Dynamic Multi-objective Cooperative Optimization of Biochemical Process Based on Kinetic Model and MOPSO

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Abstract
Dynamic optimization or optimal control problems are omnipresent in the biochemical industry, which often involve multiple and conflicting objectives. This paper presents a novel dynamic multi-objective cooperative optimization algorithm based on particle swarm optimization and kinetic model for biochemical process. The multi-objective optimization includes two objective functions: as maximizing production concentration and minimizing the production time by optimizing the initial variables. In order to improve the diversity of the Pareto solutions, a dynamic aggregate method is adopted to select the best particle and to guide its fighting. The global exploratory capability is enhanced by using incorporate adaptive inertia weight. The efficiency of the proposed method is demonstrated by some comparison rice fermentation process experiments, the results show the superiority of the proposed method to the conventional one.
Key words: MULTI-OBJECTIVE OPTIMIZATION, PSO, KINETIC MODEL, RICE VINE FERMENTATION

1. Introduction

Biochemical processes strictly are dynamic processes, where the state variables vary with the time and the position. Because of this, the traditional control strategies based on steady-state model are unable to solve such dynamic problems. In additional, practical rice fermentation processes usually require optimization of multiple targets, such as shortest time-consuming, maximum production, etc. These objectives often influence or conflict with each other, resulting in complex dynamic multi-objective optimization problems [1]. Therefore, we conducted this study to present a new method to solve the problem.

Recently, there have been a few studies that apply intelligence optimization algorithms to solve the DMOPs. Particle Swarm Optimization (PSO) is a swarm intelligence method that roughly models the social behavior of swarms [2, 3]. PSO shares many features with evolutionary algorithms that rendered its adaptation to the multi-objective context straightforward. Jia et al. applied an improved MOPSO algorithm that employed a novel diversity preservation strategy to solve two classical batch process problems [4]. Reference [5] proposed a new application of multi objective particle swarm optimization (MOPSO) with the aim of determining optimal location and size of distributed generations (DGs) and shunt capacitor banks (SCBs) simultaneously with considering load uncertainty in distribution systems. Reference [6] applied an optimized method for micro-grid system using MPSO. However, the research on its application in rice vine fermentation process, especially dynamic multi-objective cooperative optimization problems, is relatively few. There are several factors that limited its extension to in rice vine fermentation process optimization. One important factor is its strong sensitivity to parameters, resulting in repeatedly parameter adjustments. In addition, premature convergence and slow convergence rate in the later stage are two difficult problems. Therefore, how to efficiently balance the converging speed and the diversity of the population becomes quite important.

To circumvent the aforementioned problems, this paper presents a novel dynamic multi-objective cooperative optimization algorithm based on particle swarm optimization and kinetic model for rice fermentation process. In order to improve the diversity of the Pareto solutions, a dynamic aggregate method is adopted to select the best particle and to guide its fighting. The globe exploratory capability is enhanced by using incorporate adaptive inertia weight. The efficiency of the proposed method is demonstrated by some experiments.

The rest of paper is organized as follows. In Section 2, the theories of multi-objective particle swarm optimization (MOPSO) and dynamic multi-objective cooperative particle swarm optimization (DMOC-PSO) are introduced. Some detailed analysis about Kinetic model of rice vine fermentation process and the multi-objective problem are introduced in Section 3. The determination of optimizing initial variables and the steps of optimizing initial conditions by DMOC-PSO are designed in Section 4. Some experiments results are discussed in Section 5, and the conclusion is presented in Section 6.

2. Dynamic multi-objective cooperative particle swarm optimization (DMOC-PSO)

Particle swarm optimization (PSO) is an evolutionary computation optimization technique (a search method based on a natural system) developed by Kennedy and Eberhart[7-9]. The PSO algorithm is initialized by creating a swarm, i.e., population of particles (N), with random positions. Every particle is shown as a vector, $(\vec{X}_i, \vec{V}_i, \vec{P}_{best_i})$, in a D-dimensional search space where $\vec{X}_i$ and $\vec{V}_i$ are the position and velocity respectively. $\vec{P}_{best_i}$ is the personal best position found by the ith particle：

$$\vec{X}_i = (x_i^1, x_i^2, ..., x_i^D) \qquad for \quad i = 1, 2, ..., N \tag{1}$$

$$\vec{V}_i = (v_i^1, v_i^2, ..., v_i^D) \qquad for \quad i = 1, 2, ..., N \tag{2}$$

$$\vec{P}_{best_i} = (p_{besti}{}^1, p_{besti}{}^2, ..., p_{besti}{}^D) \qquad for \quad i = 1, 2, ..., N \tag{3}$$

The best position obtained by the swarm, $\vec{P}_g$ is obtained to update the next particle velocity. $\vec{P}_g = (p_g^1, p_g^2, ..., p_g^D)$. Based on $\vec{P}_{best_i}$ and $\vec{P}_g$, the next velocity and position of the ith particle are computed using (12) and (13) respectively as follows:

$$v_i^d(t+1) = w \cdot v_i^d(t) + c_1 \cdot rand_1 \cdot (p_{besti}{}^d(t) - x_i^d(t)) + c_2 \cdot rand_2 \cdot (p\,_g^d(t) - x_i^d(t)) \tag{4}$$

$$x_i^d(t+1) = x_i^d(t) + v_i^d(t+1) \tag{5}$$

where $v_i^d(t+1)$ and $v_i^d(t)$ are the next and current velocity of the i th particles respectively, $x_i^d(t+1)$ and $x_i^d(t)$ are the next and current position of the ith particle, $rand_1$ and $rand_2$ are two uniform random functions in the range [0,1]. w is the inertia factor influencing the local and global abilities of the algorithm.

As shown in Eqs. (4) and (5), when solving a single-objective optimization problem, the leader, p_g, that each particle uses to update its position, is easily identified because each particle has only one fitness value. However, multi-objective optimization problems consist of several objectives that are necessary to be handled simultaneously. Such problems arise in many applications, where two or more, sometimes competing and/or incommensurable, objective functions have to be minimized concurrently. In contrast to the single-objective optimization case, multi-objective problems are characterized by trade-offs and, thus, there is a multitude of Pareto optimal solutions, which correspond to different settings of the investigated multi-objective problem. Under these circumstances, the choice of the leader is a key point and a quality measure is very important[15]. In order to indicate how good a leader is, a dynamic aggregation method was used to guide the flight of particles in previous studies[10,12]. Here, with consideration of diversity, we select a different leader for each particle and the quality measure uses the dynamic weighted aggregating function expressed as

$$fitness = \frac{1}{\sum_{i=1}^{M} w_i f_i} \tag{6}$$

where M is the number of objectives, and f_i is the ith objective function. $w_i = \lambda_i / \sum_{i=1}^{M} \lambda_i$, $\lambda_i = Rand(0,1)$.

In this way, at each iteration and for each particle in the swarm, the fitness of each individual in the current Pareto solution set is dynamically computed and the individual with the largest fitness value is selected as the particle's leader. The technique of dynamic selection of leaders means that all Pareto solutions have the same probability of being selected as leaders; this avoids the drawback of diversity loss. The diagram of MOPSO as following：

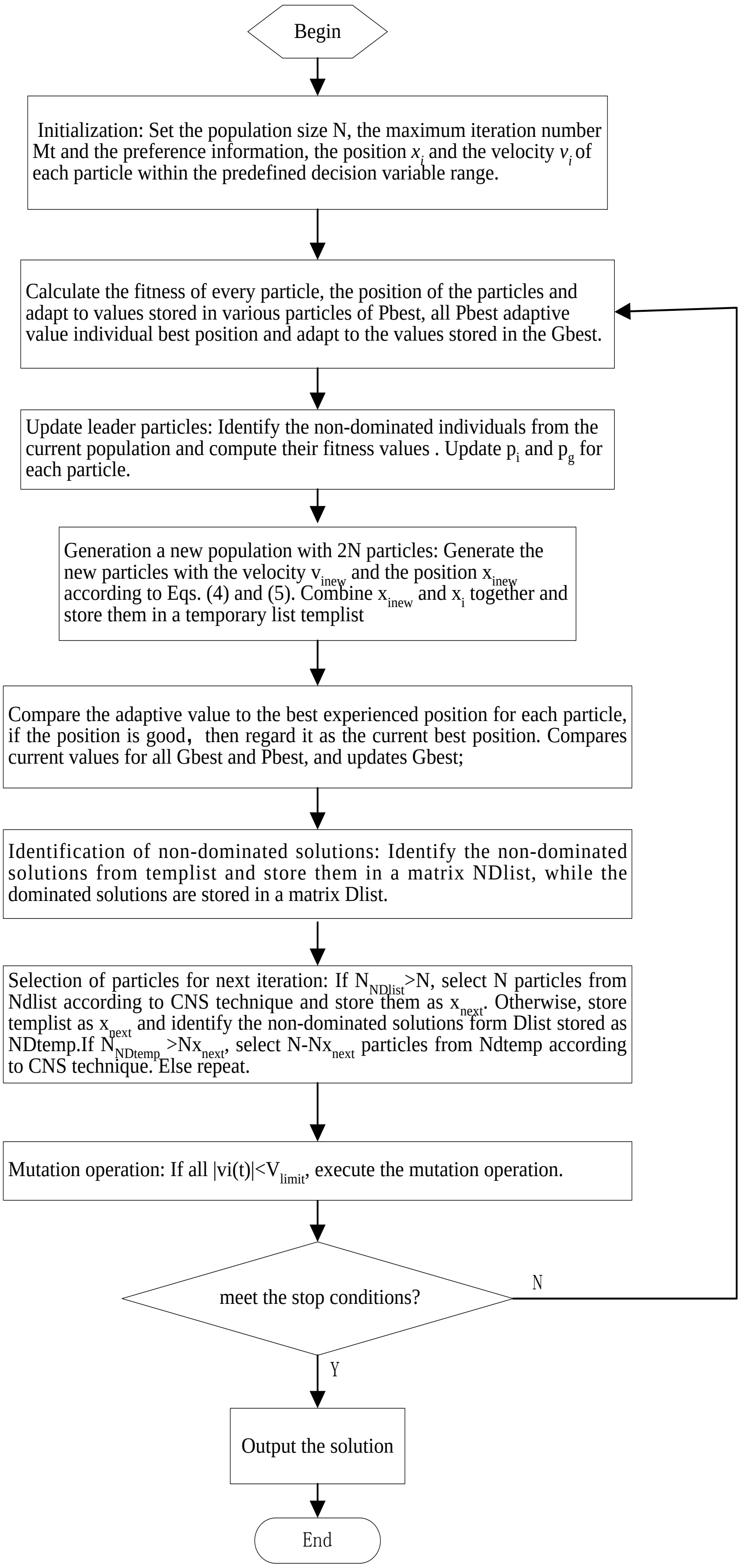

Figure 1. The diagram of DMOC-PSO

3. The multi-objective problem of biochemical process

In generally, the dynamic processes are often described by a group of differential equations as following :

$$\min_{u(t),p} = J(J_1, J_2, \cdots, J_k, \cdots J_M)^T$$

$$J_k = \varphi_k(t_f, x(t_f)) + \int_0^{t_f} \varphi_k(t, x(t), u(t))dt$$

$$s.t \quad \begin{cases} \dfrac{dx_i}{dt} = f_i(t, x(t), u(t)) & x_i(0) = x_{i,0} \quad i = 1, \cdots, n \\ u_{j,\min}(t) \le u_j(t) \le u_{j,\max}(t) \end{cases}$$

where t_f is the final time, x(t) is the vector of state variables, with the initial conditions $x(t_0)=x_0$; u(t) denotes the control variables, φ_k is performance index.

Chinese rice wine, a traditional Chinese beverage, has more than 5000 years of history, which is a typical biochemical process. The manufacture of rice wine goes through a series of processes including steeping, steaming, stirring, fermentation, squeezing, storing and blending[13,14]. Of these processes fermentation is a dynamic processes, where the state variables vary with the time and the position[15,16]. In general, the primary phase of rice wine fermentation is a typical simultaneous saccharification and fermentation (SSF) process and is also referred to as a semi-solid state and semi-liquid state fermentation process. The kinetic model of rice vine fermentation process as follows[17]:

$$\frac{dS}{dt} = -k_1 SE \tag{7}$$

$$\frac{dR}{dt} = 1.037k_2C_1 - k_5 \frac{R}{K_{s1}+R} \frac{O}{K_{s2}+O} C \tag{8}$$

$$\frac{dM}{dt} = 1.056k_3C_1 - k_6 \frac{M}{K_{s3}+M} \frac{O}{K_{s2}+O} C - k_7 \frac{M}{K_{s4}+M} C \tag{9}$$

$$\frac{dG}{dt} = 1.111k_4C_1 - k_8 \frac{G}{K_{s5}+G} \frac{O}{K_{s2}+O} C - k_9 \frac{G}{K_{s6}+G} C \tag{10}$$

$$\frac{dC}{dt} = 0.084k_5 \frac{R}{K_{s1}+R} \frac{O}{K_{s2}+O} C - 0.088k_6 \frac{M}{K_{s3}+M} \frac{G}{K_{s2}+G} C + 0.09k_8 \frac{G}{K_{s5}+G} \frac{O}{K_{s2}+O} C \tag{11}$$

$$\frac{dA}{dt} = 0.54 \frac{M}{K_{s4}+M} C - 0.51k_9 \frac{G}{K_{s6}+G} C \tag{12}$$

$$\frac{dO}{dt} = -k_5 \frac{R}{K_{s1}+R} \frac{O}{K_{s2}+O} C - k_6 \frac{M}{K_{s3}+M} \frac{G}{K_{s2}+G} C - k_8 \frac{G}{K_{s5}+G} \frac{O}{K_{s2}+O} C + O_{in} \tag{13}$$

$$\frac{dE}{dt} = -k_1 SE + (k_2 + k_3 + k_4)C_1 \tag{14}$$

$$\frac{dC_1}{dt} = k_1 SE - (k_2 + k_3 + k_4)C_1 \tag{15}$$

where the S is the starch concentration(g/L), R is the maltotriose concentration(g/L), M is the maltose concentration(g/L), G is the glucose concentration(g/L), C is the yeast concentration(g/L), A is the ethanol concentration(g/L), O is the oxygen concentration(g/L), E is the Qu(amylase) concentration(g/L), C_1 is the starch–Qu complex concentration(g/L), K_{s1}-K_{s6} are half-saturation constants(g/L), K_{s1}=5.97, K_{s2}=6.9, K_{s3}=30.9, K_{s4}=30.5, K_{s5}=6.315, K_{s6}=6.315 and k_1–k_9 are the chemical reaction rates($g/L/h$), k_1=0.007, k_2=1.659, k_3=20.818, k_4=0.685, k_5=0.643, k_6=2.929, k_7=0.886, k_8=0.412, k_9=0.062 .

For rice vine fermentation process, the two objectives are reset as maximizing alcohol concentration and minimizing the production time in this study. The objective model can be described as below:

$$\begin{aligned} &\max \quad J_1(C_0, E_0) = \int_0^{t_f} \frac{dA}{dt} dt \\ &\min \quad J_2(C_0, E_0) = t_f \\ &s.t \quad \begin{cases} C_{0\min} \le C_0 \le C_{0\max} \\ E_{0\min} \le E_0 \le E_{0\max} \end{cases} \end{aligned} \tag{16}$$

4. Dynamic Multi-objective Cooperative Optimization of Biochemical Process

4.1 Determination of optimizing initial variables

In section 3, the rice vine fermentation kinetic model (Eqs.(7)-(15))is a system of differential equations which contains 9 equations and has 9 initial state variables[S_0 R_0 M_0 G_0 C_0 A_0 O_0 E_0 C_{10}], according to the actual production process, the initial concentration of starch S_0 is easy to control, do not need optimization, set S_0=100(g/L). In addition, malt sugar, maltose, glucose, concentration of ethanol, starch and the initial concentration of the curved compounds are obvious to 0 in the initial state because of the reaction is not began, the initial concentration of dissolved oxygen is generally set to a fixed value 10(g/L), thus two initial state variables are determined for optimizing: initial concentration of yeast C_0, initial concentration of E_0. According to the reference[10], these initial conditions of state variable's scopes is:

$0.5 \le C_0 \le 10(g/L)$

$0.5 \le E_0 \le 20(g/L)$

4.2 The step of optimizing

The step of optimizing the initial conditions of rice fermentation based on DMOC-PSO and kinetic model as follows:

Step 1. Initialization: Kinetic model of rice vine fermentation process X_0=[100 0 0 0 C_0 0 10 E_0 0]. Set the population size 50, the search space dimension D is 2 (represent C_0, E_0 respectively), the maximum iteration number M=100. $c_1 \in [0.1, 2]$, $c_2 \in [0.1, 2]$, initialize the position x_i and the velocity v_i of each particle within the predefined decision variable range.

Step 2. Setting the three main initial variable ranges of wine fermentation process, $C_0 \in [0.5, 10]$, $E_0 \in [0.5, 20]$, determining a set of initial values by the rand function randomly.

Step 3. The current ethanol concentration is obtained by solving the rice fermentation kinetic equations (7-15) with the Newton Gradient Method, and calculate the fitness of each particle by Eqs.(6) , i.e. $fitness = 1/(w_1 f_1 + w_2 f_2)$, and the position and the current adaptation values of each particles are stored in each of the particles in Pbest, the individual position and adapt the value of the adaptation value of all Pbest best are stored in the G_{best}.

Step 4. The velocity and displacement of the particles are updated by using the formula (4) and (5).

Step 5. Compare the adaptive value to the best experienced position for each particle, if the position is good, then regard it as the current best position. Compares current values for all G_{best} and P_{best}, and updates $G_{best.}$

Step 6. If meet the stop conditions, then stop searching, and output the results, otherwise return step 3, continue to search.

5. Result analysis

5.1 Associative optimizing two initial variables and analyzing results

The initial yeast concentration C_0 and the initial Qu concentration E_0 are selected as the two main associative optimizing variables and are optimized by DMOC-PSO. Particle size D=2, particle scope=[05 10; 0.5 20], swarm size N=50, Max loop count M=100, the other related parameters are set in subsection 4.2. The optimized results are shown in figure 2, From the figure, it can be seen clearly that these versus of starch concentration, Maltotriose concentration, Maltose concentration, Glucose concentration, Yeast concentration, Qu concentration and Ethanol concentration changing follow to varying of the time in different initial conditions respectively. The final optimized result is: the optimal initial yeast concentration is 5.2503 (*g/L*), and the optimal initial Qu concentration is 9.7072(*g/L*), the maximizing alcohol concentration is 38.6809 (*g/L*), the optimal minimizing the production time is 59.2735h.

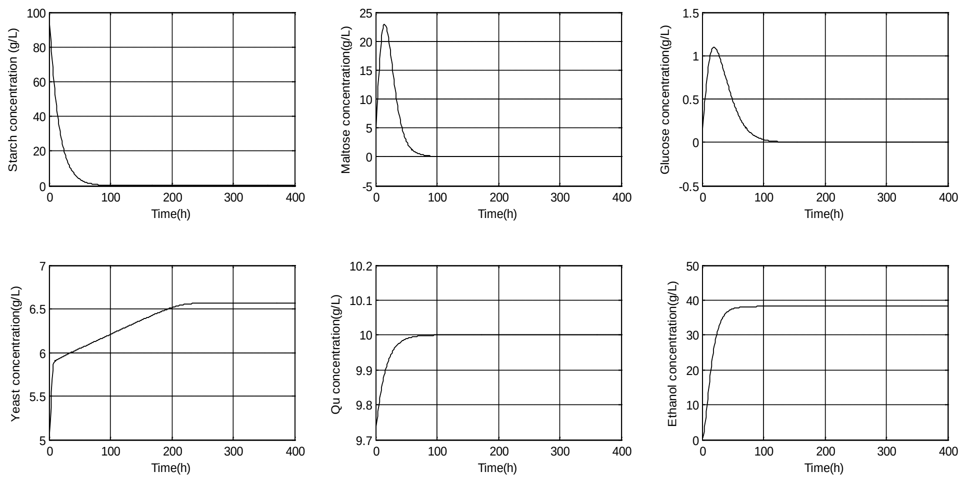

Figure 2. Associative optimizing process of two initial variables

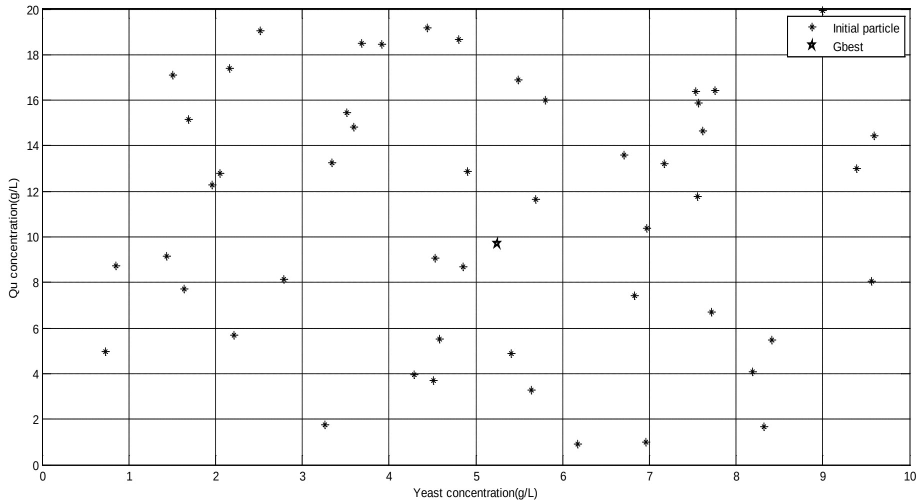

Figure 3. Associative optimizing process of two initial variables

5.2 The comparison of associative optimizing methods for three initial variables

In order to illustrate the effectiveness of this method, the classical Newton method[18], MPSO algorithm[5,6]are adopted separately to optimize the process in this study. In MPSO algorithm, set $c_1 = c_2 = 2$, the other parameters are set as in DMOC-PSO. The comparison results are shown in Figure 4 and Table 1.

Figure 4 illustrates the comparison results of associative optimizing methods for two initial variables, only DMOC-PSO can obtain the global optimal among the other algorithms for this process. Table 1 shows that the other methods are into the local optimum, and the optimal solution obtained by DMOC-PSO optimization method is largest than other methods. Thus the effectiveness of this design is demonstrated from the simulation, and these results can be provided a reference in an actual vine production process.

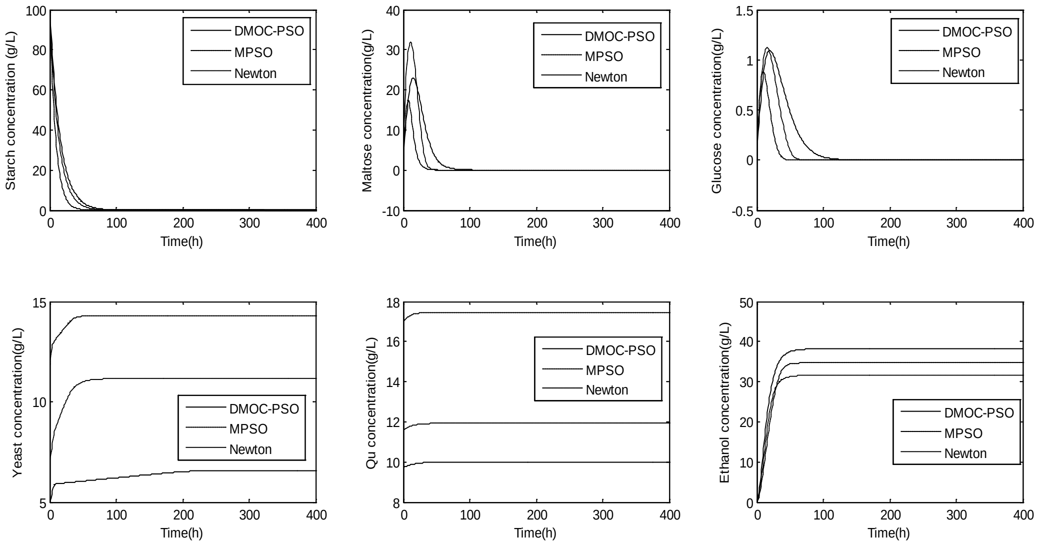

Figure 4. The comparison of optimizing results in three methods

Table 1. Optimized results of the three methods

Method / Item	Newton	MPSO	DMOC-PSO
Optimized Initial Yeast concentration (g/L)	6.4415	12.8385	5.2503

Optimized Initial Qu concentration (g/L)	11.9942	17.4953	9.7072
Optimized Ethanol concentration(g/L)	32.1994	34.8137	38.6809
Optimized Time(h)	50.1305	59.2681	59.2735

6 . Conclusions

Although many other factors, such as types of rice, rice feed-in quantity, ventilated air flow rate, etc., also affect the quality of roasted rice, the initial Yeast concentration and Qu concentration were considered to be the two major operating variables dominating the performance of the rice vine fermentation process. In this paper, an improved dynamic multi-objective cooperative optimization (DMOC-PSO) has been proposed and applied for the rice vine fermentation process, and the two objectives are reset as maximizing alcohol concentration and minimizing the production time by looking for a suitable two initial variables. In order to improve the diversity of the Pareto solutions, a dynamic aggregate method is adopted to select the best particle and to guide its fighting. The global exploratory capability is enhanced by using incorporate adaptive inertia weight. Some comparison experiments are demonstrated, and the results show that the efficiency of the proposed method is superior than other methods. This method not only can be used in a rice vine fermentation process, but also can be used in the other biochemical process.

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Nomenclature

S starch concentration (g/L)
R maltotriose concentration (g/L)
M maltose concentration (g/L)
G glucose concentration (g/L)
C yeast concentration (g/L)
A ethanol concentration(g/L),
O oxygen concentration(g/L)
E Qu(amylase) concentration(g/L)
C_1 starch–α-amylase complex concentration (g/L)
k_1–k_9 chemical reaction rates ($g/L/h$)
K_{s1}-K_{s6} half-saturation constants(g/L/h)

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