Optimal Model of C4 Olefins based on Neural Network Pick, Want

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Abstract: In the field of chemical industry and medicine, C4 olefin has high utilization value. In the preparation of C4 olefin, different catalyst and temperature combinations have a significant impact on the yield of C4 olefin. Therefore, it is of important practical significance to choose reasonable catalyst and temperature combinations in production. For problem 1, the neural network is used to machine learn the training set separated from the processed data, and find the sum of squares of the difference between the predicted value and the actual value of each model by least squares method, and obtain the optimal prediction model after comparison. Then the five parameter combination input model with a certain step length was predicted to obtain all the different temperature and catalyst combinations to obtain the corresponding C4 olefin yield.By comparison, when the catalyst combination was 150mg 3wt%Co / SiO2-170mg HAP-ethanol concentration of 0.3 ml/min and a temperature of 370 degrees, the C4 olefin yield reached a maximum of 0.99976. When the temperature was controlled below 350 degrees, the results were continuously optimized by shortening the step length of the temperature, and finally obtained the C4 olefin yield reached a maximum of 0.27202 when the catalyst was 190mg 3wt%Co / SiO2-190mg HAP-ethanol concentration of 1.9 ml/min and a temperature of 349 degrees. For problem 2, the two experiment were designed to verify the optimal model and the C4 olefin yield as high as possible. Experiments 1,2 were designed to verify whether the catalyst combination with the peak C4 olefin yield, predicted by Problem 3 models, was close to the actual C4 olefin yield. Second, to compensate for the variables that cannot be explored in Annex 1, we designed three experiments based on the data in Annex 1. Finally, this paper explores the sensitivity of the model to improve the future by exploring the advantages and disadvantages of the four independent variables in the catalyst.

Keywords: Interpolation fit; Multiple linear regression analysis; Neural network; Combinatorial optimization

1. Introduction

In the chemical and medical fields, the preparation of C 4 olefin using ethanol has a strong application value, and during this preparation process, different Co load, Co / SiO2 and HAP loading ratio, ethanol concentration and temperature will affect the specific proportion and content of C4 olefin. Therefore, it is very practical and valuable to explore the different combinations of catalyst used in this preparation process.

Combined with a series of experimental results of a chemical laboratory for different catalysts at different temperatures, the following problems are solved through mathematical modeling:

The catalyst combination with the highest possible yield with the temperature and when under the same experimental conditions The catalyst for the C4 olefin yield below 350 degrees.

Design 5 additional experiments and give a reasonable explanation.

2. Model Establishment and Solution

2.1. Establishment and solution of the problem 1 model

2.1.1. Establishment of the problem 1 model

Neural network model preparation.

The process of ethanol coupling to prepare C4 olefin is a highly nonlinear process, the direct use of the linear model is obviously groundless, while considering the nonlinearity of this process, using the easy solvable nature of the linear model to reduce time complexity and improve the real linearity of the control strategy [1]. Based on the idea of "limit learning machine" (ELM), a new model is proposed: first makes the nonlinear transformation of the input five parameters x to obtain the intermediate variable Z, and then establishes a linear weighted model between Z and the output Y (namely the olefin yield), which ensures the nonlinearity and can quickly solve the problem with the nature of the linear model to improve the real-time; the mathematical description is as follows:

$$Z = \mathrm{g}(X) \tag{1}$$

$$Y = \mathrm{WZ} + \mathrm{B} = \mathrm{f}(\mathrm{Z}) \tag{2}$$

Where, g is a nonlinear map and f is a linear map

The core idea of the model is to include all the nonlinearities in it, and the linear relationship is between the final output y of the output z of the nonlinear map, to facilitate the solution.

The standard ELM uses the structure of a single-layer feed forward neural network; specifically the composition of the SLFN includes the input layer, implied layer and output layer, where the output function of the implied layer is defined as follows:

$$f_L = \sum_{i=1}^{l} w_i g_i(x_i) = g(x_i)W \tag{3}$$

$x_i = (i = 1,2,3,4,5)$ indicates that the 5 parameters are the input to the neural network and W is the output weight, called feature mapping, acting to map the data of the input layer from its original space to the feature space of the ELM:

$$g(x) = G(v, x) = H_{l \times q} \tag{4}$$

Where v is the parameter of the feature map;

Based on the above analysis, the following predictive model can be established for the ethanol value loss:

$$Y = f(g(X)) = \ldots + + bw_1 g(x_1) w_2 g(x_2) w_n g(x_n) \tag{5}$$

x_i The values representing the i th feature of the sample, the weights of the i th feature of the sample, and b is biased x_i

What we need to understand is that the feature mapping of the input layer to the implied layer in the ELM is random or artificially given and not adjusted, so the feature mapping of the ELM is random. According to the universal approximation theorem, ELM is infinitely close to any continuous objective function, feature mapping can be any nonlinear fragment continuous function such as RBF function, sigmod function, LU function, etc., the core of ELM algorithm is to solve the output weight to minimize the error function. Moreover, ELM has strong generalization due because the random initialization of feature mapping parameters in the algorithm enhances the mutual independence of each input feature, creating a larger solution space facilitating the finding of the correct objective function for learning [4].

Neural network model[3] The establishment.

With the help of Matla b software, the data input after the analysis and processing is directly allowed to conduct machine learning, predict with the neural network model, and finally determine the optimal model. The specific operation steps are as follows:

Organize the attachment data (emulate problem 2, ignore the data group containing quartz sand), take the final nine sets of data as validation datasets, and the other as training datasets into the neural network in Matlab software for machine learning;

Multiple runs to find a better neural network model and substitute the data of the validation set to get the prediction value, and analyze the error separately with the actual value. Using least squares as shown in Table 1, select the optimal model through comparison, and selecting the optimal model through error analysis can effectively avoid over fitting and enhance the persuasion of the model.

Table 1. Comparison of the different training algorithms

Training algorithm	Absolute error and	Error sum of squares
The levingberg-marquart method	0.222619629	0.040129977
The bayesian regularization method	0.111319629	0.010523969
Quantifying the conjugate gradient method	0.736319629	0.522282627

The superior results of machine learning are shown in Figure 1. After 31 iterations of convergence, when the 25th occurrence circle represents the validation group MSE (mean square error) reaches the minimum, then the occurrence of W and b are the best W and b to fit the data. Data training further represents the model by the size of the goodness-of-fit.

Neural network model after increasing temperature constraints.

A temperature constraint is added that changes the range of temperature, where the value range of this parameter becomes 250,350 degrees, and its analytical solution is similar to the first small question.

Delete the data group greater than 350 degrees in the data, and take the last nine sets of data as the validation dataset. All the rest are used as the training dataset, input the training dataset, and start machine learning using Matlab;

After running the neural network model, the data of the validation set are replaced with the prediction results, and the actual value are analyzed respectively. The data in the model 3 is negative value, so the error is discarded in advance, and the least squares square sum of error is obtained as shown in Table 2. By comparison and choosing the optimal prediction model, the error analysis can effectively avoid over fitting and enhance the persuasion of the neural network model.

Table 2. Comparison of the different training algorithms after increasing the temperature constraints

Training algorithm	Absolute error and	Error Sum of squares
The Levingberg-Marquart method	0.004740424	0.000294
The Bayesian regularization method	0.010948596	0.000142

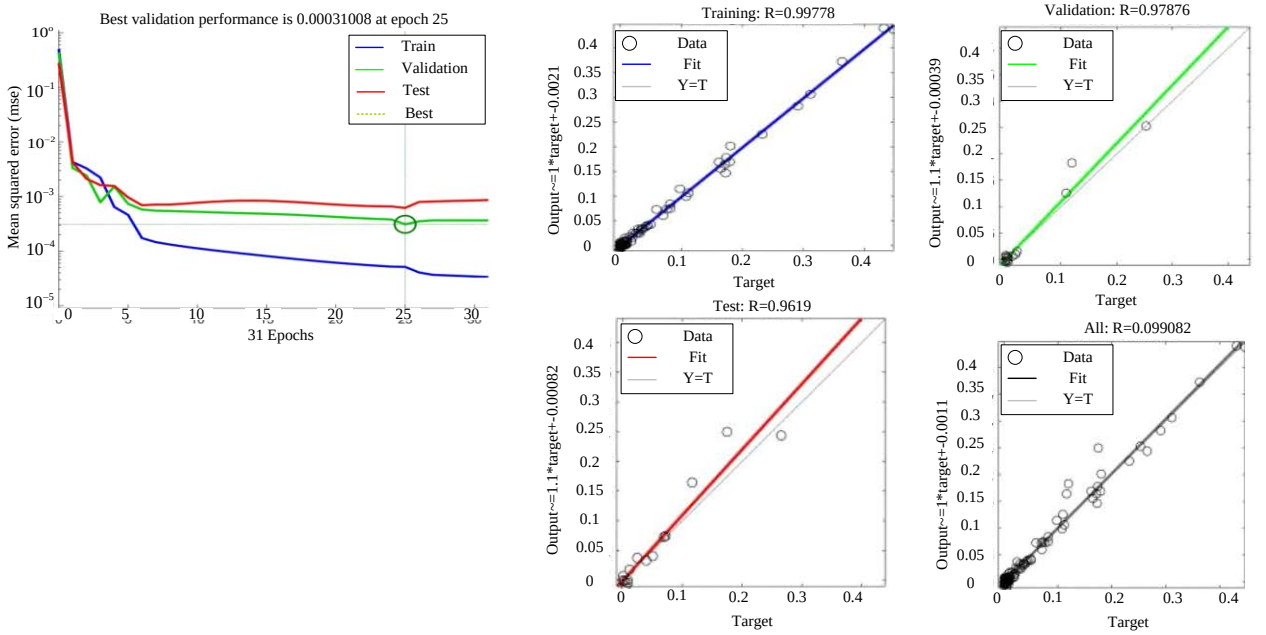

Figure 1. Results after the training of the neural network model

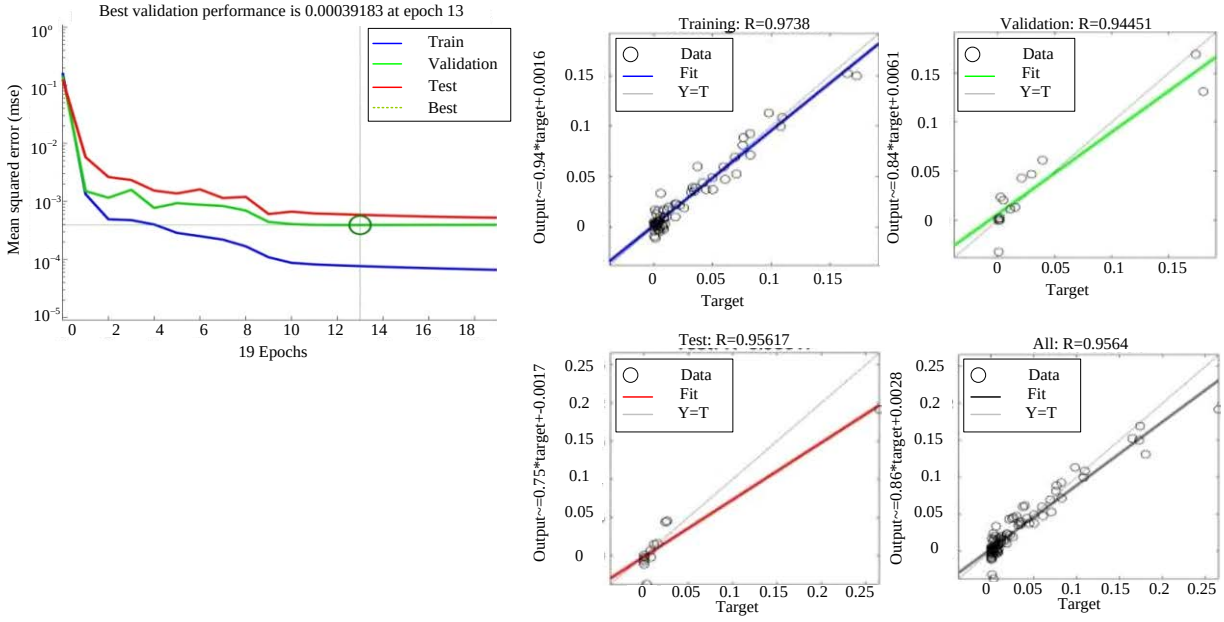

Figure 2. Results after training of the neural network model after increasing temperature constraints

The better results of machine learning are shown in Figure 4. After 19 iterations of convergence, when the 13th circle representative validation group MSE (mean square error) reaches the minimum, the W and b are the best W and b to fit the data; the fit value to the real value, the higher the goodness degree of fit shows that the better the fit of the model.

2.1.2. Solution of the problem 3 model

~ For the attachment data, the range and step length of the five parameters were determined, namely temperature at 20 from 250450 degrees, ethanol concentration at 0.01 within 0.3~2.1ml/min, Co load from 0.01 from 0.01 to 0.05, C 0 / SiO2 mass from 10 to 200 m g, and HAP at 20 from 10 to 200 m g. The refined data set of the five parameters was input separately, predicted with the optimal prediction model obtained above, finally listing the predicted C4 olefin yield of 104 different combinations

of 500 catalysts and temperatures, comparing the C4 olefin yield size of these combinations, finding the highest value of C4 olefin yield of 0.99976 as shown in Table 3
Taken together, the C4 olefin yield in the range of five parameters with a selected catalyst combination of 150mg 3wt%Co / SiO2-170mg HAP- -ethanol concentration of 0.3 ml/min, and a temperature of 370 degrees, reached a peak of 0.99976.

Table 3. Different parameters with the highest C 4 olefin yield take the values

Parameter	Numeric value
Temperature (degree)	370 degrees
Catalyst combination	The concentration of 150mg 3wt%Co / SiO2-170mg HAP-ethanol was 0.3 ml/min
The yield of C4 olefin	0.99976

After increasing the temperature constraint, only the temperature was changed so that it was iterated at 10 as a step length within 250,340 degrees, the refined data set of the five parameters was input separately, and the C4 olefin yield of 95,000 catalysts and temperature combinations was predicted by the optimal prediction model, respectively.
Comparing the size of C4 olefin yield in different combinations, the highest value of C4 olefin yield was 0.24572 at the temperature was below 350 degrees. The corresponding catalyst combination was: 190mg 3wt%Co / SiO2-190 L-mg HAP-ethanol concentration of 1.9 ml/min and the temperature was: 340 degrees.
The results were further improved: when the temperature interval was reduced to 335 to 349 degrees, the step length was shortened to 1 degree, and the other parameters were unchanged, then the new data sets of five parameters were input, and the C4 olefin yield of 142,500 catalysts and temperature combinations were predicted by the optimal prediction model, respectively.

Table 4. The different parameters with the highest C4 olefin yield after increasing the temperature constraint are taken

Parameter	Mumeric value
Temperature (degree)	349 degrees
Catalyst combination	The 190mg 3wt%Co / SiO2-190mg HAP-ethanol concentration was 1.9 ml/min
The yield of C4 olefin	0.27202

Comparing the size of C4 olefin yield under different combinations, the maximum value of 335-349 degrees at the temperature range of 330-27202 was found as shown in Table 4, with the corresponding catalyst combination of 190mg 3wt%Co / SiO2-190mg HAP-ethanol concentration of 1.9 ml/min and a temperature of 349 degrees. By comparing the results before the optimization, the relatively higher C4 olefin yield in the catalyst combination and temperature.

2.2. Establishment and solving of the four-way problem model

2.2.1. Establishment of the problem four model

This paper considers the design of five additional experiments from two aspects as shown in Table 5:
The first two experiments were designed to verify the rationality of the optimal model and its predictive values established by the problem three, starting with the C4 olefin yield as high as possible.
The design of the last three experiments is based on analyzing the data in Annex 1, considering the deficiencies of the experimental design given in the topic and the problems still to be explored.

Table 5. The five experimental data are added in Table 5

Group	Catalyst and temperature combination
1	150mg 3wt%Co / SiO2-170mg HAP-ethanol concentrations of 0.3 ml/min and 370 degrees
2	190mg 3wt%Co / SiO2-190mg HAP-ethanol concentrations were 1.9 ml/min as well as 349 degrees
3	The concentration of 50mg 1wt%Co / SiO2-90mgHAP-ethanol was 1.68 ml/min
4	The 100mg 2wt%Co / SiO2100mg HAP-ethanol concentration was 1.68 ml/min
5	67mg 1wt%Co / SiO2-33mg HAP-ethanol concentration was 1.68 ml/min

2.2.2. Solution of the problem four-way model

Experiment 1 was designed to verify whether the catalyst combination of the C4 olefin yield between the peak C4 olefin yield and the temperature in the actual experiment using the 250 to 450 degrees range were close to this peak; in like manner, Experiment 2 was designed to verify whether the combination of catalysts at the temperature below 350 degrees of the C4 olefin yield and the temperature in the actual experiment were close to the peak; The last three experiments were designed based on the analysis of the Annex 1 data, The deficiencies of the experimental design given in the topic and the questions to be explored are considered.
The specific reasons for setting the experimental data are as follows:
Experiments were performed at 1:150mg 3wt%Co / SiO2-170mg HAP-ethanol concentrations of 0.3 ml/min and 370 degrees
Experiments were performed at 2:190mg 3wt%Co / SiO2-190mg HAP-ethanol concentrations of 1.9 ml/min and 349 degrees
In order to verify the model in Question 3, the design data were tested to obtain the actual C4 olefin yield, and

the C4 olefin yield was compared with the C4 olefin yield predicted by Q 3, so as to verify the feasibility and rationality of the model.

Experiment 3:50mg 1wt%Co / SiO2-90mgHAP-ethanol concentration of 1.68 ml/min

Because only one set of experimental data of quartz sand appears in the attachment, and the other independent variables of the group are different, we cannot simply study the effect of quartz sand on the experimental results with the control variable method, so we can design a set of experiments, control variables to verify the impact of different catalyst carriers on the experimental results, that is, under other conditions, replace quartz sand with HAP catalyst carrier.

Experiment 4:100mg 2wt%Co / SiO2100mg HAP-ethanol concentration of 1.68 ml/min

Out of the seven catalyst combinations assembled in II, their Co load was 1wt%, which cannot explore the effect of altered Co load on the experimental results, so we can design a set of experiments to study the Co load under the same conditions.

Experiment 5:67mg 1wt%Co / SiO2-33mg HAP-ethanol concentration was 1.68 ml/min

There are equal and unequal catalyst combinations of loading modes I, Co / SiO2 and HAP, while the quality of Co / SiO2 and HAP in the loading mode II did not explore the experimental situation of unequal Co / SiO2 and HAP in the catalyst combination, so we need to design a set of experiments to change the relative quality of both under other conditions.

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