Korean J. Chem. Eng., **29**(7), 851-854 (2012)
DOI: 10.1007/s11814-011-0256-5

Degrees of freedom analysis and parameter optimization of state feedback of first-order affine singular control for bioprocess systems

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(*Received 18 April 2011 • accepted 3 October 2011*)

Abstract−The state feedback optimization of first-order affine nonlinear singular control systems is formulated as a time-invariant parameter optimization problem. Degrees of freedom (DF) is applied to the differential balance equations with initial control or its time derivatives and switching times as parameters, and uncovered that the state feedback optimization problem has -2 DF, clarifying admissible singular control structures. Using these two novel concepts, we considered end-point optimization problems in fed-batch fermentation problem to illustrate the state feedback optimization of the feed flow rate.

Key words: State Feedback, Singular Control, Degrees of Freedom, Optimization, Bioprocess

INTRODUCTION

The singular optimal control is a problem of which optimal control strategy is not explicitly obtained by optimal control theory such as Pontryagin's minimum principle (PMP) [1]. First-order affine singular control system is a special one with one singularity [2]. Feed rate control problems are typical of the first-order affine singular control system. It includes process optimizations of autocatalytic reactions, multiple reactions, extraction processes, bioreactors, semi-batch reactors and fed-batch cultures. Optimization of these processes usually leads to an open-loop solution for the singular feed rate, except for processes of order less than or equal to three where the solution can be obtained in feedback form. Open-loop optimization is well known to engineers for its difficulty in application due to errors arising from high dependency on initial conditions. However, most practical problems, especially in fed-batch fermentation process, consist of more than four differential balance equations [3-5]. Therefore, feedback optimization of the first-order singular feed rate problems has continuously been issued and a few feedback laws have been developed [6,7]. For example, Palanki et al. [6] derived a feedback control law based on PMP and singular control theory. In addition, even though many optimization methods dealing with discrete-time control system have been proven to be convenient for computer implementation, the optimization method based on state feedback control law is attractive in that accurate solution could be obtained.

This research is to develop a state feedback formulation of the first-order affine nonlinear singular control systems. Analyzing DF of the state feedback concepts of Palanki's work [6], we have found the state feedback law has -2 DF and this restricted admissible optimal control structure, making zero DF. In addition to this, a parameter optimization problem with initial control or its time derivatives and switching times as parameters has been formulated to replace the first-order affine nonlinear singular optimization problem. Fed-batch optimization as an example was demonstrated to verify the usefulness of the state feedback optimization, coupling the parameter optimization formulation and admissible control structures analyzed by DF.

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METHODS

1. Problem Formulation

A singular control problem with one control variable is expressed by the following formulation:

$$\mathrm{IP} = \operatorname*{Min}_{F(t)} \mathrm{G}[\underline{\mathbf{x}}(\mathrm{t}_f)]$$
$$\dot{\underline{\mathbf{x}}} = \underline{\mathrm{f}}(\underline{\mathbf{x}}) + \underline{\mathrm{g}}(\underline{\mathbf{x}})\mathrm{F}, \quad \underline{\mathbf{x}}(\mathrm{t}_0) = \underline{\mathbf{x}}_0 \tag{1}$$

where $\underline{\mathbf{x}}$, $\underline{\mathbf{x}}_0$, IP and F are the state vector, the initial state vector, the performance index , and control variable, respectively. In general, the performance index has an integral form over the entire trajectory. However, this integral form can be transformed into the terminal cost form, increasing one differential equation in the constraint condition. Therefore, the following mathematical illustrations can be applied to the problem with performance index over the entire trajectory. According to PMP [1], the adjoint vector and its final values are as follows:

$$\mathrm{H} = \underline{\lambda}^T[\underline{\mathrm{f}}(\underline{\mathbf{x}}) + \underline{\mathrm{g}}(\underline{\mathbf{x}})\mathrm{F}]$$
$$\dot{\underline{\lambda}} = -\partial\mathrm{H}/\partial\underline{\mathbf{x}}, \quad \underline{\lambda}(\mathrm{t}_f) = \partial\mathrm{IP}/\partial\underline{\mathbf{x}}(\mathrm{t}_f) \tag{2}$$

The necessary condition is minimization of the Hamiltonian and the partial derivative of H with respect to F, is

$$\partial\mathrm{H}/\partial\mathrm{F} = \underline{\lambda}^T\underline{\mathrm{g}}(\underline{\mathbf{x}}) = \phi \tag{3}$$

which is called 'a singular control problem' because $\partial^2\mathrm{H}/\partial\mathrm{F}^2=0$, which does not yield any information on the optimal control variable. Eqs. (1), (2) and (3) constitute the two-point boundary value problem. Since the Hamiltonian is linear in F, the optimality depends on the sign of the switching function, ϕ.

$$F=\begin{cases} F_{max} & \text{when } \phi<0 \\ F_{min}=0 & \text{when } \phi>0 \\ F_{singulr} & \text{when } \phi=0 \text{ over finite time interval(s), } t_q<t<t_{q+1} \end{cases} \quad (4)$$

On the singular region, the time derivatives of the switching function are also zero.

$$d^{2q}\phi/dt^{2q}=\phi^{2q}=0 \quad (5)$$

where q is the order of singularity. Differentiation continues until the control variable appears linearly. For many chemical and biological processes, q is 1. Henceforth, q is assumed to be 1.

2. Feedback Control Law

For a systematic formulation, Lie brackets are usually adapted for the nonlinear optimization problem. Given two vector fields, $\underline{f}(x)$ and $\underline{g}(x)$, $[\underline{f},\underline{g}](\underline{x})$ is the Lie bracket defined as follows: $[\underline{f},\underline{g}](\underline{x})=(\partial\underline{g}/\partial\underline{x})\underline{f}(x)-(\partial\underline{f}/\partial\underline{x})\underline{g}(\underline{x})$ where $\partial\underline{f}/\partial\underline{x}$ and $\partial\underline{g}/\partial\underline{x}$ are the Jacobians. The time derivatives of the switching function and the singular control with first order of singularity obtained from Eq. (5) are as follows:

$$\begin{aligned}
\phi^{(0)} &= \underline{\lambda}^T ad_f^0 \underline{g}(\underline{x}) = \underline{\lambda}^T \underline{g}(\underline{x}) = 0 \\
\phi^{(1)} &= \underline{\lambda}^T ad_f^1 \underline{g}(\underline{x}) = \underline{\lambda}^T [\underline{f},\underline{g}](\underline{x}) = 0 \\
\phi^{(2)} &= \underline{\lambda}^T \{ad_f^2 \underline{g}(\underline{x}) + [\underline{g}, ad_f^1 \underline{g}](\underline{x})F\} \\
&= \underline{\lambda}^T \{\underline{f},[\underline{f},\underline{g}](\underline{x}) + \underline{g},[\underline{f},\underline{g}](\underline{x})F\} = 0
\end{aligned} \quad (6)$$

For an n[th] order optimal control problem, the singular control from Eq. (6) has n−3 independent adjoint variables due to the two equality conditions ($\phi^{(0)}=0$ and $\phi^{(1)}=0$), which are linear in adjoint variables and cancellation of one adjoint variable in $F_{singular}$. Therefore, for processes with orders higher than 3, the singular control depends on n−3 adjoint variables in addition to the state vector. Therefore, the singular control is an open-loop form unless there are means to eliminate all adjoint variables so that the singular control expression depends entirely upon the state vector only. Thus, to implement the singular control requires on-line solution of two-point split boundary value problem to obtain the adjoint variables. For example, the shooting method, a popular algorithm to solve the TPBVP correctly, has a main drawback in that fairly accurate estimations of adjoint variable values at the initial time and each time nodes are necessary and poor guesses lead to a convergence problem.

Palanki et al. [6] derived the feedback form of the singular control for the system of Eq. (1):

$$F_{singular}=\psi_1(\underline{x}, F, dF/dt, \ldots, d^{n-3}F/dt^{n-3}) \quad (7)$$

However, the feedback control entails new variables, dF/dt, … and $d^{n-3}F/dt^{n-3}$ due to more time derivatives of the switching function. The detailed calculation procedure is illustrated below. Palanki et al. [6] state that the unknown initial values of these time derivatives of control variable do not affect the performance index critically and demonstrated insensitivity to it through a case study of 4[th] order control problem. However, this demonstration of insensitivity to a single parameter (dF/dt at t=0) for a single 4[th] order process with fixed parameters is not a proof for all situations for all processes of higher orders. Thus, the feedback control proposed requires extensive and exhaustive testing to demonstrate insensitivity of all initial values of time derivatives of F.

3. Analysis of dF/dt, … $d^{n-3}F/dt^{n-3}$ Based on Degrees of Freedom (DF)

$\phi^2(t)$ contains the control variable F and $\phi^3(t)$ does dF/dt. In general, $\phi^n(t)$ contains from F to dF^{n-2}/dt. In addition, the switching function and its time derivatives are linear to adjoint variables, as shown in Eq. (6). Following DF theory, n number of constraint equations is needed to calculate n number of unknown variables. For this reason, N number of equality equations can be deduced from time derivatives of the switching function $\phi(t)$ up to (n− 1)[th] order, and $\phi(t)$ to calculate n number of adjoint variables.

$$\phi(t)=\phi^{(1)}(t)=\phi^{(2)}t=\ldots=\phi^{(n-1)}(t)=0 \quad (8)$$

$$Q\underline{\lambda}^T=0 \quad (9)$$

where Q is the matrix obtained from $\phi(t)$ and its (n− 1) derivatives, which is composed of state variables and control variable F and its time derivatives.

Adjoint variable vector must not be zero from Eq. (9) due to the non-triviality of adjoint variables. Therefore, the determinant of Q must be zero, leading to Eq. (10).

$$\det(Q)=0 \quad (10)$$

Since Q is a function of state variables and control variable and its time derivatives, the calculation of Eq. (10) results in Eq. (7). Eq. (7) can be reformulated for $d^{n-3}F/dt^{n-3}$ as follows:

$$F^{(n-3)}=d^{n-3}F/dt^{n-3}=\psi_2(\underline{x}, F, dF/dt, \ldots, d^{n-4}F/dt^{n-4}) \quad (11)$$

For the open-loop control for processes with order of singularity of 1, a second order derivative of $\phi(t)$, not higher, leads to the singular feed rate. Thus, we can say that (n−3) numbers of equality conditions $\phi^{(3)}(t)=\phi^{(4)}(t)=\ldots=\phi^{(n-1)}(t)=0$ are added to three equality constraints, $\phi(t)=\phi^{(1)}(t)=\phi^{(2)}(t)=0$ for a total of n equations. The unknown (n−3) initial values $\underline{F}_0$ are the free parameters. However, due to nontriviality condition of Eq. (9), the number of independent constraint equations is (n−1) out of n equations, Eq. (8). Therefore, DF is -2 ((n−3) free parameters minus (n−1) equations).

To convert to a zero DF problem, more free parameters need to be identified and this can be obtained from switching times. This means zero DF depends on control structure. Admissible control structures have already been illustrated in terms of DF [8]. Even though the singular feed rate is formulated as a state feedback form, additional (n−3) equality conditions $\phi^{(3)}(t)=\phi^{(4)}(t)=\ldots=\phi^{(n-1)}(t)=0$ entails unknown (n−3) initial values $\underline{F}_0$ as free parameters. Therefore, reformulation of the open-loop form singular feed rate into state feedback form does not influence DF of the two-point boundary value problem, which was defined by Eqs. (1) and (2). This means that admissible control structures with zero DF follow the rules already reported in the reference [8].

4. Time-invariant Parameter Optimization of State Feedback Control for End-point Fed-batch Optimization Problems

Eq. (11) can be expressed as (n−3)[th] ordinary differential equations (ODE):

$$\begin{aligned}
&F=F_1, \\
&\dot{F}_1=F_2, \dot{F}_2=F_3, \ldots, \dot{F}_{n-3}=F_{n-2} \\
&\dot{F}_{n-3}=\psi_3(\underline{x}, F_1, F_2, \ldots, F_{n-1})
\end{aligned}$$

$$\underline{F}_0=[F_1^*, F_2^*, F_3^*, \ldots, F_{n-3}^*]_{t=0} \qquad (12)$$

The singular control, $F=F_1$, is obtained from Eq. (1) and Eq. (12) as a $(2n-3)^{th}$ order system of ODE but the initial values $\underline{F}_0=[F_1^*, F_2^*, F_3^*, \ldots, F_{n-3}^*]_{t=0}$ are unknown parameters, as illustrated below.

$$IP=\underset{[F_{1,0}^*\ldots F_{n-2,0}^* F_{n-3,0}^*]}{\mathrm{Min}} G[\underline{\mathbf{x}}(t_f)]$$

$$\begin{bmatrix} \dot{\underline{\mathbf{x}}} \\ \dot{F}_1 \\ \vdots \\ \dot{F}_{n-2} \\ \dot{F}_{n-3} \end{bmatrix} = \begin{bmatrix} \underline{f}(\underline{\mathbf{x}})+\underline{g}(\underline{\mathbf{x}})F_1 \\ F_2 \\ \vdots \\ F_{n-1} \\ \psi_3(\underline{\mathbf{x}}, F_1, F_2, \ldots, F_{n-1}) \end{bmatrix} = \begin{bmatrix} \underline{g}(\underline{\mathbf{x}}) & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \vdots & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_{n-1} \\ F_n \end{bmatrix}$$

$$+\begin{bmatrix} \underline{f}(\underline{\mathbf{x}}) \\ 0 \\ 0 \\ 0 \\ \psi_3 \end{bmatrix}, \begin{bmatrix} \underline{\mathbf{x}} \\ F_1 \\ \vdots \\ F_{n-2} \\ F_{n-3} \end{bmatrix}(t_0) = \begin{bmatrix} \underline{\mathbf{x}}_0 \\ F_{1,0}^* \\ \vdots \\ F_{n-2,0}^* \\ F_{n-3,0}^* \end{bmatrix} \qquad (13)$$

The optimization problem formulated by two-point boundary value problem (Eqs. (1) through (3)) is transformed into a state feedback form with additional parameters which need to be optimized for the performance index $IP=\underset{[F_{1,0}^*\ldots F_{n-2,0}^* F_{n-3,0}^*]}{\mathrm{Min}} G[\underline{\mathbf{x}}(t_f)]$. The control variable to be optimized is changed from time-variant feed flow rate F(t) to time-invariant parameters $[F_{1,0}^* \cdots F_{n-2,0}^* F_{n-3,0}^*]$.

5. Implementation

Although a shooting method can be applied to find switching times and free parameters $\underline{F}_0$ for a control structure so that IP is minimized, unless $(n-1)$ constraints as shown above are considered explicitly, the singular control is not assured to be on a singular arc. For example, Modak and Lim [8] suggested a one-dimensional numerical algorithm to estimate switching times so that the first necessary condition $\lambda^T \underline{g}(\underline{x})=0$ is accurately met on the singular arc. However, the backward integration of adjoint variables is unstable, which decreases robustness of computation of the two-point boundary value problem and makes difficulty in its successful implementation in the closed feedback control system.

The parameter optimization with state feedback control (Eq. (12)) is applicable to a singular control region. In a nonsingular region, the manipulated control, F_{max} or F_{min}, must be taken for the optimal control. Therefore, switching times must be calculated between each control, along with the initial time-invariant parameters $[F_{1,0}^* \cdots F_{n-2,0}^* F_{n-3,0}^*]$. Admissible control structure must be estimated *a priori* and DF theory about the control structure [8] can give a guide to the estimation. The exact control structure and switching times can be calculated, off-line, by solving two-point boundary value problem. With this information, the on-line control scheme in terms of state variables only could be set up. The efficiency of the feedback scheme depends on the switching times and parameters calculated *a priori.* During on-line feedback control, simple calculation of constraint conditions at switching times can be helpful to determine the accuracy of the feedback control. The constraint conditions are $\phi(t)=\phi^{(1)}(t)=0$ at the entrance time to a singular arc and $\phi(t)=0$ at the switching time between F_{max} (or F_{min}) and F_{max} (or F_{min}) [8]. Once the constraint conditions are seriously violated during on-line feedback control, switching time adaptation by intermittent off-line calculation could increase the performance of the closed feedback control.

6. Case Study

The following is a case study dealing with penicillin fed-batch fermentation with the performance index to be maximized at the final process time, $IP=\underset{F(t)}{\mathrm{Min}} PV(t_f)$. The used mathematical model is a modified version of that suggested by Bajpai and Reuss [9].

$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \frac{d}{dt}\begin{bmatrix} XV \\ SV \\ PV \\ V \end{bmatrix} = \begin{bmatrix} \mu x_1 \\ -\sigma x_1 \\ \pi x_1 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ S_F \\ 0 \\ 1 \end{bmatrix} F$$

$\mu=0.11s/(s+0.006)$, $\pi=0.0055s/(10s^2+s+0.0001)$, $\sigma=\mu/0.47+\pi/1.2+0.029s/(s+0.0001)$ $[XV, SV, PV, V](t_0)=[2g, 5g, 0g, 2L]$, $[S_F, F_{max}, F_{min}, V_{max}, t_f]=[10wt\%, 3L/h, 0L/h, 5L, 25h]$, where X, S, and P stand for the concentrations of cells, substrate, penicillin concentration, respectively, V the culture volume, S_F the feed substrate concentration, F the feed flow rate, and t_f the final operation time.

Referring to DF analysis of admissible control structure [8], the concatenation of F_{max} - F_{min} - $F_{singular}$ - F_{min} could be an admissible control structure. Before applying Eq. (13), the performance index and first time-derivative of feed flow rate $\dot{F}_1$ must be identified. To derive $\dot{F}_1$ using Eqs. (8) and (9), the condition, $\phi^{(3)}(t)=0$, should first be added to the conditions $\phi(t)=\phi^{(1)}(t)=\phi^{(2)}(t)=0$. Extending Lie bracket formulation of Eq. (6) yields the condition $\phi^{(3)}(t)=0$, as below:

$$\underline{\lambda}^T\{ad_f^3\underline{g}(\underline{x})+([g, ad_f^2 g](\underline{x})+[f,[g, ad_f^1\underline{g}]](\underline{x}) \\ +[g,[g, ad_f^1\underline{g}]](\underline{x})F)F+[g, ad_f^1\underline{g}](\underline{x})\dot{F}\}=0 \qquad (14)$$

Applying Eq. (9) to the set of Eqs. (6) and (14) gives rise to the condition of $\dot{F}_1$.

Now, the optimization problem is defined according to Eq. (13), where the initial feed rate $F_{1,0}^*$ and switching times must be calculated to meet the performance index.

Fig. 1 shows the simulation results. Switching times are [3 0.008 hr 6.6464 hr 18.341 hr 0.00490 hr] and the performance index IP= $=\underset{F(t)}{\mathrm{Min}} PV(t_f)$ is 0.8667 g. Backward integration of adjoint variables was carried out to calculate switching functions, whenever the optimization function *fminsearch* in MATLAB completes the optimization problem. The switching function signs (Fig. 1, switching time) with respect to each feed flow rate make sure that the feed flow rate strategy along with the calculated initial feed rate $F_{1,0}^*$ and switching times is optimal.

DISCUSSION

This research adopts the state feedback concepts of Palanki's work [6]. However, novelty can be said as follows. First, introducing degrees of freedom concept, we've found the state feedback law has -2 DF. Furthermore, admissible fist-order affine singular control structures are clarified to the state feedback optimization problem, making zero DF. This restricts the optimal control strategy candidates of the feedback optimization and reduces calculation time of the off-line optimization. Second, the optimization problem is explicitly formulated as a parameter optimization problem in the frame-

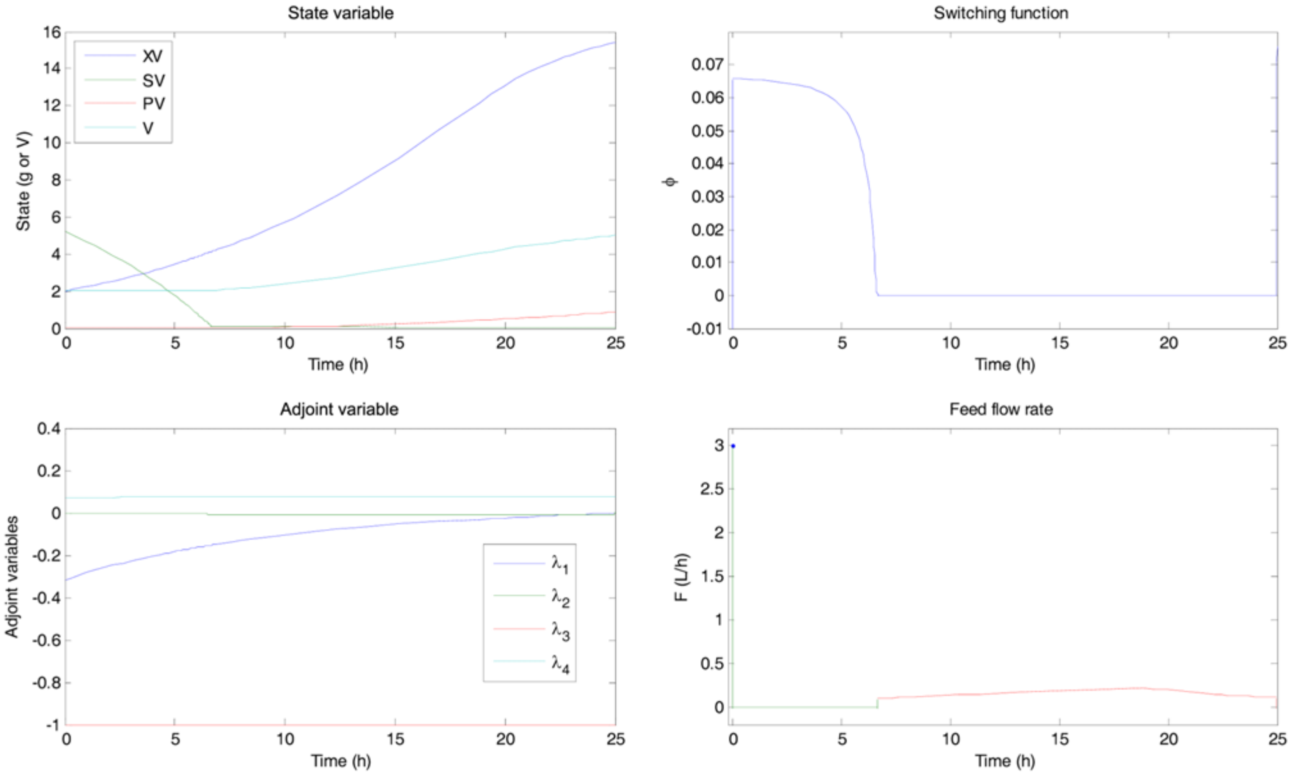

Fig. 1. Time Profiles of state and adjoint variables, switching function, and feed rate (Maximal metabolite at the fixed final time, variable yields). μ**=0.11s/(s+0.006),** π**=0.0055s/(10s**^{2}**+s+0.0001),** σ**=**μ**/0.47+**π**/1.2+0.029s/(s+0.0001) [XV, SV, PV, V](t**$_0$**)=[2g, 5g, 0g, 2L], [S**$_f$**, F**$_{max}$**, F**$_{min}$**, V**$_{max}$**, t**$_f$**]=[10wt%, 3L/h, 0L/h, 5L, 0, 25h]. Switching times: [3 0.008 6.6464 18.341 0.00490]. Final state variables: [XV, SV, PV, V](t**$_f$**)=[15.43g, 0.0023g, 0.8667g, 5.0000L].**

work of initial control or its time derivatives and switching times. This formulation can help to calculate accurate initial control or its time derivative values to optimize the first-order affine nonlinear singular systems with end-point performance index, even though optimization of these parameters is not illustrated in Palanki's work [6]. Through this case study, we can assure that the state feedback control of fed-batch process is realizable by optimizing parameters such as initial feed rate or its time-derivatives and switching times. The calculation time to solve the feedback optimization problem with state variable only is very fast compared with the case for solving the two-point boundary value problem with state and their adjoint variables. Moreover, the state feedback optimization reduces errors due to uncertainties arising from many initial conditions and parameters, which appears in open-loop optimization algorithm or model itself. Successful implementation of the feedback control in the fed-batch process depends on an accurate measurement of state variables and the reliability of model parameters. Adaptive feedback control scheme coupling the state feedback control suggested in this research with an efficient estimation of kinetic parameters of the model is expected to further improve the optimization of fed-batch fermentation.

ACKNOWLEDGEMENTS

This research was supported by grants from the Marine Biotechnology Program funded by the Ministry of Land, Transport and Maritime Affairs, Korea and by INHA UNIVERSITY Research Grant.

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