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Model of Ethanol Coupling to C4 Olefins Based on PSO-GA Algorithm

Enjie Fang[1], Jing Zhang[2]

[1]School of Mechanical Engineering and Automation, Fuzhou University, Fuzhou, Fujian, 350116, China

[2]College of Computer and Data Science, Fuzhou University, Fuzhou, Fujian, 350116, China

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Abstract: In order to explore the combination scheme and temperature setting of catalyst for ethanol coupling preparation of C4 olefins, the C4 olefin yield is taken as the objective function and the corresponding constraints are established. Then, the improved particle swarm optimization algorithm based on genetic algorithm is used to find the global optimal solution, and then the C4 olefin yield optimization model is established. The final result is obtained by MATLAB programming: under the optimal scheme, the C4 olefin yield can reach 47.98%.

1. Introduction

Olefins are widely used in chemical products and pharmaceutical production industries. Ethanol is the raw material for manufacturing C4 olefins in industry. In the production process, the catalyst combination (the combination of CO/SiO2 and HAP loading ratio, CO loading and ethanol concentration) and temperature will affect the C4 olefin yield and C4 olefin selectivity. Therefore, it is of far-reaching significance and value to find the optimal scheme and explore the conditions and process of ethanol catalytic coupling to produce C4 olefins. In this paper, the improved particle swarm optimization algorithm based on genetic algorithm is used to find the global optimal solution, and then the optimization model of C4 olefin yield is established to maximize the C4 olefin yield under the same experimental conditions.

2. Model Establishment and Solution

In this paper, the catalyst combination scheme and temperature should be designed to make the C4 olefin yield as high as possible, and the optimal scheme should be designed when the temperature is less than 350℃. According to the formula, C4 olefin yield, ethanol conversion and C4 olefin selectivity can be realized on the basis of linear fitting function. The product of ethanol conversion and C4 olefin selectivity linear fitting function is taken as the objective function, and the corresponding constraints are established. The improved particle swarm optimization algorithm based on genetic algorithm is used to find the global optimal solution.

2.1 Establishment of objective function and constraints

If the linear fitting function of ethanol conversion is Y_1, the linear fitting function of C4 olefin selectivity is Y_2, and the C4 olefin yield is $R = Y_1 Y_2$, the objective function is $\max\ R$.

Because the ethanol conversion and C4 olefin selectivity are between 0 and 1, there are constraints:

$$0 \leqslant Y_1, Y_2 \leqslant 1$$

$$0 \leqslant R \leqslant 1$$

If the temperature, Co / SiO2 weight, CO load, HAP weight and addition speed are t_1, t_2, t_3, t_4, t_5 respectively, there are constraints:

$$t_1, t_2, t_3, t_4, t_5 \geqslant 0$$

To sum up, the optimization model is established:

$$\max\ R$$

$$s.t.\begin{cases} 0 \leqslant Y_1, Y_2 \leqslant 1 \\ 0 \leqslant R \leqslant 1 \\ t_1, t_2, t_3, t_4, t_5 \geqslant 0 \end{cases} \quad (1.)$$

2.2 Improved particle swarm optimization algorithm based on genetic algorithm

In this paper, an improved particle swarm optimization algorithm based on genetic algorithm is adopted. The algorithm combines the advantages of PSO and GA, and avoids some of their shortcomings. It is not easy to fall into the local best when solving the optimal solution, and has better performance of solving the global optimal solution. The algorithm flow chart is as follows:

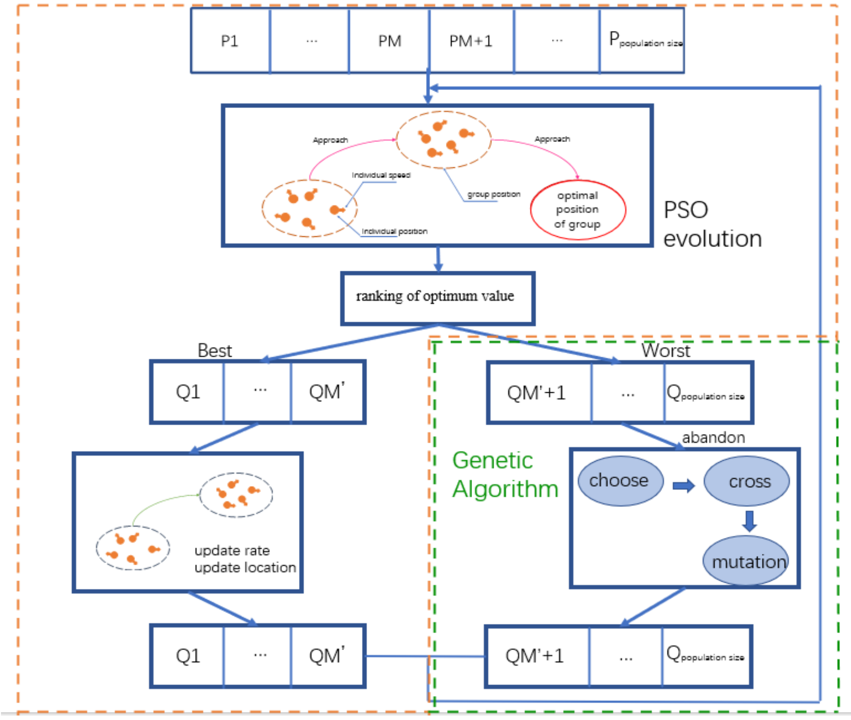

Figure 1: Flow chart of pso-ga algorithm

The process can be represented by pseudo code as follows:

```
Improved particle swarm optimization algorithm based on genetic algorithm
    Input: Initialize feasible region D, Optimization objective function {f_1(x); f_2(x); ...; f_s(x)}
    Output: x_1, x_2, x_3, x_4, x_5, {f(x_1, x_2, x_3, x_4, x_5)}
      function  OPS(D, [f(x_1, x_2, x_3, x_4, x_5)])
      For each particle i
      Initialize velocity V_i and position X_i
      end for
      gBest = min(pBest)
      While iter ≤ M
          For i=1 to size
          update the velocity and position of particle i
          Evaluate particle i
          if fit(X_i) > fit(pBest)
              pBest = X_i
          if fit(pBest) < fit(gBest)
              gBest = pBest_i
              end for
          end while
    end procedure
```

2.3 Solution of optimization model

In this paper, PSO-GA algorithm is implemented by MATLAB to search the optimal solution of the optimization model. The results are as follows:

Table 1: Catalyst and temperature scheme with the highest C4 olefin yield

temperature	Co / SiO2 weight	Co load	Weight of HAP	Adding speed	C4 olefin yield
399.28(°)	277.89(mg)	43%	271.64(mg)	0.2529(ml/min)	47.98%

3. Conclusion

This paper designs the catalyst combination scheme and temperature to make the C4 olefin yield as high as possible, takes the C4 olefin yield as the objective function, and establishes the corresponding constraints. Then, the improved particle swarm optimization algorithm based on genetic algorithm is used to find the global optimal solution, and then the C4 olefin yield optimization model is established. The final result is obtained by MATLAB programming: under the optimal scheme, the C4 olefin yield can reach 47.98%.

The particle swarm optimization (pso-ga) algorithm is improved based on genetic algorithm, which makes the particle swarm optimization algorithm have excellent global optimization ability, can well avoid the defect that the particle swarm optimization algorithm is easy to fall into the local optimal solution, and make the model more objective and comprehensive; However, both particle swarm optimization algorithm and genetic algorithm belong to heuristic models, which will cause the fluctuation and non uniqueness of the solution.

In actual production, the C4 olefin yield of C4 olefins prepared by ethanol coupling is not only affected by catalyst and temperature, but also by environmental factors. Therefore, more influencing factors can be added to this model to make the model have stronger practical applicability and bring broader social benefits.

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