Original Research Article

Research on Catalyst Selection Based on Simulated Annealing Algorithm

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Abstract: In this paper,the effect of catalyst selection on C4 olefin yield was studied based on simulated annealing algorithm. Firstly,using the processed data,through the influence model of different components of the catalyst and the combination method of multiple linear regression,the comprehensive influence model of the catalyst on the yield of C4 olefins is obtained.Then,through the simulated annealing algorithm,it is found that when t=405℃,the C4 olefin yield reaches the highest,52.92%.Finally,when the reaction temperature needs to be less than 350℃,it is found that when t=350℃,the C4 olefin yield reaches the highest,20.79%.
Keywords: Simulated annealing model; Optimal combination; Catalyst performance

1. Introduction

C4 olefins are widely used in the production of chemical products and medicine.Their traditional production methods use fossil energy as raw materials.However,with the shortage of fossil energy output and the aggravation of its impact on the environment,the energy supply gradually tends to be diversified,and the development of new clean energy becomes more and more urgent.Ethanol is the raw material for the production of C4 olefins.It not only has a wide range of sources and is green and clean,but also the use of ethanol to prepare C4 olefins can bring huge economic benefits[1].However,in the preparation process,the catalyst combination and temperature will have an impact on the selectivity and yield of C4 olefins.Therefore,it is of great significance and value to explore the process conditions for the preparation of C4 olefins by ethanol catalytic coupling through the combination design of catalysts.

2. Comprehensive impact model

2.1 Model establishment

We know the comprehensive influence function $f(\delta_1,T)$ of CO loading and temperature,the comprehensive influence function $g(\delta_2,T)$ of ethanol concentration and temperature,the amount of Co/SiO2,the loading ratio of Co/SiO2 and AHP and the comprehensive influence function $\varphi(\delta_3,\delta_4,T)$ .In order to obtain the comprehensive influence model of the three,we carry out linear multivariate combination treatment on the three[2].

$$H(\delta_1,\delta_2,\delta_3,\delta_4,T)=\omega_1 f(\delta_1,T)+\omega_2 g(\delta_2,T)+\omega_3\varphi(\delta_3,\delta_4,T) \quad (1)$$

Since there is an influence of temperature in the three formulas we obtained,that is,the change of temperature may affect the simultaneous change of the three formulas.At the same time,considering the possible temperature error in the actual observation and measurement,we introduce the temperature correction coefficient γ ,that is:

$$H(\delta_1,\delta_2,\delta_3,\delta_4,\gamma T)=\omega_1 f(\delta_1,\gamma T)+\omega_2 g(\delta_2,\gamma T)+\omega_3\varphi(\delta_3,\delta_4,\gamma T) \quad (2)$$

The goal of this problem is to solve the combination of temperature and catalyst when the C4 olefin yield is maximum under two given conditions.Therefore,we need to express the objective function,that is:

$$\min H(\delta_1,\delta_2,\delta_3,\delta_4,\gamma T)_{Ethyleneconversionrate}\cdot H(\delta_1,\delta_2,\delta_3,\delta_4,\gamma T)_{C4olefinselectivity} \quad (3)$$

Because the model is complex,we need to set the definition domain of the parameters in the model to improve the calculation speed of the model.The specific parameter range can be determined according to the analysis of the impact of different variables.

(1)Setting of temperature range

Firstly,for the temperature T,we can judge that when the temperature is low,the ethanol conversion rate and C4 olefin selectivity are also relatively low,and the C4 olefin yield should also be relatively low at this time.When the temperature increases,the overall ethanol conversion rate and C4 olefin yield show an increasing trend,and the C4 olefin yield should also show an increasing trend. According to this trend and combined with our fitted function,it can be obtained that when T>400℃,the yield of C4 olefins may continue to increase.Therefore,in order to better find the best temperature and reduce our calculation time,we set the temperature range to

$$250 < T \leq 500 \quad (4)$$

(2)Setting of Co load range

We can find that the C4 olefin yield has reached the maximum within the known variation range of Co load,and further from our

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analysis results,the C4 olefin yield continues to decline when the co load continues to increase.Comprehensively,we set the range of Co load as

$$0.5 \le \delta_1 \le 5 \tag{5}$$

(3)Determination of ethanol concentration

Through our analysis of the impact of different ethanol concentrations,we can find that when the ethanol concentration is greater than 1.68ml/min,the conversion rate of ethanol and the yield of C4 olefins continue to decline,but the selectivity of C4 olefins shows an upward trend.Combined with the relationship between Fig.7 and our fitting,we can find that when the ethanol concentration is greater than 2.1ml/min,C4 olefin selectivity may also increase.Since C4 olefin yield is the product of ethanol conversion rate and C4 olefin selectivity,with the increase of C4 olefin selectivity,C4 olefin yield may also show an upward trend when ethanol reaches a certain concentration.Therefore,with the continuous increase of ethanol concentration,C4 olefin yield may have a maximum value.In order to ensure the accuracy of the model,we set the range of ethanol concentration δ_2 as

$$0.3 \le \delta_2 \le 4 \tag{6}$$

(4)Determination of Co/SiO2 content and range of Co/SiO2 and charge ratio

According to our analysis results on the influence of Co/SiO2 content δ_3 and Co/SiO2 and HAP loading ratio δ_4 ,when the Co/SiO2 content is greater than 50mg or the Co/SiO2 and HAP loading ratio is greater than 1,the C4 olefin yield shows a continuous downward trend.At the same time,under this condition,The conversion rate of ethanol and C4 olefin selectivity also show a downward trend.Through the image,we can also find that the three should still show a downward trend with the increase of influence conditions.Therefore,considering comprehensively,we set the range of Co/SiO2 content δ_3 and Co/SiO2 and HAP loading ratio δ_4 as:

$$10 \le \delta_3 \le 200 \tag{7}$$

$$0.49 \le \delta_4 \le 2.03 \tag{8}$$

At this point,we can get the complete expression of our model

Objective function:

$$\min H(\delta_1,\delta_2,\delta_3,\delta_4,\gamma T)_{Ethyleneconversionrate} \cdot H(\delta_1,\delta_2,\delta_3,\delta_4,\gamma T)_{C4olefinselectivity} \tag{9}$$

$$\text{s.t.}\begin{cases} H(\delta_1,\delta_2,\delta_3,\delta_4,T) = \omega_1 f(\delta_1,T) + \omega_2 g(\delta_2,T) + \omega_3 \varphi(\delta_3,\delta_4,T) \\ 250 < T \le 500 \\ 0.5 \le \delta_1 \le 5 \\ 0.3 \le \delta_2 \le 4 \\ 10 \le \delta_3 \le 200 \\ 0.49 \le \delta_4 \le 2.03 \end{cases} \tag{10}$$

2.2 Model solution

Firstly,in this model,considering the particularity of temperature in this model,we take the temperature correction coefficient as $\gamma = 0.9$ .Secondly,it is necessary to solve the value of the model parameter ω_i .According to the processed data,we bring the value of δ_i and temperature T in each group of data into our known $f(\delta_1,T)$, $g(\delta_2,T)$ and $\phi(\delta_3,\delta_4,T)$,and 114 groups of parameters can be obtained:

$$\begin{cases} f_i & i = 1,2,\dots,114 \\ g_i & i = 1,2,\dots,114 \\ \varphi_i & i = 1,2,\dots,114 \end{cases} \tag{11}$$

At this time,for $H(\delta_1,\delta_2,\delta_3,\delta_4,\gamma T)$,we can regard ω_i as an independent variable.At this time,the formula is a multivariate linear function about ω_i .Therefore,we can obtain the parameter value according to the 114 groups of data obtained by us through the method of multivariate linear fitting.

We import the data into Matlab.Through MATLAB multiple linear regression,the parameter value is:

$$\begin{cases} \omega_1 = [0.16112,0.038035]' \\ \omega_2 = [0.54379,0.63744] \\ \omega_3 = [0.35258,1.0062]' \\ z_1 = 1.2843 \\ z_2 = -12.24 \end{cases} \tag{12}$$

For this problem,the model we build is more complex,so it is difficult to find a better solution by using the general algorithm,and the efficiency of the solution is low.For finding the optimal solution of the problem,we use simulated annealing algorithm to solve it.

Let’s briefly explain several quantities in the process[3].

(1)Metropolis guidelines

If newy<beginning_y,then accept the new solution;If newy>beginning_y,then calculateΔf=beginning_x<newy,and calculate $p = e^{-\Delta f/T_i}$,and then randomly generate a random number r that obeys uniform distribution in the interval[0,1].If r<P,accept the new solution newy;

(2)Attenuation function of control temperature

The attenuation function can take many forms.A common attenuation function is $T_{K+1} = \alpha T_k$ .Where α is a constant,which can be taken as 0.5-0.99.Its value determines the cooling process.Slowing down the speed of temperature attenuation may lead to an increase in the number of iterations of the algorithm process,so that the transformation accepted by the algorithm process,the neighborhood visited and the solution space searched will increase,and then return to the optimal solution.However,the solution time will increase greatly.At present,it is generally 0.95.

We imported the model into Matlab and solved it by programming.When the temperature is t=405℃,the maximum yield of C4 olefin is 52.92%.At this time,the conversion rate of ethanol is 83.8%and the selectivity of C4 olefin is 63.42%.See Table 1 for the detailed composition of the catalyst.

Tab1 Composition of catalyst when T=405 degrees.

Co load	Ethanol concentration	Co/SiO2 content	HAP content	Co/SiO2 and HAP loading ratio
3.728	0.300	200	161.576	1.238

We set the temperature condition to T=350 degrees,put our model into Matlab again,and solved it by programming.When T=350 degrees,the maximum yield of C4 olefin is 20.79%.At this time,the conversion rate of ethanol is 52.35%,and the selectivity of C4 olefin is 39.71%.See table 2 for the detailed composition of the catalyst.

Tab2 Composition of catalyst when t=350 degrees.

Co load	Ethanol concentration	Co/SiO2 content	HAP content	Co/SiO2 and HAP loading ratio
3.703	0.301	200	162.823	1.228

3. Model Evaluation

In this paper,each component of the catalyst is put together to make a linear combination,and again through the multiple function regression model,the comprehensive influence model of the catalyst on the yield of C4 olefins is accurately established,and the catalyst combination and reaction temperature with the highest yield of C4 olefins are found through the simulated annealing algorithm,The catalyst combination with the highest C4 olefin yield when the reaction temperature is less than 350□was also obtained by changing the temperature conditions.The disadvantage of the model is that when the reaction temperature is greater than 410□,there is not much data in the model,resulting in the lack of accuracy when the reaction temperature is greater than 410,so the model can not judge the C4 olefin yield at all temperatures.

References:

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