Biochemical Engineering Journal 24 (2005) 115–123

Biochemical Engineering Journal

www.elsevier.com/locate/bej

On-line states and parameter identification of acetone–butanol–ethanol fermentation process

A. Jahanmiri *, H. Rasooli

Department of Chemical Engineering, Shiraz University, Iran

Received 12 January 2004; received in revised form 2 February 2005; accepted 4 February 2005

Abstract

In the present work, the use of extended Kalman filter (EKF) to infer the outlet compositions and growth rate of the acetone–butanol–ethanol fermentation process from outlet gas CO_2 measurement has been discussed. In order to tune the filter (Q matrix), different methods consist of trial and error; Loan, Mont Carlo simulations and continuous case have been investigated for process noise covariance matrix. The reliability of the developed estimator is discussed with respect to disturbance on CO_2 concentration. The performance of the estimator has been evaluated by comparison with other filters such as Wiener and linearized Kalman filter as well as simulation and experimental results. The results show, EKF estimator provides good agreement with the composition values measured off-line while Q is adjusting by Loan method.

Keywords: Kalman filter; Fermentation; State estimation; Acetic acid; Ethanol; Bioreactor

1. Introduction

Biotechnology deals with the use of living organisms to manufacture valuable products. As such, it has ancient roots in the agricultural and brewing arts. However, recent developments in genetic manipulative techniques and remarkable advances in bioreactor design and computer-aided process control have founded a ‘new technology’ which considerably extends the present rang of technical possibilities and it is expected to revolutionize many facets of industrial, agricultural and medical practices [1].

There is no doubt that the extended Kalman filter (EKF) has had success in the process industries since the first reported applications from the early 1970s. Yet the number of reported industrial applications is relatively low. Applications in the area of inferential estimation for bioprocesses include the work by Mou and Cooney [2], Stephanopoulos and San [3], and Bastin and Dochain [4]. In the study by Mou and Cooney [2], elemental cell balances based on an empirically derived molecular formula for the biomass formed the inferential model that related secondary outputs such as the carbon dioxide evolution rate (CER) to the biomass (primary output) growth. In the antibiotic fermentation considered by them, a different correlation was used in the production phase to account for the time-varying process behavior resulting from the changing maintenance activity of the culture. To account for noise in real time measurements and also simultaneously estimate critical parameters of the culture such as specific growth rate and the culture states, Stephanopoulos and San [3] proposed the extended Kalman filter approach. They recommended compensation of the secondary measurements for the maintenance activity if the latter was significant. The EKF is, however, known to be very sensitive to modeling errors and can generate biased estimates of the states in the presence of model plant mismatch. In a different approach to simultaneous state and parameter identification, Ramirez [5] and Chattaway and Stephanopoulos [6] used the Kalman filter coupled with the sequential parameter updating strategy Ljung and Soderstrom [7] to perform the state and parameter estimation. Park and Ramirez [8] have also successfully applied the preceding strategy to regulate nutrient levels in a bioreactor. They assumed, however, that the primary state variables such as the biomass and

* Corresponding author. Tel.: +98 71 12303071; fax: +98 71 12303071.
E-mail address: jahanmir@shirazu.ac.ir (A. Jahanmiri).

1369-703X/$ – see front matter © 2005 Published by Elsevier B.V.
doi:10.1016/j.bej.2005.02.006

Nomenclature

A	acetone concentration (g/L)
AA	acetic acid concentration (g/L)
B	butanol concentration (g/L)
BA	butyric acid concentration (g/L)
D	dilution rate (h^{-1})
E	ethanol concentration (g/L)
f	process model (vector function)
F	flow rate (L/h)
H	measurement model (vector function)
H	measurement matrix (vector)
I	Monte Carlo simulation number
$k_1, \ldots, k_{15}, K_{AA}, K_{BA}$	model parameters
K	Kalman gain matrix (vector)
K_S	limitation constant
P	state covariance matrix
Q	process noise covariance matrix (vector)
R	measurement noise covariance matrix (scalar)
S	glucose concentration (g/L)
S_0	glucose concentration in the feed (g/L)
u	input (scalar)
V	bioreactor volume (L)
w, v	process and measurement noise
X	state vector
X	biomass concentration (g/L)
Z	measurement vector

Greek letters

Φ	transition matrix
μ	specific growth rate (h^{-1})
μ_m	maximum specific growth rate (h^{-1})

Superscripts

$\wedge$	model estimation
T	transpose matrix

substrate concentrations were measurable on an on-line basis.

2. Mathematical model of the process

For theoretical analysis of the process and development of control strategies, a mathematical model was built which can describe all important growth phase of the yeast.

2.1. Reactor model

The reactor model is derived from the liquid and gas phase balances of the main components in the cell-retention continuous-flow culture system. A fermentation kinetics model was developed on the basis of the following assumptions derived from the available knowledge of acetone–butanol–ethanol (A–B–E) fermentation process [9]:

(1) Carbon substrate limitation only.
(2) No nitrogen and nutrient limitation.
(3) Product inhibition.
(4) Acetic acid and butyric acid are intermediate metabolites and are reduced to acetone and butanol, respectively.
(5) Acetone and butanol are also synthesized directly from carbon substrate.
(6) Fermentation is performed at (a) optimal temperature of 37 °C; (b) optimal pH of 4.5; (c) under anaerobic conditions.
(7) All the cells are metabolically active and viable.

A set of general equations based on mass balances around the bioreactor system can describe the fermentation kinetics of *C. acetobutylicum*. Respecting the above assumptions, the reactor model is given by the balances:

$$\frac{dX}{dt} = \mu_m \frac{S}{S+K_S}(-0.153B\mathrm{BA} + 2.16)X \quad (1)$$

$$\frac{dS}{dt} = D(S_0 - S) - k_3\mu X - k_4 X - k_1 \frac{S}{S+K_S}\frac{\mathrm{BA}}{\mathrm{BA}+K_{BA}}X - k_2 \frac{S}{S+K_S}\frac{\mathrm{AA}}{\mathrm{AA}+K_{AA}}X \quad (2)$$

$$\frac{d\mathrm{BA}}{dt} = -D\mathrm{BA} + k_5\left[k_3\mu_m \frac{S}{S+K_S} f(I)X + k_4 X\right] - k_6 \frac{\mathrm{BA}}{\mathrm{BA}+K_{BA}}\frac{S}{S+K_S}X \quad (3)$$

$$\frac{d\mathrm{AA}}{dt} = -D\mathrm{AA} + k_8\left[k_3\mu_m \frac{S}{S+K_S} f(I)X + k_4 X\right] - k_9 \frac{\mathrm{AA}}{\mathrm{AA}+K_{AA}}\frac{S}{S+K_S}X \quad (4)$$

$$\frac{dB}{dt} = -DB + k_7\left[k_3\mu_m \frac{S}{S+K_S} f(I)X + k_4 X\right] + k_{14}\frac{\mathrm{BA}}{\mathrm{BA}+K_{BA}}\frac{S}{S+K_S}X \quad (5)$$

$$\frac{dA}{dt} = -DA + k_{10}\left[k_3\mu_m \frac{S}{S+K_S} f(I)X + k_4 X\right] + k_{15}\frac{\mathrm{AA}}{\mathrm{AA}+K_{AA}}\frac{S}{S+K_S}X \quad (6)$$

$$\frac{dE}{dt} = -DE + k_{11}\left[k_3\mu_m \frac{S}{S+K_S} f(I)X + k_4 X\right] \quad (7)$$

$$\frac{d\mathrm{CO_2}}{dt} = k_{16}\left[X\left(\frac{S}{S+K_S}\right)\right] \quad (8)$$