PSO-based Parameter Estimation of Nonlinear Kinetic Models for β-Mannanase Fermentation

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Original scientific paper
Received: March 12, 2007
Accepted: June 14, 2008

Particle swarm optimization (PSO), as a novel evolutionary algorithm involved in social interaction for global space search, was firstly used in kinetic parameter estimation. Based on three developed nonlinear kinetic equations for bacterial cell growth, total sugar utilization and β-mannanase production by *Bacillus licheniformis* under the support of a batch fermentation process, various PSO algorithms as well as gene algorithms (GA) were developed to estimate kinetic parameters. The performance comparison among these algorithms indicates the improved PSO (Trelea 1) is most suitable for kinetic parameter estimation of β-mannanase fermentation. In order to find the physical-chemical-meanings of kinetic parameters from many optimized results, multiobjective optimization with a normalized weight method was adopted. The 9 desired parameters in equations were obtained by the Trelea 1 type PSO with two batches fermentation data, and the results predicted by the models were also in good agreement with the experimental observations.

Key words:
Particle swarm optimization, parameter estimation, kinetic model, β-mannanase, multiobjective optimization

Introduction

As is well known, kinetic models play an important role in the analysis, design and operation of chemical/biochemical processes. Besides their important roles in chemical reaction process,[1] the kinetic equations, in a specific microbial fermentation process can both theoretically elucidate the characteristic of cell growth and metabolic mechanism in certain conditions and quantitatively describe the change of fermentation behavior.[2] Therefore, the establishment of models and estimation of kinetic parameters was always the key to the fermentation research until now. Among these studies, the kinetic models are usually divided into two classes: structured model and unstructured model. The latter one, characterized as a set of nonlinear equations, is frequently applied to simulate one kind of microbial fermentation processes for its simplicity and clear biological or physicochemical meanings of kinetic parameters.[3–8] Parameter estimation is important for determining unknown kinetic equations.[9] A number of algorithms, such as nonlinear least square regression,[3] simplex algorithm[5–6] and genetic algorithm (GA),[7–8] have been successfully developed to estimate parameters of these unknown equations. Unfortunately, these algorithms often brought some unexpected problems, such as weak simulated veracity, complex concept and codes, or long computed time.

Particle swarm optimization (PSO), as a novel global search algorithm, was initially proposed by Kennedy and Eberhart [10] when they devoted themselves to simulation on social behavior of bird flocking using the computer. PSO, one of the evolutionary algorithms, also maintains many similarities shared with GA: initializing step and updating generations. As a famous saying, the new coming from the old is better than the old; the PSO algorithm has many advantages over GA in some aspects. Unlike GA, PSO can directly search for the optima in the multidimensional space without crossover and mutation operation,[11] and may make particles keeping memory (position and velocity). Moreover, PSO is proved simple in concept, easy to implement and computationally efficient.[12] In view of these advantages of PSO, a lot of applied papers about PSO have been recently published.[13–14] But few papers are concerned with the application of PSO in chemical/biochemical process research field. In this paper various PSO-based algorithms were employed in parameter estimation of nonlinear kinetic models for an important industry enzyme – β-mannanase fermentation by *Bacillus licheniformis*.

Materials and methods

Culture conditions

β-Mannanase fermentation by *Bacillus licheniformis* was carried out in a $V = 6.6$ L fermenter [15] (Bioflo-IIc, New Brunswick Scientific Co., USA)

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containing 4.5 L production medium (pH 7) of the following composition (g L^{-1}): konjac powder, 34; meat peptone, 30; corn steep liquor, 5; $(NH_4)_2SO_4$, 5; Na_2HPO_4, 4; KH_2PO_4, 0.3; $MgCl_2$, 0.6; $CaCl_2$, 3; and $FeSO_4$, 0.01. Konjac powder was purchased from Dazhou Wufeng Co. (Sichuan, China) and the amount of glucomannan in konjac powder was w = 82.4 %. Batch fermentation was carried out at θ = 30 °C, aeration at 1:1 L L^{-1} min^{-1}, and dissolved O_2 at 40 % saturation. Inoculum (φ = 10 % in volume) was taken from a culture grown in an inoculum medium (pH 7.5) that had a composition (γ/g L^{-1}) of beef extract, 5; peptone, 10; yeast extract, 5; and NaCl, 5. The later cultures were incubated at θ = 30 °C with shaking at 180 rpm for 16 h.

Analyses

The konjac glucomannan concentration was expressed as the total sugar concentration and analyzed after hydrolysis in C = 6 mol L^{-1} HCl for 1 h, followed by detection of reducing sugar carried out in accordance with the method of Bernfeld.[16] Cell density was measured turbidometrically at 560 nm and converted into cell dry mass using a calibration curve. β-mannanase activity was determined according to the method of Akino.[17] One unit of β-mannanase activity was defined as the amount of enzyme which released 1 μmol reducing sugar as equivalent to D-mannose per min. Then the β-mannanase activity was converted into a protein concentration using a calibration curve.

Results and discussion

Kinetic models of β-mannanase fermentation

The fermentation process data of cell growth, total sugar utility and β-mannanase synthesis are shown in Fig. 1.

From Fig. 1, some important information was shown as follows: (1) the curve of cell growth was quite similar to the pattern of Monod equation except a short lag phase in initial four hours; (2) the trend of the curve for β-mannanase synthesis also extremely coincided with the formula of Monod equation; (3) as the cell grew, the total sugar concentration decreased, which obviously suggested that the total sugar was the limiting substrate for cell growth.

According to Feng,[5] a low fraction of total sugar (about 20 %) could not be taken in by the bacteria because the total sugar (konjac glucomannan) was not fully hydrolyzed by β-mannanase. Therefore, the total sugar (γ_S) was divided into two

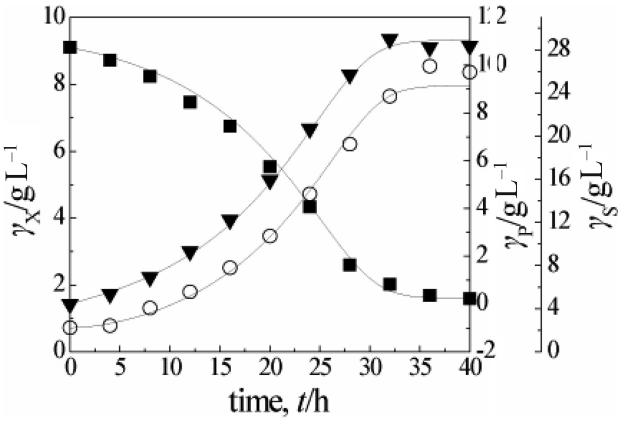


Fig. 1 – *Kinetics of cell growth, enzyme synthesis and substrate utilization in a batch fermentation process (γ_{S_0} = 28 g L^{-1}) for β-mannanase production by Bacillus licheniformis. Symbols represent cell concentration γ_X (g L^{-1}) (○), enzyme concentration γ_P (g L^{-1}) (▼) and total sugar concentration γ_S (g L^{-1}) (■), which were observed in the fermentation experiment. The simulated results (–) were calculated from eqs. (5)-(7) after the optimal kinetic parameters in Table 2 were obtained by PSO.*

portions: available part (γ_{S_a}) and unavailable part (γ_{S_u}), as shown in eq. (1).

$$\gamma_S = \gamma_{S_a} + \gamma_{S_u} \tag{1}$$

The latter (γ_{S_u}) was regarded as a part of the initial total sugar (γ_{S_0}):

$$\gamma_{S_u} = f_s \gamma_{S_0} \tag{2}$$

According to the information of cell growth and metabolism, a modified Monod equation with a lag phase [18] was applied in the experiment (eq. (3)), and a cell growth equation was established according to *Malthus*' law,[19] which was based on the assumption that cell growth rate has a linear relation with the cell concentration, as shown in eq. (4).

$$\mu = \mu_m \frac{\gamma_{S_a}}{K_S + \gamma_{S_a}} \left[1 - \exp\left(-\frac{t}{t_L}\right)\right] \tag{3}$$

$$\frac{d\gamma_X}{dt} = \mu \gamma_X \tag{4}$$

By incorporating eq. (3) into eq. (4), the cell growth equation for β-mannanase fermentation is shown in eq. (5):

$$\frac{d\gamma_X}{dt} = \mu_m \frac{\gamma_{S_a}}{K_S + \gamma_{S_a}} \left[1 - \exp\left(-\frac{t}{t_L}\right)\right] \gamma_X \tag{5}$$

When the inducing effect of the total sugar and the correlation between cell growth and enzyme production were taken into consideration, the model for β-mannanase synthesis was similar to Monod equation, as listed in eq. (6):

$$\frac{\mathrm{d}\gamma_{\mathrm{P}}}{\mathrm{d}t} = \frac{q_{\mathrm{m}}\gamma_{\mathrm{S_a}}\gamma_{\mathrm{X}}}{K_{\mathrm{P}} + \gamma_{\mathrm{S_a}}} \tag{6}$$

As to material balance, there were usually three ways for substrate utilization: supporting cell growth, supplying β-mannanase production and providing energy for cell maintenance.[20] Consequently, the substrate utilization kinetic equation was expressed as follows:

$$\frac{\mathrm{d}\gamma_{\mathrm{S}}}{\mathrm{d}t} = -\frac{1}{Y_{\mathrm{X/S}}}\frac{\mathrm{d}\gamma_{\mathrm{X}}}{\mathrm{d}t} - \frac{1}{Y_{\mathrm{P/S}}}\frac{\mathrm{d}\gamma_{\mathrm{P}}}{\mathrm{d}t} - m\gamma_{\mathrm{X}} \tag{7}$$

In short, three nonlinear kinetic equations for cell growth, enzyme synthesis and total sugar utilization were respectively developed in eqs. (5-7).

Optimization algorithms and cost function

Various optimization algorithms were used to estimate kinetic parameters for β-mannanase fermentation by *Bacillus licheniformis*. After the original PSO was introduced by Kennedy and Eberhart,[10] a number of improved versions depending on certain problems were presented. For example, the PSO, one of the most popular versions, was developed by Shi and Eberhart:[21]

$$v_{k+1} = w_{\mathrm{ab}}v_k + c_1\,\mathrm{rand}()(p_{ik} - x_{ik}) + \\ + c_2\,\mathrm{RAND}()(p_{gk} - x_{gk})] \tag{8}$$

$$x_{k+1} = x_k + v_{k+1} \tag{9}$$

According to Shi and Eberhart, [21] the inertia weight w plays a key role on the performance of PSO. Their optimization results indicated that w, which started with a large value 1.4 and linearly decreased to 0, led to a best performance of the Shi-type PSO.

Subsequently, Clerc and Kennedy[22] contributed to a PSO with constriction coefficient, which was used in some optimization problems in a multidimensional complex space. And the explosion, stability and convergence of PSO were elaborately analyzed. The updated equations of velocity and position in the Clerc-type PSO was listed as follows:

$$v_{k+1} = \chi[v_k + \varphi_1\,\mathrm{rand}()(p_{ik} - x_{ik}) + \\ + \varphi_2\,\mathrm{RAND}()(p_{gk} - x_{gk})] \tag{10}$$

$$x_{k+1} = x_k + v_{k+1} \tag{11}$$

In eq. (10), the constriction coefficient χ was calculated as follows:

$$\chi = \begin{cases} \sqrt{\dfrac{2\kappa}{\varphi - 2 + \sqrt{\varphi^2 - 4\varphi}}}, & \text{for } \varphi = \varphi_1 + \varphi_2 > 4 \\ \kappa, & \text{for } \varphi = \varphi_1 + \varphi_2 \le 4 \end{cases} \tag{12}$$

where $0 \le \kappa \le 1$, and the standard value ($\kappa = 1$) was adopted in this work.

An improved deterministic PSO algorithm was introduced by Trelea,[23] and the algorithm was simply expressed as follows:

$$v_{k+1} = a v_k + b(p_{ik} - x_{ik}) + b(p_{gk} - x_{gk}) \tag{13}$$

$$x_{k+1} = c x_k + d v_{k+1} \tag{14}$$

After dynamic analysis and optimization experiments, Trelea[23] emphasized two important parameters of the algorithm, a and b, and divided them into two parameter sets: Trelea 1 ($a = 0.6$; $b = 1.7$) and Trelea 2 ($a = 0.729$; $b = 1.494$). Additionally, both c and d were generally set as 1.

The five types of PSO algorithms (Original, Shi-type, Clerc-type, Trelea 1 and Trelea 2) as well as GA were respectively employed in the kinetic parameter optimization for β-mannanase production from *Bacillus licheniformis*.

The objective cost function for kinetic parameter estimation was expressed as:

$$f_{\mathrm{cost}} = \sum_n \left(\frac{\gamma^0_{\mathrm{S}_i} - \gamma^{\mathrm{s}}_{\mathrm{S}_i}}{\gamma_{\mathrm{S_M}}}\right)^2 + \sum_n \left(\frac{\gamma^0_{\mathrm{X}_i} - \gamma^{\mathrm{s}}_{\mathrm{X}_i}}{\gamma_{\mathrm{X_M}}}\right)^2 + \\ + \sum_n \left(\frac{\gamma^0_{\mathrm{P}_i} - \gamma^{\mathrm{s}}_{\mathrm{P}_i}}{\gamma_{\mathrm{P_M}}}\right)^2 \tag{15}$$

where $\gamma^0_{\mathrm{S}_i}$, $\gamma^0_{\mathrm{X}_i}$ and $\gamma^0_{\mathrm{P}_i}$ are the observed mass concentrations of substrate, cell and enzyme, respectively, and $\gamma^{\mathrm{s}}_{\mathrm{S}_i}$, $\gamma^{\mathrm{s}}_{\mathrm{X}_i}$ and $\gamma^{\mathrm{s}}_{\mathrm{P}_i}$ are the corresponding simulated concentrations; $\gamma_{\mathrm{S_M}}$, $\gamma_{\mathrm{X_M}}$ and $\gamma_{\mathrm{P_M}}$, which are set as 29 g $\mathrm{L^{-1}}$, 9 g $\mathrm{L^{-1}}$ and 11 g $\mathrm{L^{-1}}$, respectively, at $\gamma_{\mathrm{S_0}}$ = 28 g $\mathrm{L^{-1}}$ (or 19 g $\mathrm{L^{-1}}$, 6 g $\mathrm{L^{-1}}$ and 7 g $\mathrm{L^{-1}}$, respectively, at $\gamma_{\mathrm{S_0}}$ = 17.5 g $\mathrm{L^{-1}}$ in validated experiment), are the approximately maximum concentrations of substrate, cell and enzyme, respectively, according to the experiment data; n = 11.

The simulated concentrations were obtained by solving nonlinear differential equations (eqs. (5)-(7)) using a fourth and fifth order Runge-Kutta method.

Kinetic parameter estimation by various optimizers

According to our previous work,[5] the varying scopes of kinetic parameters were chosen and listed in Table 1. A population of 24 particles was used

Table 1 – *The varying scopes of kinetic parameters of β-mannanase fermentation*

Parameters	μ_m	K_S	t_L	q_m	K_P	f_S	$Y_{X/S}$	$Y_{P/S}$	m
Unit	h^{-1}	g L^{-1}	h	h^{-1}	g L^{-1}	–	g g^{-1}	g g^{-1}	g g^{-1} h^{-1}
Scope	[0.01, 1]	[1, 5]	[1, 5]	[0.01, 1]	[4, 7]	[0.01, 1]	[0.01, 1]	[0.01, 1]	[0.00001, 1]

Table 2 – *The performance comparison of various optimizers*[*]

Optimizer	1	2	3	4	5	6	Time, *t*/min
Original PSO	0.01374	0.01485	0.02349	0.02561	0.02770	0.02863	5-7
Shi-type PSO	0.01007	0.01225	0.01235	0.01445	0.01484	0.01707	4-5
Clerc-type PSO	0.01986	0.01991	0.02303	0.03089	0.03462	0.03555	1-3
Trelea 1 PSO	0.00887	0.01316	0.01421	0.01483	0.01509	0.01592	1-3
Trelea 2 PSO	2.16763	2.48320	2.58365	2.91974	3.35858	4.38063	3-5
GA	0.02283	0.02285	0.02572	0.02634	0.02740	0.02927	1-3

[*] The computing time was obtained from the PC (CPU: Intel Pentium 4 3.0G; Memory: 2.0G).

for searching 9-dimension space to minimize the objective cost function using the PSO algorithms (the same conditions for GA), as shown in Fig. 2. The various PSO algorithms and GA were respectively tested for the performance of optimization, and the optimized results with iteration of 250 times (the best six values in 30 runs for every algorithm) are shown in Table 2. The trajectories of the best global position, whose change reflected the ability of global optimization, were respectively shown in Fig. 3.

When the iteration times are at the same level (250 times), the less the value of the cost function in reasonable computing time, the better the performance of the optimizer. In Table 1 and Fig. 3, it is obvious that each PSO (except Trelea 2) is more suitable for kinetic parameter estimation of *β*-mannanase fermentation than GA. The performance of PSO with Trelea 1 type was the best among all PSO algorithms, which agrees with the experimental results of Trelea.[23] If the computing time is insignificant, the Shi-type PSO or the original PSO, as the alternative algorithm, may be considered in optimizing kinetic parameters. Due to the important effect of the inertia weight *w*, furthermore, the Shi-type PSO is superior to the original one both in the optimal accuracy and in the computing time.

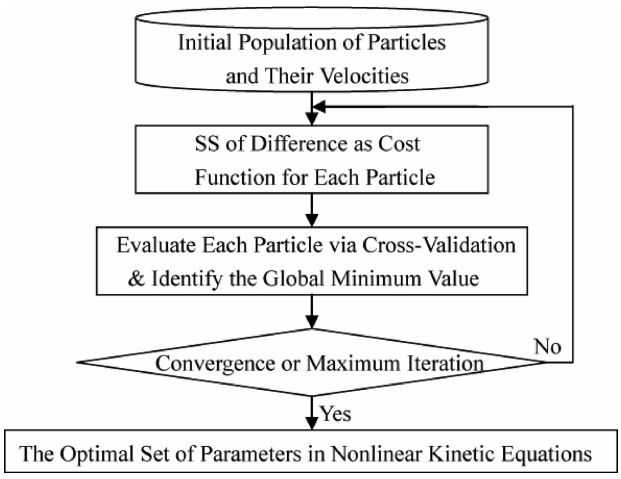


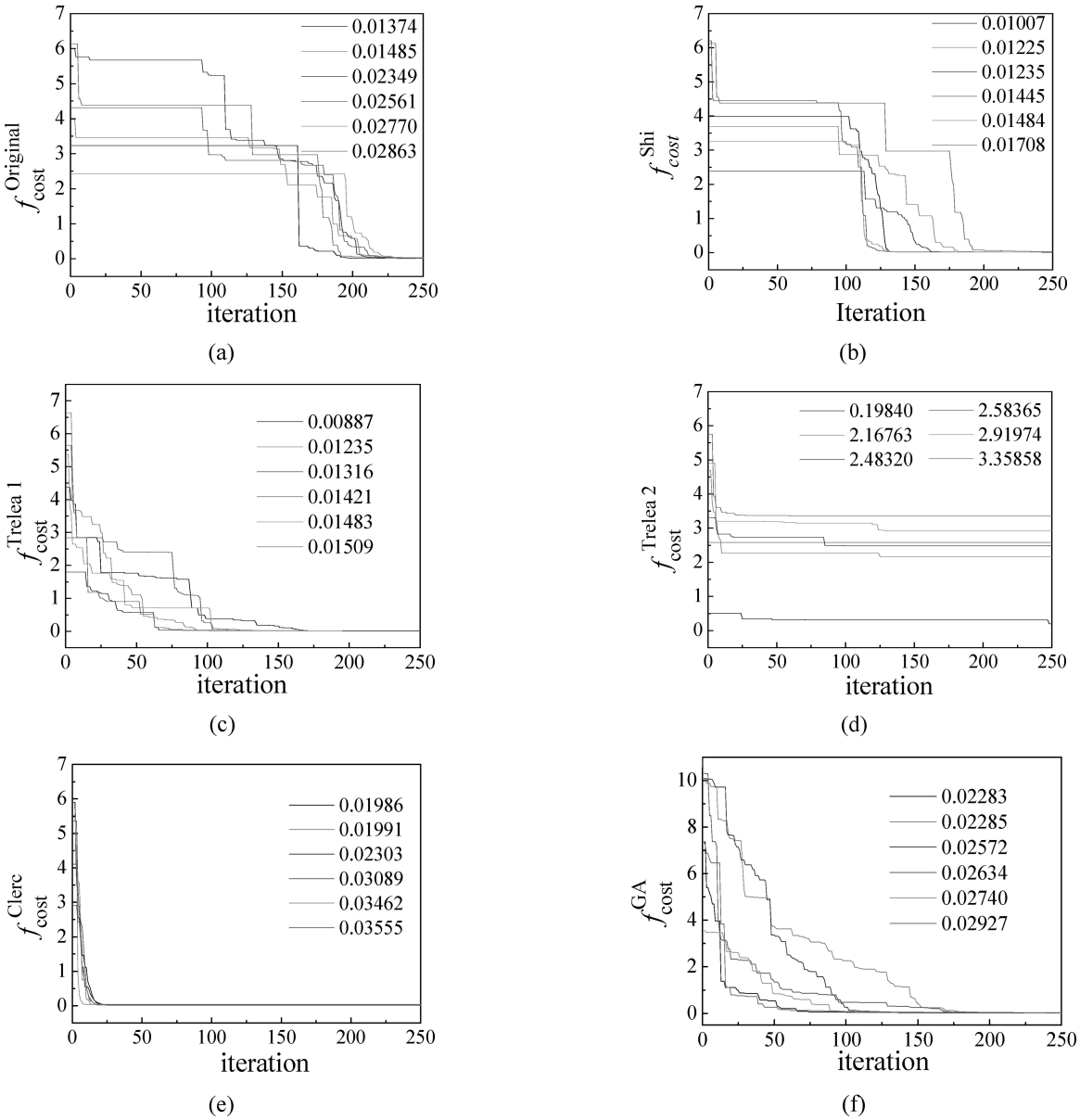
Fig. 2 – *PSO-based kinetic parameter estimation*

Multiobjective optimization and verification

As is well known to all, the kinetic parameters have their own physical-chemical meanings. The values of the optimal parameters estimated by the optimizer, however, were quite different for the same batch data (at γ_{S_0} = 28 g L^{-1}). That means these relatively optimal parameters need to be screened and verified further using the other batch fermentation data (at γ_{S_0} = 17.5 g L^{-1}).

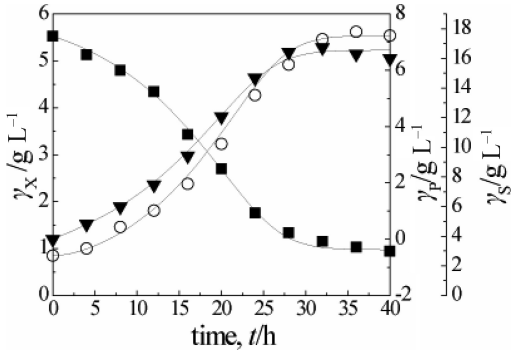
In order to find the more suitable kinetic parameters, which may support two fermentation processes with different amount of carbon source, multiobjective optimization with a normalized weight method was used. The total objective function was defined as follows:

$$F_{\text{total}} = (f^1_{\text{cost}} + f^2_{\text{cost}})/2 \qquad (16)$$



F i g . 3 – *Trajectories of the best global position for various optimizers*

The multiobjective problem was solved by the Trelea 1 PSO. The five best ones in 20 runs were summarized in Table 3. The optimal kinetic parameters were obtained as: μ_m = 0.1062 h^{-1}; K_S = 2.7203 g L^{-1}; t_L = 3.1313 h; q_m = 0.2184 h^{-1}; K_P = 7.0000 g L^{-1}; f_S = 0.1764; $Y_{X/S}$ = 1.0000 g g^{-1}; $Y_{P/S}$ = 0.6906 g g^{-1}; m = 0.00001 g $g^{-1}h^{-1}$. Comparisons of the optimal simulation values with the experimental results (at γ_{S_0} = 28 g L^{-1} and at γ_{S_0} = 17.5 g L^{-1}) are respectively shown in Fig. 1 and Fig. 4. Obviously, the simulation results with the optimal kinetic parameters were in good agreement with the experimental data because the sum of square (SS) of difference (f^1_{cost} = 0.0158 and f^2_{cost} = 0.0126) was very tiny.



F i g . 4 – *Kinetics of cell growth, enzyme synthesis and substrate utilization in a batch fermentation process (γ_{S_0} = 17.5 g L^{-1}) for β-mannanase production by Bacillus licheniformis. Symbols represent cell concentration γ_X (g L^{-1}) (○), enzyme concentration γ_P (g L^{-1}) (▼) and total sugar concentration γ_S (g L^{-1}) (■), which were observed in the fermentation experiment. The simulated results (–) were calculated from eqs. (5)-(7) using the known kinetic parameters in Table 2.*

Table 3 – *Results of multiobjective optimization using the Trelea 1 PSO*

Item		1	2	3	4	5
Parameter	μ_m	0.1062	0.1103	0.1098	0.1102	0.1102
	K_S	2.7203	2.8614	2.8583	2.8584	2.8607
	t_L	3.1313	3.6766	3.5996	3.6672	3.6703
	q_m	0.2184	0.2207	0.2201	0.2207	0.2207
	K_P	7.0000	7.0000	7.0000	7.0000	7.0000
	f_S	0.1764	0.1769	0.1763	0.1769	0.1769
	$Y_{X/S}$	1.0000	1.0000	1.0000	1.0000	1.0000
	$Y_{P/S}$	0.6906	0.6902	0.6903	0.6902	0.6902
	m	0.00001	0.00001	0.00009	0.00001	0.00001
Objective	f^1_{cost}	0.0158	0.0163	0.0162	0.0163	0.0163
	f^2_{cost}	0.0126	0.0118	0.0119	0.0118	0.0118

Conclusion

In this work, various PSO algorithms as well as GA were employed to optimize the kinetic parameters for β-mannanase fermentation model, and the performance analysis of these optimizers suggests the PSO can be efficiently used to estimate the kinetic parameters for the unstructured models in fermentation research. For a specific optimization problem, the selection of the parameter set in PSO algorithm is quite important. Compared with the other algorithms, the PSO with Trelea 1 frequently gives smarter performance, stronger robustness and better veracity. The desirable and physical-chemical-meanings of kinetic parameters (μ_m = 0.1062 h^{-1}; K_S = 2.7203 g L^{-1}; t_L = 3.1313 h; q_m = 0.2184 h^{-1}; K_P = 7.0000 g L^{-1}; f_S = 0.1764; $Y_{X/S}$ = 1.0000 g g^{-1}; $Y_{P/S}$ = 0.6906 g g^{-1}; m = 0.00001 g $g^{-1}h^{-1}$) were found by multiobjective optimization of the Trelea 1 PSO using two batches fermentation data. The simulation results with the estimated kinetic parameters were in good agreement with the experimental data. More applications of PSO in facilitating chemical/biochemical processes will be witnessed in the coming years.

ACKNOWLEDGEMENTS

The authors wish to thank the Tianjin Science & Technology Commission of China for their financial support through Project No. 05YFGZGX04600 and this research is supported by National Key Technology R&D program (2007BAD42B02) and International Science and Technology cooperation program (2006DA62400).

List of symbols

a – constant in eq. (13)
b – constant in eq. (13)
C – concentration, mol L^{-1}
c – constant in eq. (14)
c_1 – positive constant in eq. (8)
c_2 – positive constant in eq. (8)
d – constant in eq. (14)
f^1_{cost} – objective cost function at γ_{S_0} = 28 g L^{-1}
f^2_{cost} – objective cost function at γ_{S_0} = 17.5 g L^{-1}
f_s – fraction
F_{total} – total objective cost function in multiobjective optimization
φ_1 – positive constant in eq. (10)
φ_2 – positive constant in eq. (10)
k – iteration time of PSO
κ – constant in eq. (9)
K_P – constant in eq. (6), g L^{-1}
K_S – Monod constant for cell growth, g L^{-1}
m – maintenance coefficient, g g^{-1} h^{-1}
n – account number of collecting data in a batch fermentation
p_{ik} – weight average of particle's own previous best position in PSO
p_{gk} – weight average of globally best position in PSO
γ_P – β-mannanase concentration, g L^{-1}
q_m – coefficient in eq. (6), h^{-1}
γ_S – substrate concentration, g L^{-1}
γ_{S_0} – initial substrate concentration, g L^{-1}
γ_{S_u} – unavailable substrate concentration, g L^{-1}
γ_{S_a} – available substrate concentration, g L^{-1}
t – fermentation time, h

t_L – lag time, h
μ – specific growth rate, h^{-1}
μ_m – maximum specific growth rate, h^{-1}
v – particle velocity
w – mass fraction, %
w_{ab} – inertia weight in PSO
x – particle position
χ – constriction coefficient in the Clerc-type PSO
γ_X – cell mass concentration, g L^{-1}
$Y_{P/S}$ – β-mannanase yield on carbon substrate, g g^{-1}
$Y_{X/S}$ – biomass yield on carbon substrate, g g^{-1}
θ – temperature, °C

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