefficients matrix, $D$ the dilution rate, $F$ the feed rate vector with $\text{dim}(F) = n$ and $Q$ the gaseous outflow rate vector with $\text{dim}(Q) = n$. The reaction rates are defined as $\varphi(\hat{\xi}) = H(\hat{\xi})\hat{\rho}(\hat{\xi})$ to take advantage of any possible knowledge of the kinetic model, $H(\hat{\xi})$ being a $(m \times r)$ matrix of known functions of the state and $\hat{\rho}(\hat{\xi})$ a vector of $r$ unknown functions of the state.

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

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

(2a)

$$\frac{d\hat{\rho}}{dt} = [KH(\hat{\xi})]^{\top}\Gamma(\hat{\xi} - \hat{\xi})$$

(2c)

The structure for the regression Equation (2b) obeys stability requirements for some related linear time varying (LTV) perturbed system.

A difficulty in the application of this methodology is in the tuning of the gain matrices $\Omega$ and $\Gamma$, which are design parameters at the disposal of the user for the control of the stability and tracking properties of the algorithm. This problem is discussed by Pomerleau and Perrier who 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 assuming that the estimated kinetics follow a second-order dynamic response to the true reaction kinetics changes. It will be shown that, under mild restrictions, the method proposed imposes a piecewise second-order dynamics to the convergence of the estimator (i.e. with natural period of oscillation and damping coefficients which change in each sampling interval).

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Second-order dynamics based tuning

The kinetics estimator can be based 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\(^{4,5}\).

(i) Denoting by subscript s the redimensioned vectors and matrices related to such sub-space, a reformulated dynamical model is conveniently adopted by considering the transformation \( \Phi = K_s(z) \), where \( K_s \) is the relevant yield coefficients matrix of dimension \( r \times m \).

This leads to:

\[
\frac{d\psi}{dt} = H(z)\rho - D\psi + K_s^{-1}(F_s - Q_s(z)) \tag{3}
\]

(ii) The kinetics estimator can then be re-written as:

\[
\frac{d\hat{\psi}}{dt} = H\hat{\rho} - D\psi + K_s^{-1}(F_s - Q_s - \Omega_s(\psi - \hat{\psi})) \tag{4a}
\]

\[
\frac{d\hat{\rho}}{dt} = H^T\Gamma_s(\psi - \hat{\psi}) \tag{4b}
\]

Equation (4a) is obtained by direct transformation of Equation (2a), whereas Equation (4b) is the result of the same type of stability considerations which led to Equation (2b).

The dynamics of the observation error is obtained by subtracting Equation (4a) from Equation (3):

\[
\frac{d(\psi - \hat{\psi})}{dt} = H(\rho - \hat{\rho}) + \Omega_s(\psi - \hat{\psi}) \tag{5}
\]

Assuming that matrix \( \Gamma_s \) is such that \([H(z)]^T \Gamma_s \) is a constant matrix, then differentiating Equation (4b) gives:

\[
\frac{d^2\hat{\rho}}{dt^2} = H^T\Gamma_s \frac{d(\psi - \hat{\psi})}{dt} \tag{6}
\]

Moreover, if \( H(z) \) is a diagonal matrix, then combining Equations (4b), (5), and (6) and setting:

\[
\Omega_s = \text{diag}(-\omega_s) \quad \text{and} \quad \Gamma_s = H(z)^T \text{diag}(\gamma_s) \tag{7a,b}
\]

with \( \omega_s, \gamma_s \in \mathbb{R}^r \), the following result is obtained:

\[
\tau_i \frac{d^2\hat{\rho}_i}{dt^2} + 2\zeta_i \tau_i \frac{d\hat{\rho}_i}{dt} + \hat{\rho}_i = \rho_i, \quad i = 1, \ldots, r \tag{8a}
\]

with

\[
\zeta = (\gamma h)^{0.5} \quad \text{and} \quad \xi = 0.5(\gamma h)^{0.5} \tag{8b,c}
\]

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

Remark 1

Equations (8b) and (8c) show that each parameter follows a second-order dynamic response to the true parameter changes with a natural period of oscillation \( \tau_i \) and a damping coefficient \( \zeta \). Nevertheless, they are functions of the system state, and hence are time variant.

Remark 2

In the general case of \( H \) being a varying state dependent matrix, the algorithm is restricted to the condition \( m = r \). The other restriction to be obeyed is that \( H \) is diagonal. Both conditions, however, are observed in a large and significant number of bioprocess reactions.

Remark 3

In the restricted number of cases where the matrix product \( KH \) (with dimensions \( r \times r \)) is time independent, the transformation to be performed should be \( \psi = [KH]^{-1} \psi \). For such cases it can be immediately concluded that both \( m > r \) and \( m < r \) can be accommodated.

The application of this methodology to the estimation problems of completely unknown and of partially known reaction rates is summarized in Table 1.

Case study – Baker's yeast fed-batch fermentation

The process model

Yeast growth may be characterized by three metabolic pathways:

\[
S + O \xrightarrow{\mu_s} X + C \tag{9a}
\]

\[
S \xrightarrow{\mu_i} X + C + E \tag{9b}
\]

\[
E + O \xrightarrow{\mu_e} X + C \tag{9c}
\]

where \( S \): glucose; \( C \): oxygen; \( X \): biomass; \( E \): ethanol; \( G \): carbon dioxide and \( \mu_s, \mu_i, \mu_e \): specific growth rates for the three pathways. Pathways (9a) (9b) and (9c) refer respectively to the respiratory growth on glucose (oxidative pathway), fermentative growth on glucose (reductive pathway) and the respiratory growth on ethanol (oxidative pathway).

Table 1 Second-order dynamics based tuning for estimation of reaction kinetics

<table>
<thead>
<tr>
<th>Fully unknown rates</th>
<th>Partially unknown rates</th>
<th>Specific growth rates</th>
<th>Kinetic terms</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho(z) )</td>
<td>( \rho(z) )</td>
<td>( \rho(z) )</td>
<td>( \rho(z) )</td>
</tr>
<tr>
<td>( H(z) )</td>
<td>( f_i )</td>
<td>( \text{diag}(f_i) )</td>
<td>( \text{diag}(g_i) )</td>
</tr>
<tr>
<td>( \tau_i )</td>
<td>( \gamma_i )</td>
<td>( \gamma_i )</td>
<td>( \gamma_i )</td>
</tr>
<tr>
<td>( \zeta )</td>
<td>( \xi )</td>
<td>( \xi )</td>
<td>( \xi )</td>
</tr>
</tbody>
</table>

\( \gamma \), product of reactants concentration in reaction \( i \).
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 dynamic model (Equation 1):

$$\frac{d}{dt} \begin{bmatrix} X \\ S \\ E \\ C \\ G \end{bmatrix} = \begin{bmatrix} 1 & -k_1 & -k_2 & 0 & \mu_1^c \\ -k_3 & 1 & 1 & 0 & \mu_1^e \\ -k_5 & k_7 & k_8 & k_9 & \mu_2^c \\ 0 & 0 & 0 & 0 & \mu_2^e \\ 0 & DS_m & 0 & 0 & \end{bmatrix} \begin{bmatrix} X \\ S \\ E \\ C \\ G \end{bmatrix} - \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ D S_m \end{bmatrix}$$

(10)

where $S_m$ is the substrate concentration in the feed, $OTR$ is the oxygen transfer rate and $CTR$ is the carbon dioxide transfer rate.

The kinetic model proposed by Sonnenleitner and Käppeli$^3$ was used for simulation purposes. It is assumed that the baker’s yeast fed-batch process can only be either in an ethanol production state or in an ethanol consumption state, this meaning that the yeast can only grow by two pathways simultaneously: pathways (9a) and (9b) corresponding to ethanol production, and pathways (9a) and (9c) corresponding to ethanol consumption.

The kinetics estimator

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

$$\frac{d\hat{p}}{dt} = H\hat{p} - D\hat{y} + K_{z1}^{-1}(F_1 - Q_1) - \Omega_1(\psi - \hat{y})$$

(11a)

$$\frac{d\hat{\mu}}{dt} = \Xi T_2(\psi - \hat{\psi})$$

(11b)

where $\psi = K_{z1}^{-1}\xi_0$, $\xi_0 = [C \ G]^T$, $(F_1 - Q_1) = [OTR - CTR]^T$, and with the estimated specific growth rates vector $\mu$ switching between $[\mu_1^e, \mu_2^e]$ and $[\mu_1^c, \mu_2^c]$.

The use of Equations (11) requires the on-line knowledge of biomass concentration. This is achieved by means of a ‘Luenberger-type asymptotic observer’$^b$ which enables the on-line estimation of $X$, $S$ and $E$ from measurement of $C$ and $G$:

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

(12a)

$$\hat{\xi}_2 = \hat{Z} + K_2K_1^{-1}\xi_1$$

(12b)

with

$$\xi_1 = [C \ G]^T$$

$$\hat{\xi}_2 = [\hat{X} \ \hat{S} \ \hat{E}]$$

$$(F_1 - Q_1) = [OTR - CTR]^T$$

and $(F_2 - Q_2) = [0 \ DS_m \ 0]^T$

As such, the estimation procedure consists of two steps, viz: (i) state estimation from available process measurements and (ii) specific growth rate estimation.

The process model and the kinetic model adopted were implemented in a process simulator$^{3,4}$ which supplied this two-step estimation algorithm with the simulated measured variables $C$, $G$, $CTR$, $OTR$, $S_m$ and $F$ at sampling times of 6 min.

Second-order dynamics based tuning

For this case of specific growth rate estimation, and as discussed above (Table 1, $h_i = X$; remark 1), the gain matrix elements $\gamma$ cannot be made strictly constant. A suitable approximation consists of employing the gain matrices given by:

$$\gamma_i = \frac{1}{\tau_i^2 X_m^2}$$

and $\alpha_i = \frac{2\xi_i}{\tau_i}$

(13a,b)

where $\tau$ and $\xi$ are the desired natural period of oscillation and damping coefficient, and $X_m$ is a mean value of biomass estimates over each time interval. The $\gamma$ parameters are thus taken as piecewise functions of the biomass, i.e., $\gamma$ remains constant between measurements, being adjusted at each sampling period.

Both the state observer (Equations (12)) and the kinetics estimator (Equations (11)) 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 Euler’s discretization approach and the tuning method proposed by Pomerleau and Perrier$. Basically, this method consists of 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:

$$\gamma_i = \frac{(p_i - 1)^2}{\tau_i^2 X_m^2}$$

and $\omega_i = \frac{2(p_i - 1)}{T}$

(14a,b)

where $p_i$ is the desired double pole of the error system ($0 < p_i < 1$), $X$ is the biomass estimate and $T$ 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 Figure 1 are obtained
Figure 1 Specific growth rates estimation, using the second-order dynamics based tuning, with $\tau = 0.01$ and $\zeta = 0.5$. ITAE index values for estimates of $\mu_e$, $\mu_f$, and $\mu_r$, respectively = 0.10, 0.02, 0.05. (solid lines = true; dotted lines = estimates).

Figure 2 $\mu_r^e$ estimates for different coefficients ($\tau = 0.01$).

Figure 3 $\mu_r^e$ estimates for different damping coefficients' natural periods of oscillation ($\zeta = 0.8$) with similar natural periods of oscillation ($\tau = 0.01$) and damping coefficients ($\zeta = 0.5$) for the three components. The influence of $\tau$ and $\zeta$ on the dynamics of convergence can be assessed from the plots in Figures 2 and 3. This influence is in agreement with the characteristics of a typical second-order dynamics response: for decreasing $\tau$ the response becomes faster and for decreasing $\zeta$ the response becomes more oscillatory.

For the alternative pole placement procedure, the best results are obtained when the double poles are close to zero (no significant improvement is obtained when $p < 0.01$). In Figure 4 the three specific growth rates (estimated vs. 'true') are represented for $p = 0.01$.

The information in Figures 1 and 4 suggests that the second-order dynamics' approach produces better results than the pole placement method. This is confirmed by the error indices 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 beyond the scope of this paper. Work is in progress which aims in particular 
at establishing an adaptive procedure which may lead to 
rigorous second-order convergence.

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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 \( i \)
\( H(\xi) \) \((m \times r)\) 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
\( S_F \) glucose feed concentration
\( T \) sampling period
\( X \) biomass concentration
\( X_c \) average value of biomass concentration over the sampling period
\( a \) specific reaction rates vector
\( \phi \) reaction rates vector
\( \mu \) specific growth rates vector
\( \mu_i \) vector of estimated specific growth rates
\( \mu_i^* \) specific growth rate for the fermentative growth on glucose pathway
\( \mu_i^g \) specific growth rate for the respiratory growth on ethanol pathway
\( \mu_i^r \) specific growth rate for the respiratory growth on glucose pathway
\( \rho(t) \) vector of unknown time-varying parameters
\( \rho \) vector of estimated parameters
\( \tau \) natural period of oscillation
\( \Omega, \Gamma \) diagonal elements of \( \Omega \) and \( \Gamma \)
\( \Omega \), \( \Gamma \) gain matrices
\( \xi \) predicted state vector of concentrations
\( \xi_i \) vector of measured concentrations
\( \xi_i^* \) vector of non-measured concentrations
\( \xi_i^e \) estimated state vector of non-measured concentrations
\( \delta \) damping coefficient

References

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