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Control of fed-batch bioreactors by a hybrid on-line optimal control strategy and neural network estimator

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ABSTRACT

It is known that the performance of an optimal control strategy obtained from an off-line computation is degraded under the presence of model–plant mismatch. In order to improve the control performance, a hybrid neural network and on-line optimal control strategy are proposed in this study and demonstrated for the control of a fed-batch bioreactor for ethanol fermentation. The information of unmeasured state variables obtained from the neural network as an on-line estimator is used to modify the optimal feed profile of the fed-batch reactor. The simulation results show that the neural network provides a good estimate of unmeasured variables and the on-line optimal control with the neural network estimator gives a better control performance in terms of the amount of the desired ethanol product, compared with a conventional off-line optimal control method.

1. Introduction

In recent years, an optimal control technique has been widely applied to control a fed-batch bioreactor for fermentation processes. Following such a control approach, the optimal operation policy in terms of a reactor feed rate is obtained by solving an optimal control problem with an objective to maximize the amount of a desired product or to minimize an operating time. Most previous studies primarily concentrated on the development of numerical solution methods for solving the formulated optimal control problems. These methods include simultaneous approach, sequential approach, and iterative dynamic programming method [1–6].

It has been known that the limitation of an optimal control approach is the existence of model–plant mismatches, a particularly important issue in designing a model-based control technique. Due to the model–plant mismatch problem, the pre-specified optimal control profile obtained from off-line calculation may not give the optimal performance when implemented to real processes. To enhance the efficiency of the process operation, it is necessary to recalculate a new optimal control profile via an on-line computation. Following an on-line optimal control approach, feedback information from the process to be controlled is usually employed to compute the updated optimal control profile for the remaining batch time. However, in reality, some process variables are immeasurable or can be even measured but with less accuracy and long time delay. To overcome this difficulty, a state estimation from available information is involved with the on-line optimal control strategy.

In order to estimate the unmeasured state variables, a variety of methods can be applied. For example, Ramirez [7] presented an optimal state and parameter estimation technique for a comprehensive model of a batch fermentation process. The sequential parameter estimation with Kalman filter was shown to be capable of estimating the entire states of the process. Neeleman and Van Boxtel [8] applied a backward and forward extended Kalman filter with off-line biomass measurements to estimate the specific growth rate that enables the calculation of kinetic parameters. The use of backward filtering to reduce the sensitivity of the estimator to initial conditions combined with the recursive forward estimation of parameters provided superior performance in biomass prediction. In addition, Cunha et al. [9] applied the principle component analysis (PCA) to improve the prediction of final process productivity. It is noted that most of these estimation techniques depend heavily on the exact knowledge of the system's dynamic model. Due to the limited understanding of nonlinear and complicated systems like biological processes, such estimators may not perform well as expected [10]. As a consequence, an attractive alternative technique such as a neural network (NN) based method is presented to handle the above situation. The advantage of NN is that any prior knowledge about the relationships that exist between the states of the system is not required; it can learn sufficiently accurate models and provides

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Nomenclature

J	performance index
K_p	kinetic constant of product (g/L)
K_s	kinetic constant of substrate (g/L)
p	product concentration (g/L)
s	substrate concentration (g/L)
t	time (h)
u	feed rate (L/h)
V	volume of reactor (L)
x	cell mass concentration (g/L)
Y	yield coefficient

Greek symbols

μ	specific growth rate (h^{-1})
η	specific productivity (h^{-1})

good estimation when model equations are not known or only partial state information is available [11]. However, there are limited efforts concerning the use of NN for bioprocesses, especially in an on-line optimal control implementation [12,13].

Therefore, the aim of this work is to develop the control approach based on the idea of an on-line optimal control strategy. The proposed on-line optimal control technique is incorporated with a NN for the estimation of unmeasured process variables and applied to modify the optimal feed rate policy of substrate in a fed-batch bioreactor for ethanol production. The performance of the on-line optimal control strategy with NN estimator is demonstrated via simulation studies in case of disturbance rejection and model–plant mismatch.

2. Model of fed-batch bioreactor

The present study is focused on the production of ethanol in a fed-batch bioreactor. The process model developed by Hong [14] for describing the ethanol fermentation by *Saccharomyces cerevisiae* in a fed-batch culture is used in simulation studies. The mathematical model consists of four differential equations describing the changes in concentration of cell mass (x), substrate (s: glucose), and product (p: ethanol), and in liquid volume (v), as shown

$$\frac{dx}{dt} = \mu x - \frac{x}{v}u \tag{1}$$

$$\frac{ds}{dt} = -\frac{\mu x}{Y} + \frac{(s_0 - s)}{v}u \tag{2}$$

$$\frac{dp}{dt} = \eta x - \frac{p}{v}u \tag{3}$$

$$\frac{dv}{dt} = u \tag{4}$$

$$\mu = \frac{\mu_0 s}{(1 + p/K_p)(K_s + s)} \tag{5}$$

Table 1
Initial conditions and kinetic parameters of bioreactor model for ethanol production.

Initial conditions	Kinetic parameters (g/L)
$x(0) = 1$ g/L	$K_p = 16.0$
$s(0) = 150$ g/L	$K_s = 0.22$
$p(0) = 0$ g/L	$K_p{}' = 71.5$
$v(0) = 10$ L	$K_s{}' = 0.44$
$\mu_0 = 0.408\ h^{-1}$	
$\eta_0 = 1\ h^{-1}$	

$$\eta = \frac{\eta_0 s}{(1 + p/K_p')(K_s' + s)} \tag{6}$$

where μ is the specific growth rate, η is the specific productivity, Y is the yield coefficient ($= 0.1$), s_0 is the substrate concentration in feed stream, and u is the feed rate of substrate which is the only manipulated variable in this process.

Table 1 shows the initial conditions and kinetic parameters of the process. It is noted that for the process considered, the maximum value of substrate feed rate (u) is 12 L/h, the liquid volume of the reactor is limited by 200 L, and the operating time of the fed-batch reactor (t_f) is fixed to be 63 h.

3. Formulation of an optimal control problem

The optimal control problem of a fed-batch bioreactor for a fixed final time is formulated to find a substrate feed rate $u(t)$ over $t \in [t_0, t_f]$ maximizing the amount of a desired product of ethanol at the end of batch run. This can be mathematically stated as

$$\max_{u(t)} \quad J = p(t_f) \times v(t_f) \tag{7}$$

subject to

$$\text{bioreactor model equations (Eqs. (1)–(6))} \tag{8}$$

$$0 \leqslant v(t) \ \text{(L)} \leqslant 200 \tag{9}$$

$$0 \leqslant u(t) \ \text{(L/h)} \leqslant 12 \tag{10}$$

where t_f denotes the final time of the operation, $p(t_f)$ and $v(t_f)$ are the product (ethanol) concentration and the liquid volume within the reactor at the end of batch, respectively. Eqs. (9) and (10) show the upper and lower bounds on the reactor volume and the feed rate, respectively.

3.1. Solution method via a sequential approach

In this study, the optimal control problem as formulated earlier is solved by using a sequential approach in which the control variables are discretized in order to transform a dynamic optimization problem into a nonlinear programming problem (NLP). Typically, a piecewise constant approximation with equally spaced time intervals is made for the control variables. The main advantage of the sequential approach is that only the control profile is considered as a decision variable and therefore, the resulting NLP problem is a small scale optimization problem [15]. The basic algorithm of the sequential approach can be summarized in Fig. 1. With the initial guess of the decision variables (in this problem, i.e. the value of feed rate at each time interval), an integrator based on Gear's type method is used for solving the process model providing the value of the objective function and constraints. Gradient information of the objective function and constraints with respect to the decision variables is evaluated using an adjoint variable approach. Then, a NLP solver [16]