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OPTIMIZATION ALGORITHM AND ITS CONVERGENCE FOR MICROBIAL CONTINUOUS FERMENTATION

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ABSTRACT. Based on the producing 1, 3-propanediol from microorganism continuous fermentation, we study the algorithm and its convergence for the optimal model in this paper. First, taking the zero of the optimality function as the terminal criteria, an algorithm for the discrete time system of the optimal model is given with the step-size determined by Armijo line search and the search direction by gradient method. By the result that the discrete time system converges to the continuous time optimal model, the optimality function of the discrete time system is a consistent approximation to the one of the continuous time optimal model and an algorithm for the optimal model is given too. The convergence of the algorithm is proved. At last, it shows that the optimal model describes the experiment correctly and the algorithm is feasible by comparing the computing value with the dates in laboratory.

1. Introduction. 1,3-propanediol (1,3-PD) possesses potential applications on a large commercial scale; especially as a monomer of polyesters or polyurethanes, its microbial production has been given worldwide attention for its low cost, high production and no pollution, etc. It is considered to be one of the bulk chemicals, which is likely to be produced by bioprocesses on large scales. If we can find an optimum way to get a higher concentration of 1,3-PD by the mathematical method (but not chemical experimentation), a lot of money and time could be saved. A great contribution has been made by GBF (National Research Institute for Biotechnology). A kinetic model for substrate and energy consumption of microbial growth under the substrate-sufficient condition was formed by Drs. An-ping Zeng and Deckwer in 1995 [**1**]. In 2000, Xiu et al. modified the parameters in the kinetic model by the least squares method [**9**]. Based on the modified

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model, many results were given. In particular, in 2003, Sun et al. studied the phenomena and characterization of oscillation in microbial continuous ferment [**8**]. The optimal control in microbial continuous ferment was studied through numerical calculation by genetic algorithm in 2004 [**10**]. Recently, the property, parameter identification and optimal control of the impulse system in microbial fed-batch ferment were analyzed [**2**–**5**]. Taking the final concentration of 1,3-PD as the objective function, the optimal control in microbial continuous ferment was discussed, and the optimality condition was given in 2006 [**6**]. In the same year, we gave a discrete time system corresponding to the continuous one and formed a discrete time optimal control model. Its optimality function which was a consistent approximation to the one of the continuous time optimal control model was defined [**7**]. Then, the next problem was how to construct an effective algorithm by which we can get the optimum operating condition. When the optimum operating condition is taken in the laboratory, the higher concentration of 1,3-PD will be obtained. In this paper, taking the zero of the optimality function as the terminal criteria, an algorithm (Algorithm 1) for the discrete time system of the optimal model is given with the step-size determined by Armijo line search and the search direction by the gradient method. This algorithm is ready for Algorithm 2. By the result that the discrete time system converges to the continuous time optimal model, the optimality function of the discrete time system is a consistent approximation to the one of the continuous time optimal model; an algorithm (Algorithm 2) for the optimal model is given too. The convergence of Algorithm 2 is proved by the above result. Finally, it shows that the optimal model describes the experiment correctly and the algorithm is feasible by comparing the computed value with the dates in laboratory.

2. Optimal control model for microbial continuous ferment. In 2000, a modified model was given by Xiu et al., see [**2**]:

$$(1)\qquad \begin{cases} \dot{x}_1(t) = h_1(x,u) = (\mu - D)x_1(t), \\ \dot{x}_2(t) = h_2(x,u) = D(x_{20} - x_2(t)) - q_2 x_1(t), \\ \dot{x}_3(t) = h_3(x,u) = q_3 x_1(t) - Dx_3(t), \\ \dot{x}_4(t) = h_4(x,u) = q_4 x_1(t) - Dx_4(t), \\ \dot{x}_5(t) = h_5(x,u) = q_5 x_1(t) - Dx_5(t), \end{cases} \qquad t \in [0,T]$$

where

(2)

$$\begin{cases} \mu = \mu_m \dfrac{x_2(t)}{x_2(t)+k_s}\left(1-\dfrac{x_2(t)}{x_2^*}\right)\left(1-\dfrac{x_3(t)}{x_3^*}\right)\left(1-\dfrac{x_4(t)}{x_4^*}\right)\left(1-\dfrac{x_5(t)}{x_5^*}\right), \\ q_2 = m_2 + \dfrac{\mu}{Y_2^m} + \Delta q_2^m \dfrac{x_2(t)}{x_2(t)+k_2}, \\ q_3 = m_3 + \mu Y_3^m + \Delta q_3^m \dfrac{x_2(t)}{x_2(t)+k_3}, \\ q_4 = m_4 + \mu Y_4^m + \Delta q_4^m \dfrac{x_2(t)}{x_2(t)+k_4}, \\ q_5 = q_2 \left(\dfrac{0.025}{0.06 + Dx_2(t)} + \dfrac{5.18}{50.45 + Dx_2(t)}\right). \end{cases}$$

The vector form of (1) is as follows:

$$\begin{cases} \dot{x}(t) = h_c(x,u) & t \in [0,T], \\ x(0) = \xi = (x_1^0, x_2^0, 0, 0, 0)^T, \end{cases} \tag{3}$$

where the elements of the state variable $x(t) = (x_1(t), x_2(t), \dots, x_5(t))^T \in R^5$ are biomass, substrate, product 1,3-PD, acetic acid and ethanol concentration in the reactor. The elements of the control variable $u = (D, x_{20})^T \in R^2$ are dilution rate, substrate concentration in the medium. ξ is the initial value for the state variable. $h_c(x,u) = (h_1(x,u), h_2(x,u) \dots, h_5(x,u))^T$. Let W be the solution set of (3), i.e., $W = \{x^u(t) \mid x^u(t) \text{ is the solution of (3)}\}$. The meanings of the other parameters can be found in [**9**]. In 2006, by simple translation we turned the time interval $[0,T]$ to $[0,1]$ and gave an optimal control model, taking the final concentration of 1,3-PD as the objective function [**6**]:

$$\begin{aligned} \text{(P):} \quad \max \quad & J(u) = x_3^u(1) \\ \text{s.t.} \quad & \dot{x}(t) = h_c(x(t),u), \quad t \in [0,1] \\ & x(0) = \xi \\ & x^u(t) \in W \\ & u \in U_{ad}, \end{aligned}$$

where $x_3^u(1)$ is the final value of the third element of $x^u(t)$, i.e., the final concentration of 1,3-PD in the reactor. By defining some new functions, we give the equivalence form of (P) as follows:

$$\text{(P1):} \qquad \min_{u\in U_{ad}} \left\{ f_c^0(u) \mid f_c^j(u) \le 0,\ j \in \mathbf{q}_c \right\},$$

where $f_c^0(u)$ is the intensity of 1,3-PD and it is the continuous function of u. At the same time, the existence of the optimal solution and the optimality condition of the problem (P1) are discussed and its optimality function $\theta_c(u)$ is defined.

$$\theta_c(u) \triangleq \min_{v\in U_{ad}} \overline{F}_c(u,v), \quad u \in U_{ad}, \tag{4}$$

where

$$\overline{F}_c(u,v) \triangleq \max\left\{ \bar{f}_c^0(u,v) - f_c^0(u) - \gamma\psi_c(u)_+,\ \overline{\psi}_c(u,v) - \psi_c(u)_+ \right\}$$
$$\bar{f}_c^0(u,v) \triangleq f_c^0(u) + \langle \nabla_u f_c^0(u), v-u\rangle + \delta/2\|v-u\|^2$$
$$\bar{f}_c^j(u,v) \triangleq \max_{t\in[0,1]} \{\phi_c^j(u,t) + \langle \nabla_u \phi_c^j(u,t), v-u\rangle + \delta/2\|v-u\|^2\}$$
$$\overline{\psi}_c(u,v) \triangleq \max_{j\in\mathbf{q}_c} \bar{f}_c^j(u,v)$$

(5)

$$F_c(u,v) \triangleq \max\left\{ f_c^0(v) - f_c^0(u) - \gamma\psi_c(u)_+,\ \psi_c(v) - \psi_c(u)_+ \right\}$$
$$\psi_c(u)_+ \triangleq \max\{\psi_c(u),\ 0\}$$

(6)

$$\psi_c(u) \triangleq \max_{j\in\mathbf{q}_c} f_c^j(u),$$

where $v, u \in U_{ad},\ j \in \mathbf{q}_c, \gamma, \delta \in R_+$.

In [**7**], according to the continuous system, we gave the discrete-time system:

$$\begin{cases} x_N(u,t_{k+1}) - x_N(u,t_k) = 1/Nh_c(x_N(u,t_k),u) & k \in \overline{N-1}, \\ x_N(u,0) = x(0,), \end{cases} \tag{7}$$

where $\overline{N-1} = \{0,1,\dots,N-1\}$, $t_k = k/N$. Then an optimal control for the discrete-time system was formed:

$$\text{(CPN)} \qquad \min_{u\in U_{ad}} \{f_{c,N}^0(u) \mid f_{c,N}^j(u) \le 0,\ j \in \mathbf{q}_c\}$$

and the optimality functions of (CPN) are defined as follows:

$$\theta_{c,N}(u) \triangleq \min_{v\in U_{ad}} \widehat{F}_{c,N}(u,v) \tag{8}$$

where

$$\widehat{F}_{c,N}(u,v) \triangleq \max\{\hat{f}^0_{c,N}(u,v) - f^0_{c,N}(u) - \gamma\psi_{c,N}(u)_+, \widehat{\psi}_{c,N}(u,v) - \psi_{c,N}(u)_+\} \tag{9}$$

$$\overline{F}_{c,N}(u,v) \triangleq \max\{f^0_{c,N}(v) - f^0_{c,N}(u) - \gamma\psi_{c,N}(u)_+, \psi_{c,N}(v) - \psi_{c,N}(u)_+\}. \tag{10}$$

Other functions mentioned above can be found in [**7**].

Lemma 1. *If $\hat{u}$ is the optimal solution of* (P1), *then $\theta_c(\hat{u}) = 0$.*

Lemma 2. *Suppose $\{u_N\}_{N\in\mathcal{N}} \in U_{ad}$ satisfies $u_N \xrightarrow{\mathcal{N}} u$ as $N \to +\infty$. Then $\theta_{c,N}(u_N) \xrightarrow{\mathcal{N}} \theta_c(u)$ as $N \to +\infty$, where $\theta_c(u)$ is defined by* (4), *and $\theta_{c,N}(u_N)$ is defined by* (8).

The proof of Lemmas 1 and 2 can be found in [**7**]. By [**7**, Theorem 6] and the definitions of $F_c(u,v)$ and $\overline{F}_{c,N}(u,v)$, we can get

Lemma 3. *There exist constants L_s and $N_0 \in \mathcal{N}$ such that*

$$F_c(u_i, u_{i+1}) \leq \overline{F}_{c,N}(u,v) + L_S/N \tag{11}$$

holds for all $N > N_0$.

3. Optimization algorithm and its convergence. Taking the zero of the optimality function of (CPN) as a terminal criteria and imitating the gradient method to get a search direction, an algorithm for (CPN) is as follows:

Algorithm 1.

Parameters $\delta, \gamma > 0, \alpha, \beta \in (0, 1]$.

Date $u_0 \in U_{ad}$.

Step 1. Set $N = 0$,

Step 2. Compute the optimality function value according to (8):

$$\theta_N = \min_{u \in U_{ad}} \widehat{F}_{c,N}(u_N, u),$$

where $\widehat{F}_{c,N}(u, v)$ is defined by (9).

If $\theta_N > -\varepsilon$, stop.

Else compute $h_N = u_N^* - u_N$, with

$$u_N^* = \arg \min_{u \in U_{ad}} \widehat{F}_{c,N}(u_N, u).$$

Step 3 Compute the step-size

$$\lambda_N = \max_{k \in N} \{\beta^k \mid \overline{F}_{c,N}(u_N, u_N + \beta^k h_N) - \beta^k \alpha \theta_N \leq 0\}. \tag{12}$$

Step 4 Set $u_{N+1} = u_N + \lambda_N h_N$, replace N by $N + 1$, and go to Step 2.

Theorem 1. *Suppose $\{u_N\}_{N=0}^{+\infty}$ is a sequence constructed by Algorithm 1 in solving* (CPN)*, with the same values of the parameters $\gamma, \alpha, \beta, \delta$, with $\delta > 0$ as in the definition of $\theta_c(u)$. If the accumulation point $\hat{u}$ of $\{u_N\}_{N=0}^{+\infty}$ satisfies $\theta_c(\hat{u}) < 0$, then there exists an $N_1 \in \mathcal{N}$ and a $\rho > 0$ such that*

$$\overline{F}_{c,N}(u_N, u_{N+1}) \leq -\rho$$

for all $N \geq N_1$.

Proof. According to Lemma 1, there exists a $-\theta_c(\hat{u})/2 > 0$ and $N_1 \in \mathcal{N}$ such that

$$\theta_N = \theta_{c,N}(u_N) - \theta_c(\hat{u}) \leq -\theta_c(\hat{u})/2$$

for all $N \geq N_1$. This means

$$\theta_N \leq \frac{\theta_c(\hat{u})}{2}.$$

By (12) in Algorithm 1, we have that

$$\overline{F}_{c,N}(u_N, u_{N+1}) \leq \beta^k \alpha \theta_N \leq \beta^k \alpha \frac{\theta_c(\hat{u})}{2} \triangleq -\rho < 0. \qquad \square$$

By Lemma 1, we see that the problem (P1) can be solved by the following algorithm in which Algorithm 1 defines the "inner" loop. For every $N \in \mathcal{N}$, we can get a sequence $\{u_N\}_{N=0}^{+\infty}$ with u_N satisfying $\theta_{c,N}(u_N) = 0$. The inequality (13) in Algorithm 2 assures that every accumulation point $\hat{u}$ of $\{u_N\}_{N=0}^{+\infty}$ satisfies $\theta_c(\hat{u}) = 0$.

Algorithm 2.

Parameters $\alpha, \beta, \omega \in (0,1)$, $\gamma, \delta, \sigma > 0$, constant $L_S > 0$, $\varepsilon > 0$.

Date $u_0 \in U_{ad}$, $N_0 \in \mathcal{N}$.

Step 1 Set $i = 0$, $N = 0$, go to inner loop.

inner loop Step 1 Set $N = N_i$, $u_N = u_i$.

inner loop Step 2 Compute the optimality function value according to (8)

$$\theta_N = \min_{u \in U_{ad}} \widehat{F}_{c,N}(u_N, u).$$

and the search direction $h_N = u_N^* - u_N$, with u_N^* computed according to

$$u_N^* = \arg \min_{u \in U_{ad}} \widehat{F}_{c,N}(u_i, u).$$

inner loop Step 3 If $\theta_N > -\varepsilon$, set $u_N^* = u_N$, and go to inner loop Step 5.

Else, compute the step-size λ_N according to

$$\lambda_N = \max_{k \in N} \{\beta^k | \overline{F}_{c,N}(u_N, u_N + \beta^k h_N) - \beta^k \alpha \theta_N \leq 0\}.$$

inner loop Step 4 Set $u_N^* = u_N + \lambda_N h_N$.

inner loop Step 5 If

$$\overline{F}_{c,N}(u_N, u_N^*) \leq -\sigma(L_S/N)^\omega \tag{13}$$

go out inner loop, go to Step 2.

Else, set $N_i = \min\{N' \in \mathcal{N} \mid N' > N\}$ and go to inner loop Step 1.

Step 2 Set $u_{i+1} = u_N^*$, if $\|u_i - u_{i+1}\| < \varepsilon$, stop. Else, set $N_{i+1} = \min\{N' \in \mathcal{N} \mid N^{'} > N\}$, replace i by $i+1$ and go to inner loop Step 1.

Theorem 2. *If* $\{u_i\}_{i=0}^{+\infty}$ *is a sequence constructed by Algorithm* 2 *in solving* (P1)*, then every accumulation point* $\hat{u}$ *of* $\{u_i\}_{i=0}^{+\infty}$ *satisfies* $\theta_c(\hat{u}) = 0$.

Proof. First we know that, by Lemma 2,

$$F_c(u_i, u_{i+1}) \leq \overline{F}_{c,N}(u_i, u_{i+1}) + L_S/N \tag{14}$$

holds for all $N > N_0$. Consequently, we conclude from (13), that

$$F_c(u_i, u_{i+1}) \leq -\sigma(L_S/N)^\omega + L_S/N = -(L_S/N)^\omega(\sigma - (L_S/N)^{1-\omega}).$$

Because $1 - \omega > 0$, there exists $i_0 \in N^+$,

$$F_c(u_i, u_{i+1}) \leq 0, \tag{15}$$

which holds for all $i \geq i_0$.

Now suppose that, for some $K \subseteq \mathbf{N}$, $u_i \xrightarrow{K} \hat{u}$, as $i \to +\infty$, and that $\theta_c(\hat{u}) < 0$.

By Theorem 1, there exist $i_1 \in K$, $\rho > 0$, for all $i \in K$, $i \geq i_1$, such that

$$\overline{F}_{c,N_i}(u_i, u_{i+1}) \leq -\rho < 0.$$

Inserting this into (14), we have that

$$F_c(u_i, u_{i+1}) \leq L_S/N - \rho.$$

Since $L_S/N \to 0$ as $N \to +\infty$, there exists $i_2 \geq i_1$,

$$F_c(u_i, u_{i+1}) \leq -\frac{\rho}{2} < 0, \tag{16}$$

which holds for all $i \geq i_2$.

Now we must consider two cases.

Case (i). If $\psi_c(u_i) > 0$ for all $i \geq i_2$, then $\psi_c(u_i)_+ = \psi_c(u_i) > 0$. By the definition of $F_c(u_i, u_{i+1})$ and (16), we know that

$$\psi_c(u_{i+1}) - \psi_c(u_i)_+ = \psi_c(u_{i+1}) - \psi_c(u_i) \leq F_c(u_i, u_{i+1}) \leq -\frac{\rho}{2} < 0.$$

This means that the sequence $\{\psi_c(u_i)\}_{i=i_2}^{+\infty}$ is monotonically decreasing, and $\psi_c(u_i) \to -\infty$ as $i \to +\infty$, which contradicts the fact that $\psi_c(u_i) > 0$ for all $i \geq i_2$.

Case (ii). There exists an $i_3 \in N^+$, $i_3 \geq i_2$, such that $\psi_c(u_{i_3}) \leq 0$. Then $\psi_c(u_{i_3})_+ = 0$. It follows (15) that $\psi_c(u_{i_3+1}) \leq 0$ and $\psi_c(u_i) \leq 0$ for all $i > i_3$. Then, according to (16), we have

$$\begin{aligned} f_c^0(u_{i+1}) - f_c^0(u_i) - \gamma\psi_c(u_i)_+ = f_c^0(u_{i+1}) - f_c^0(u_i) \leq F_c(u_i, u_{i+1}) \\ \leq -\frac{\rho}{2} < 0. \end{aligned}$$

This means that the sequence $\{f_c^0(u_i)\}_{i=i_3}^{+\infty}$ is monotonically decreasing, and $f_c^0(u_i) \to -\infty$ as $i \to +\infty$, which contradicts the fact that, by continuity of $f_c^0(u)$, $f_c^0(u_i) \xrightarrow{K} f_c^0(\hat{u})$ as $i \to +\infty$. □

4. Numerical example and analysis. Taking parameters: $\alpha = 0.5$, $\beta = 0.5$, $\omega = 0.5$, $\gamma = 1$, $\delta = 1$, $\sigma = 1$, $N_0 = 2^8$, $L_S = 100$, $\varepsilon = 10^{-6}$, the computing values and the dates in the laboratory are listed in Table 1. Where the first column is the initial

TABLE 1. Comparison between the results in laboratory and computing.

u_0	date in laboratory	computing value	$\widehat{u}$
0.1, 1568	638.16	733.876	0.116, 1565.72
0.1, 1883	555.11	732.83	0.131, 1581.05
0.1, 1287	505.28	728.32	0.122, 1570.33
0.45, 607	124.38	587.69	0.093, 1520.32
0.15, 1443	484.35	730.78	0.122, 1568.45
0.35, 1395	127.4	698.35	0.098, 1566.58
0.5, 861	93.6	728.65	0.112, 1565.55
0.08, 152	53	691.23	0.125, 1577.26
0.47, 435	170	634.76	0.112, 1654.34

value u_0 in the algorithm, it is the initial date in the laboratory too. The second column is final concentration of 1,3-PD in the laboratory. The third column is the computing concentration of 1,3-PD, and the fourth column is the computing value of optimal control $\hat{u}$, i.e., the optimal operating condition. From Table 1, no matter how to choose the initial value u_0, the computing value $\hat{u}$ is around $u = (0.1, 1568)$; meanwhile, the highest final concentration of 1,3-PD is obtained. From the date in laboratory (the first and second column in Table 1), the highest final concentration of 1,3-PD is obtained when the initial date is $u = (0.1, 1568)$. This illuminates the fact that the computational optimal controls are convincing, and the model describes the experiment in essence; the algorithm is feasible.

While the appropriate control $\hat{u}$ is chosen, the computing values of concentration of 1,3-PD (the fourth column) can be obtained. Obviously, the concentration of 1,3-PD is higher than one in the laboratory in Table 1. This shows that the appropriate control can improve the final concentration of 1,3-PD and the appropriate control can be computed by the model and the algorithm. This indicates that model and the algorithm are valid too.

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