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Research on Chemical Process of Ethanol Coupling to Prepare C4 Olefins Based on DEA Model

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Abstract: The effects of different catalyst combinations and temperatures on ethanol conversion and C4 olefin selectivity were discussed.Firstly,the data envelopment analysis is carried out,and the CCR model is established according to the relevant data. Then the optimal target value of DEA is obtained by linprog function in MATLAB.Finally,the specific effects of different catalyst combinations and temperatures on genetic conversion and C4 olefin selectivity were obtained.

Keywords: Data Envelopment Model; Control Variable Method; Chemical Process Conditions

1. Introduction

C4 olefins are widely used in the production of chemical products and medicine.Ethanol is the raw material for the production of C4 olefins.During the preparation process,the catalyst combination(i.e.the combination of CO loading,Co/SiO2 and HAP loading ratio,ethanol concentration)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.The effects of different catalyst combinations and temperatures on ethanol conversion and C4 olefin selectivity were discussed.

2. Model Establishment and Solution

2.1 Problem Analysis

The factors affecting the degree of reaction are mainly composed of catalyst combination and temperature.In order to make the influence of different catalyst combination and temperature on the reaction more clear,we use the way of control variables to control the two factors of catalyst combination and temperature respectively.C4 olefin is our target product and ethanol is our preparation raw material.We can use these two as the support point to judge the degree of reaction and as dependent variables to measure the influence of catalyst combination and temperature.Data envelopment analysis(DEA)is used to evaluate the multi index input and multi index output problems in this paper.

2.2 Model Establishment

2.2.1Model Selection

Data envelopment analysis has many modes,mainly CCR mode,BBC mode,cross mode and A&P mode.The CCR model is characterized by immutable scale and does not show convexity,which is relatively more suitable for the solution of this paper.

2.2.2Building Decision Units

When the catalyst combination is an independent variable,seven temperatures are taken as decision objects.Each decision unit has four inputs,namely,CO loading,HAP concentration,Co/SiO2 and HAP loading ratio,and two outputs including ethanol conversion and C4 olefin selectivity. $y_{ij}\ \ i=1,2,\cdots,7 \qquad j=1,2,3,4$ represents the j-th input of the i-th decision unit. $y_{ij}=(i=1,2,\cdots,7 \qquad j=1,2)$ represents the j-th output of the i-th decision-making unit. $u=(\ u(1)\ u(2)\ u(3)\ u(4)\ )\ v=(v(1)\ v(2))$ represent input and output weight vectors respectively.

When temperature is taken as an independent variable,14 groups of catalyst combinations are taken as decision objects.Each decision unit has one input,i.e.temperature and two outputs,i.e.ethanol conversion and C4 olefin selectivity. $x_{ij}\ (i=1,2,\ldots,4\ ;j=1)$ represents the j-th input of the i-th decision unit. y_{ij} (i=1,2,...,7;j=1,2) represents the j-th output of the i-th decision-making unit. $u=(u1)$, $v=(v1,v2)$ represent input and output weight vectors respectively.[1]

2.2.3Establish DEA Efficiency Evaluation Model

The benefit evaluation index of decision-making unit K is: $e_k=\dfrac{u^TX_k}{v^TY_k},k=1,2,\cdots,n\ (1)$

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The CCR model and linear programming model for evaluating the decision-making unit K benefits are:

$$\min \quad \theta_k \qquad s.t\begin{cases}\sum_{i=1}^{n}\lambda_i x_j \le \theta_k \cdot x_k & \forall j=1,2,\cdots,m_1\\ \sum_{i=1}^{n}\lambda_i y_j \ge y_k & \forall j=1,2,\cdots,m_2\\ \lambda_i \ge 0 & i=1,2,\cdots,n\end{cases} \quad (2)$$

If the model is solved directly,the amount of calculation is large and the results are complex.We can introduce relaxation variables s_i^-, s_i^+ and non Archimedean numbersεinto the above model.The linear programming of CCR model is modeled as:

$$\min \quad \theta_k - \varepsilon\left(\sum_{i=1}^{m_1} s_i^- + \sum_{j=1}^{m_2} s_j^+\right) \qquad s.t\begin{cases}\sum_{i=1}^{n}\lambda_i x_j + s_j^- = \theta \cdot x_k & \forall j=1,2,\cdots,m_1\\ \sum_{i=1}^{n}\lambda_i y_j - s_j^+ = y_k & \forall j=1,2,\cdots,m_2\\ \lambda_i \ge 0 & i=1,2,\cdots,n\\ s_i^-, s_j^+ \ge 0 & \forall i=1,2,\cdots,m_1;\ j=1,2,\cdots,m_2\\ \varepsilon是很小的数\end{cases} \quad (3)$$

Although$\varepsilon$is very small,but we can't know the order of magnitude of each s_i^-, s_j^+,direct calculation may produce errors. Therefore,the hierarchical sequence method is used to solve this problem.In the first stage,the minimum value of θ_k is solved,and in the second stage,the maximum value of $\sum_{i=1}^{m_1} s_i^- + \sum_{j=1}^{m_2} s_j^+$ is calculated when θ_k is known.[2]

2.3 Substitute Data to Solve

When the temperature(taking 250℃as an example)is taken as the invariant,we quantify each group of catalyst combinations,form a matrix of CO loading,HAP concentration,Co/SiO2 and HAP loading ratio in A1~A14 groups of catalysts,and take out the values of ethanol conversion and C4 olefin selectivity of each group at 250℃to form a decision matrix.Using the linprog function in MATLAB to solve it,we can get the influence degree of the corresponding catalyst combination on the reaction and the relationship between investment and interest.That is:

	A1	A2	A3	A4	A5	A6	A7	A8	A9	A10	A11	A12	A13	A14
250℃	1	0.5	0.6	0.8	0.3	0.7	1	0.7	0.6	0.8	0.2	0.4	0.9	0.4

When taking the catalyst combination as an invariant,we take the temperature as an independent variable to form a matrix,take the values of group A1 ethanol conversion and C4 olefin selectivity out to form a decision matrix,and substitute it into the matlab program to obtain:

	250	275	300	325	350
A1	0.8	0.8	1	1	1

Similarly,the corresponding optimal target value can be obtained by substituting the data of other groups into the program.[2]

2.4 Optimal Target Value Analysis

The optimal solution θ_k obtained by DEA efficiency evaluation model in CCR mode is the comprehensive technical benefit of decision unit K.According to different values of this value,the comprehensive benefit evaluation is divided into the following three cases:

1.If $\theta_k = 1, s_i^-, s_j^+ = 0 \quad \forall i, j$,it indicates that the decision-making unit is"DEA strong and effective",that is,the number of any input cannot be reduced unless the output is reduced or the number of another input is increased;The number of any one output cannot be increased unless the input is increased or the number of another output is reduced.

2.If $\theta_k = 1$, s_i^- or s_j^+ is 0,it indicates that the decision-making unit is"DEA weakly effective",and the number of inputs cannot be reduced in equal proportion,unless the number of outputs is reduced;The number of outputs cannot be increased in equal proportion unless the number of inputs is increased.

3.If $\theta_k = 1$,it indicates that the DMU is"non DEA effective"and there is a waste of resources(no rational use of resources),which is neither the best efficiency nor the best scale.[3]

At this time,there are many optimal target values,which can be analyzed with the help of images.Taking group A as an example,the obtained results are made into images as follows:

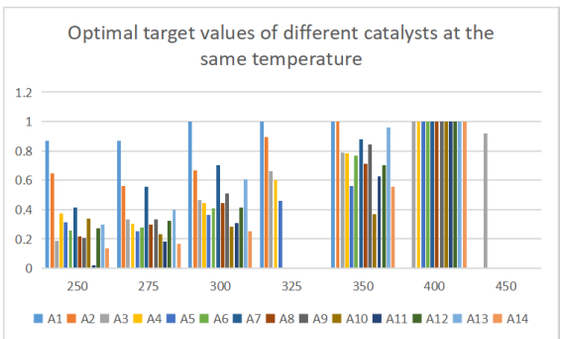

Figure1 Optimal target values of different catalysts at the same temperature

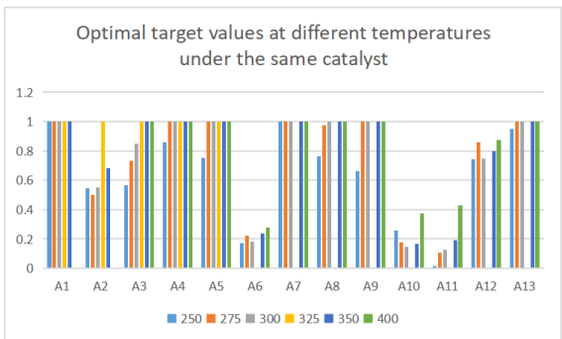

Figure2 Optimal target values of different temperatures under the same catalyst

Combined with the two groups of images,we can draw a conclusion:the catalytic effect of each group of catalysts is significantly different at low temperature,showing a decreasing trend from A1 to A14 groups,and there is little difference at high temperature;Under the same catalyst group,the higher the temperature,the higher the reaction product;When the concentration of CO/SiO2 is high,the catalytic effect decreases because the solution is acidic;When the loading ratio of CO/SiO2 and HAP is low,it will lead to high ethanol conversion but low C4 olefin selectivity,and the income is relatively low.[3]

3. Model Evaluation

The data envelopment model can specifically calculate and quantify the influencing factors,provide accurate numerical solutions to the problem,and accurately describe the relationship between catalyst,temperature and C4 olefin conversion and yield.Chemical reaction is a complex process affected by various external factors.Using ordinary chemical theory can only be qualitative analysis,but can not quantify and accurately control the conditions.Combined with mathematical modeling,we can effectively understand the role of various factors,so as to facilitate accurate control.

References:

[1] Si Shoukui and sun Zhaoliang(2019).Mathematical modeling algorithm and application/edited by -2nd Edition.-Beijing:National Defense Industry Press,reprinted in July .

[2] LV Shaopei(2018).Preparation of butanol and C by ethanol coupling_4 olefins[D].Dalian University of technology.

[3] Ge Yuena(2019).Study on C4 olefin selective stacking process[D].East China University of technology.