Problem Chosen	2023 ShuWei Cup Summary Sheet	Team Control Number
D		2023102920495

The catalytic reaction of cotton stalk pyrolysis

Abstract

Statistic models could be helpful in improving the efficiency of producing renewable energy. This essay uses statistic method to explore the effect of mixing ratio of desulfurization ash and cotton stalk on the yield of pyrolysis products in three pyrolysis combinations, establish a mechanic model of pyrolysis reaction and make prediction on pyrolysis products under different mixing ratio of three pyrolysis combinations, thus greatly facilitating the chemistry industry.

For question one, A descriptive statistical analysis on the data is performed and visualized with line chart and bar chart. Statistic Normal distribution tests were conducted on each data, with Pearson correlation coefficient being performed on them after meeting the conditions. Regard to the effect of catalyst DSA, it is found to have a significant impact on the yield ratio of Tar in all three reactions, especially on CS.

For question two, the trend of pyrolysis gas production changes is visualized to compare and analyze the changes of different gases under different mixing ratios. With normal distribution test being used Shapiro Wilk. Pearson correlation coefficient analysis is performed on the yield of each pyrolysis gas extraction and the mixing ratio. It is found that in the CS reaction, the relationship between H2, C3H8 and the mixing ratio is the most significant and shows a positive correlation.

For question three, A scatter plot of the mass ratio of the same product under different reactions is drawn and the differences in the effects of CE and LG under different mixing ratios are analyzed. A bivariate analysis of variance was performed on the experimental data when CE and LG were reactants. It was found that the catalyst had the most significant difference in the reaction between CE and LG when the mixture ratio of reactants to catalyst was 100/100.

For question four, A reaction kinetics equation is formulated by analyzing the changes of reactants and referring to relevant materials, where pyrolysis reaction are divided into three stages, with corresponding pyrolysis models being established. A nonlinear regression equation is also established for different pyrolysis products. The final kinetic equation is formed by the regression result.

For question five, a mathematical model of linear regression is formulated with further nonlinear regression prediction model being used for auxiliary examination. Subsequently, grey prediction analysis was performed on the data to test its prediction results; AI learning method is also established and trained to obtain more accurate prediction maps of product quality ratios under different mixing ratios, thus greatly improving the prediction efficiency

Keywords: descriptive statistical analysis, Pearson correlation coefficient, analysis of variance, nonlinear regression, neural network

Content

1. Introduction

1.1 Background

With the increasing population and the growing demand of renewable energy resources, biomass energy, a clean and renewable energy source initially comes from the sun, are coming into public view. As a agricultural waste with rich biomass components such as cellulose and lignin, cotton stalk is playing a significant role in solving the problem of solid waste management along with being a sustainable energy resource. Cotton stalk can convert into various forms of renewable energy when it is thermochemically decomposed at high temperatures in the absence of oxygen, which is called the pyrolysis of cotton stalk. However, the utility value and output of its products are influenced by numerous factors such as the reaction temperature, gas pressure and catalytic and so on. Therefore, how to develop the efficient utilization of cotton stalk, making the best use of its biomass energy, has become a current focus nowadays.

1.2 Restatement of the problem

The mixing ratio of reactant and catalyzer is one important factor to consider when doing pyrolysis and a slight error on small ratios would have a serious effect on the process of exploring and optimizing the experiment. Now it is required to develop a mathematical or AI learning model that can predict the precise pyrolysis process under limited data.

1) **Task 1** Find out the relationship between the yield of the pyrolysis products (tar, water, coke residue, syngas) and the mixing ratios of relevant combinations in Annex Ⅰ, then illustrate whether desulfurization has played a vital role in promoting pyrolysis of cotton stalks, cellulose and lignin as a catalyst.

2) **Task 2** Based on Annex Ⅱ, discuss how the mixing ratio of pyrolysis combinations affects the production of pyrolysis gas and draw the corresponding images of the three pyrolysis combinations.

3) **Task 3** Find out whether the yields of the products produced by the pyrolysis of CE and LG changed under the same proportion of desulfurized ash, as well as the components of the pyrolysis gas, and explain the reasons.

4) **Task 4** Build a catalytic reaction mechanism model of desulfurized ash for pyrolysis compounds like CE and LG, as well as the model of reaction kinetics to analyze.

5) **Task 5** use mathematical models or artificial intelligence learning skills to predict the production of the pyrolysis products under under limited data conditions.

2. Problem analysis

2.1 Data analysis

This essay preprocesses the data initially, performs data cleaning, and performs outlier detection.

2.2 Analysis of question one

The first question is to explore the impact of the mixing ratio of desulfurization ash catalyst with CS, CE, LG on the four pyrolysis products. This essay first conducts descriptive statistical analysis to explore the average and standard deviation data of different products under different mixing ratios, and compares the degree of change of different products; Afterwards, a scatter plot was created with the mixing ratio as the horizontal axis and the product mass ratio as the vertical axis. The trend of individual pyrolysis products with CS and different components (CE, LG) as reactants was presented on a single plot for trend analysis; Finally, correlation analysis was conducted by calculating its Pearson coefficient to quantify the correlation between the catalyst and reactant mixture ratio. The second question is to compare the importance of catalysts on different products. In order to more intuitively display the differences between each product, this article presents four types of products on a line chart using the mixing ratio as the horizontal axis and the product quality as the vertical axis, and analyzes the effects of different mixing ratios with catalysts when CS, CE, and LG are reactants, And analyze the catalyst concentration horizontally and vertically, as well as the impact of catalyst and different reactant mixtures on the products, and conduct differential analysis through paired sample T-test to further explore the differences in the role of catalysts in different pyrolysis reactions.

2.3 Analysis of question two

Question 2 requires a discussion on the impact of pyrolysis combination mixing ratio on pyrolysis gas yield. This article first conducts a descriptive statistical analysis on it. Based on the data, the mixture ratio of catalyst and reactants is used as the x-axis, and gas production and total gas production are used as the primary and secondary y-axis, respectively. A line chart for each gas production and a column chart for total gas production are created to analyze the trend of changes in gas production under different reactants and the change in total gas production, And by calculating and creating a stack diagram of the proportion of gas production, further analyze the changes in the proportion of production of pyrolysis gas stripping under the action of desulfurization ash; Subsequently, the data was subjected to a normal distribution test, and once the conditions were met, Pearson correlation coefficient analysis was performed to explore the significance of the relationship.

2.4 Analysis of question three

Question 3 requires exploring the yield of CE and LG pyrolysis products and pyrolysis gas under the same mixing ratio. This article first integrates the data for descriptive statistical analysis and plots the trend of individual product mass ratio changes with the change of CE and LG mixing ratio. Longitudinal analysis can reveal the difference of the product when CE and LG are reactants under the same proportion of desulfurization ash. In order to explore it more rigorously, this article uses the two-factor analysis of variance method to further explore the significance of the differences in CE and LG under the same proportion and explains the reasons with corresponding chemical knowledge through data review. The yield difference analysis of pyrolysis gas is the same as that of pyrolysis products.

2.5 Analysis of question four

Question 4 requires us to establish a reaction kinetics model for model compounds CE and LG and analyze it to investigate the rate at which the reactants produce pyrolysis products. This article starts from the three stages of pyrolysis reaction, gradually analyzing the time, temperature, and stage generated by each pyrolysis product. Through data preprocessing and analysis, it is confirmed that there are no abnormal values in the data. After that, a line chart is drawn with the mass fraction of each pyrolysis product as the ordinate and the type of pyrolysis product as the abscissa, and the turning points at different mixing ratios, namely the point where the slope symbol changes, are marked. Determine a new stage by analyzing before and after the turning point. Based on the results of nonlinear regression. Reverse the reaction kinetics equation of CE concentration change through the regression equation and present the final result in the form of an icon in the answer to question four.

2.6 Analysis of question five

Question 5 requires building a model to predict the products of pyrolysis reactions. This article first conducts linear regression prediction on it, and through goodness of fit testing, it is found that the prediction function of some of its products is not ideal. Therefore, the optimized model is nonlinear regression prediction, and a mathematical model with relatively ideal goodness of fit is obtained; To enrich the prediction, this article also constructs a grey prediction model for prediction; In addition, a neural network was constructed and continuously trained through machine learning to obtain a neural network model with relatively accurate output rate.

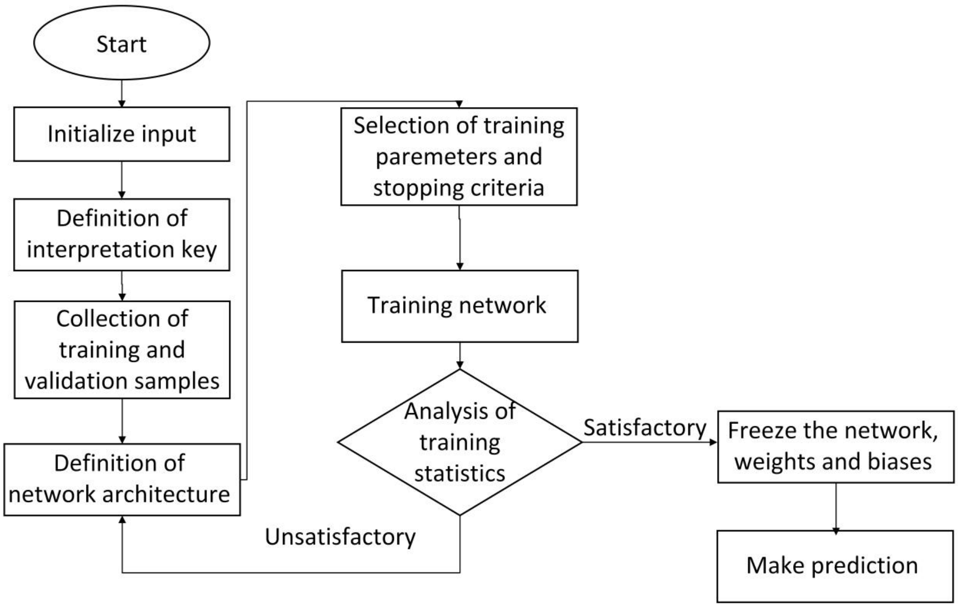


Figure 1: Flow diagram of neural network

3. Symbol and Assumptions

3. 1 Symbol Description

Notations	Descriptions
d	mean of yield of pyrolysis product
S	Standard deviation of pyrolysis product
F	ratio of pyrolysis product
s	ratio of combination of reactant and catalyst
RMSE	root-mean-square error

3.2 Fundamental assumptions

- Heat losses are ignored.
- CS, CE, LG experiments are independent.
- Every result is written down correctly without error.
- The data set can represent various cases of catalytic reaction
- All of the experiments were performed under the same environment and operating procedures

4. Solution to question one

4.1Effect of Catalyst and CS, CE, LG Mixing Ratio on Four Pyrolysis Products

4.1.1 Descriptive Statistical Analysis

To investigate the influence of the mixing ratio of desulfurization ash catalyst and CS, CE, LG on the mass ratio of four pyrolysis products, the average and standard deviation data of the four pyrolysis products were obtained through calculation, and the following table is obtained:

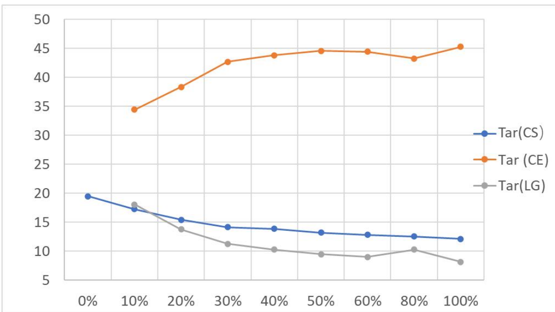
Table 1: Statistics of pyrolysis product mass ratio data

Variable name	Max	Min	Average	Standard deviation	Median	Variance
Tar yield（CS）	19.46	12.13	14.547	2.431	13.89	5.909
Water yield(CS)	31.02	26.84	28.913	1.415	28.62	2.003
Char yield(CS)	29.87	29.11	29.379	0.246	29.33	0.061
Syngas yield(CS)	28.45	24.49	27.161	1.279	27.16	1.635
Tar yield(CE)	45.28	19.46	39.569	8.322	43.24	69.26
Water yield(CE)	27.42	16.14	20.104	4.329	18.25	18.741
Char	29.21	21.43	24.637	2.02	24.59	4.081

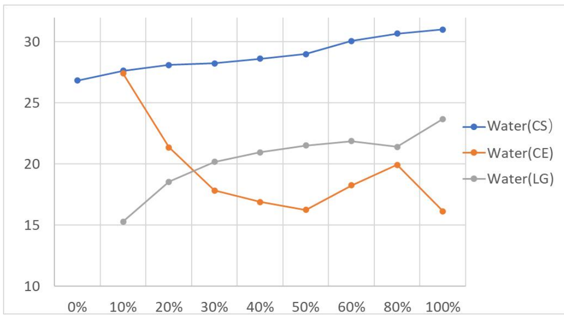
yield(CE)						
Syngas yield(CE)	24.49	12.75	15.69	3.508	14.68	12.303
Tar yield(LG)	19.46	8.19	12.207	4.049	10.3	16.397
Water yield(LG)	26.84	15.3	21.147	3.193	21.41	10.198
Char yield(LG)	58.17	29.21	54.211	9.382	57.15	88.02
Syngas yield(LG)	24.49	8.47	12.436	4.647	11.41	21.598

From the table, it can be seen that when CS is the reactant, the variance of Char is only 0.061, indicating that the catalyst has a small impact on Char, while the variance of the Tar mass ratio is 5.909, indicating that the catalyst has a significant effect on Tar in this pyrolysis reaction.

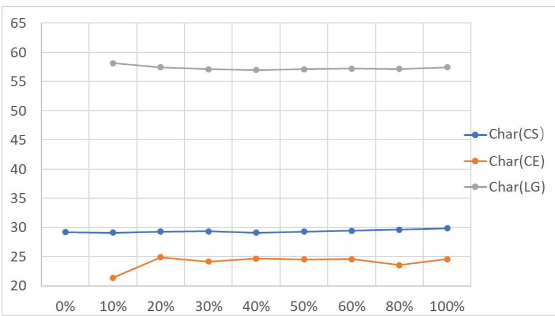
Subsequently, in order to analyze the specific trend of the catalyst's action on a single pyrolysis product, this article created a scatter plot of the quality and mixing ratio of each pyrolysis product, visualizing the impact of the catalyst on it. The changing trends of the four pyrolysis products with increasing mixing ratio were obtained as shown in the following figure:



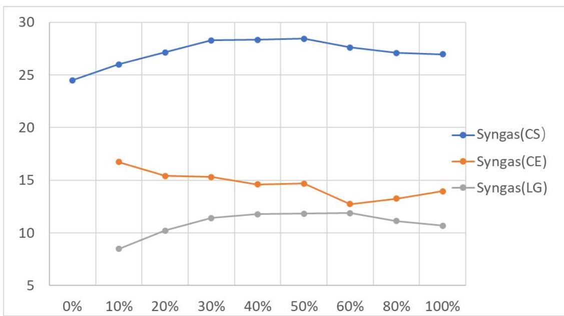
relationship between pyrolysis combination and Tar



relationship between pyrolysis combination and Water



relationship between pyrolysis combination and Char



relationship between pyrolysis combination and Syngas

Figure 2: the relationship between pyrolysis combinations and products

Taking Tar as an example, by comparing the graphs horizontally, it can be concluded that when the reaction substrate is CS, the mass ratio of tar in the product shows a decreasing trend with the increase of catalyst, and finally gradually tends to be flat, about 12.5%; When the reaction substrate is CE, the mass ratio of tar in the product shows an upward trend as the mixing ratio of the catalyst increases, and the increase is most significant when the catalyst mixing ratio is 0% -20%; When the reaction substrate is LG, as the mixing ratio of the catalyst increases, the overall mass ratio of tar in the product shows a decreasing trend, but there are slight fluctuations when the mixture ratio is high, corresponding to the variance size of Tar mentioned above.

Vertical comparison shows that the influence of CS and LG on the change trend of Tar product mass ratio is almost the same as the increase of catalyst, both of which decrease, but LG decreases more and is more unstable (or fluctuates more). The impact of CE on Tar with the increase of catalyst is completely different from that of CS and LG. The mass ratio of Tar has a significant upward trend with the increase of catalyst and is almost opposite to the trend of LG. From this, we can also speculate that in a certain reaction where the pyrolysis product is Tar, the target of the catalyst is biased towards lignin LG.

In addition, to compare the trend of changes between different products under different reactants, this article also produced a line chart of changes in the mass ratio of different products in a single reaction. This article takes CE as an example, and the rest can be found in the appendix.

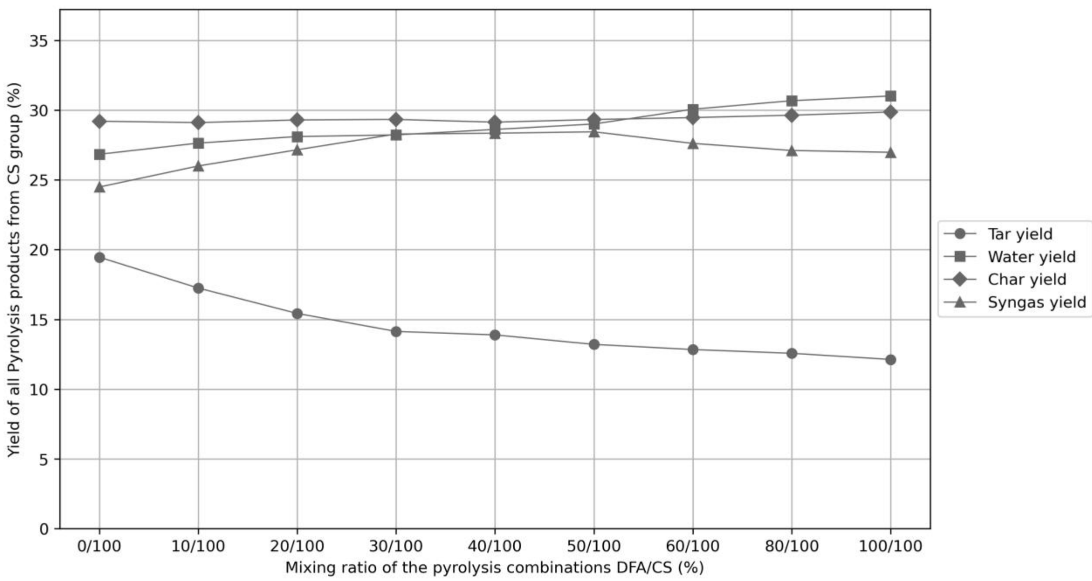


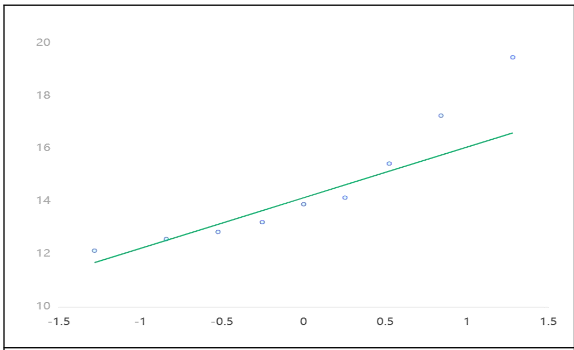
Figure 3: the relationship between pyrolysis combinations and products (CS)

From the graph, it can be seen that in the pyrolysis reaction using CS as the reactant, the degree of variation of Tar with the mixing ratio is the most significant, while the degree of variation of Char is the least significant.

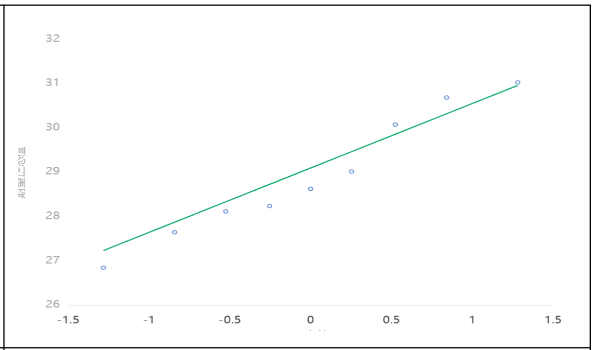
Similarly, the pyrolysis reaction results of CE and LG as reactants showed the most significant changes in Tar and the least significant changes in Char.

4.1.2 Pearson correlation coefficient analysis

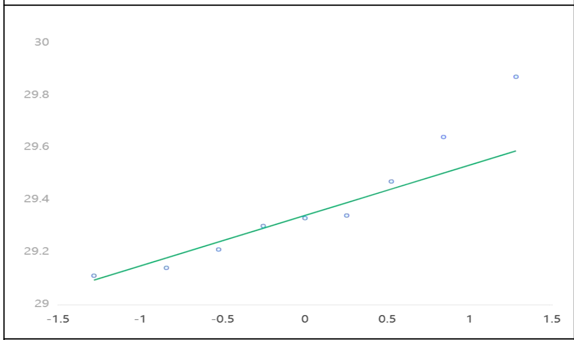
To explore the interrelationships between various categories, this article first conducts a correlation analysis. Firstly, the Shapiro Wilk method was used to analyze its normal distribution, and the results are as follows (using CS as an example, see the appendix for the rest):



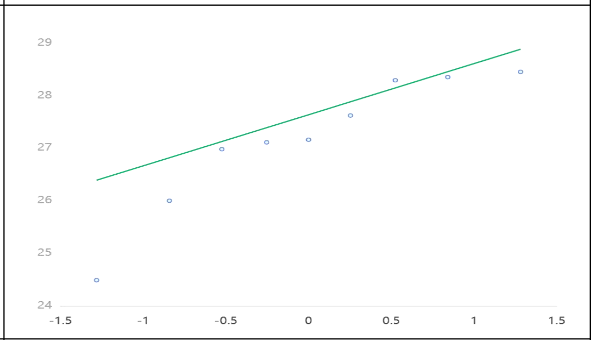
Normal distribution test of Tar (CS)



Normal distribution test of Water (CS)



Normal distribution test of Char (CS)



Normal distribution test of Syngas (CS)

Figure 4: Quantile Quantile Plot of pyrolysis products

From the graph, it can be seen that the actual values of the four pyrolysis products are almost consistent with the predicted curve under the assumed normal distribution, which can be accepted as a normal distribution. Moreover, it can be seen from the previous text that the relationship between the mixing ratio and the Tar mass ratio is approximately linear. Therefore, Pearson correlation coefficient analysis is conducted for this. The Pearson coefficient is used to measure the linear correlation between two variables, with values between -1 and 1, where 1 represents complete positive correlation, -1 represents complete negative correlation, and 0 represents no linear correlation.

Taking CS as an example, the mixing ratios of catalyst and CS are set X: {x1, x2,..., x9}, respectively. The mass ratios of Tar under different mixing ratios are set Y: {y1, y2..., y9}

$$E(X) = \frac{\sum_{i=1}^{9} X_i}{9} \tag{1}$$

$$\sigma_X = \sqrt{\frac{\sum_{i=1}^{9} (X_i - E(X))^2}{9}} \tag{2}$$

Thus, the Pearson correlation coefficient between the mixing ratio and the Tar mass ratio can be obtained based on the following formula:

$$\rho_{XY} = \frac{cov(X,Y)}{\sigma_X \sigma_Y} = \frac{\sum_{i=1}^{9} \frac{(X_i - E(X))}{\sigma_X} \frac{(Y_i - E(Y))}{\sigma_Y}}{9} \tag{3}$$

The final Pearson correlation coefficient obtained is -0.929, which shows significant significance. Therefore, it can be analyzed that the mixing ratio of catalyst and CS has a significant impact on the mass ratio of pyrolysis product Tar, and the impact of the two is negatively correlated.

By analogy, the Pearson correlation coefficients between each pyrolysis product under three different reactant mixture ratios can be obtained. After integration, the following table is obtained:

Table 2: Pearson correlation coefficient of pyrolysis products

	Tar yield	Water yield	Char yield	Syngas yield
CS	−0.929	0.985	0.845	0.513
CE	0.789	−0.771	−0.277	−0.76
LG	−0.898	0.197	0.532	−0.427

From the table, it can be seen that for the pyrolysis product Tar, whether in CS, CE, or LG, the mixing ratio of the catalyst to its mass is significantly higher than that of Tar. Among them, LG and CS have the same effect on the mass ratio, showing a negative correlation trend, indicating that the catalyst may have a significant inhibitory effect on the generation of Tar; For the pyrolysis product Water, the catalyst only has a significant impact on its quality when mixed with CS, and has a significant promoting effect on the generation of Water. However, the catalyst has a completely different effect when mixed with CE, and its effect is not significant when mixed with LG; For the pyrolysis product Char, the catalyst only had a significant impact on its mass ratio when mixed with CS, and it was positively correlated. However, the effect of mixing with CE and LG was not significant; For the pyrolysis product Syngas, the relationship between the catalyst mixing ratio and it is not significant, and it is positively correlated with the CS mixing ratio, while negatively correlated with the CE and LG mixing ratio.

Summary: When the catalyst is mixed with CS, the relationship between the mixing ratio of the catalyst and Tar, Water, Char, Syngas is significant, and the catalyst significantly promotes its thermal decomposition and the generation of Water and Char; Moreover, the influence of catalyst mixing with CS and LG on pyrolysis products is generally similar, with the most obvious relationship being similar to the mass ratio of Tar and Char. However, the correlation coefficient brought by catalyst mixing with CS and mixing with CE is generally opposite, indicating that CE in CS may play a dominant role in the pyrolysis reaction.

4.2 The Importance of Catalysts in Different Pyrolysis Reactions

4.2.1 Paired-Samples T Test

Paired sample T-test can be used to compare whether there is a significant difference in the average values of two types of experimental subjects under different conditions. To investigate the effect of the mass ratio of catalysts to individual products in pyrolysis reactions, this article uses paired sample T-test method for individual analysis.

In the pyrolysis reaction using CS as the reactant, the effects of catalysts on the mass generation ratios of Tar, Water, Char, and Syngas were calculated separately. Taking Tar as an example, assuming d is the average value of the difference in mass ratio before and after Tar under different mixing ratios, S is the standard deviation of the difference in mass ratio before and after Tar under different mixing ratios, u is the assumed mean difference, and n is the number of sample observations. By calculating the formula:

$$d=\frac{\sum_{i=1}^{n} d_i}{n} \quad (1)$$

$$S_d = \sqrt{\frac{\sum_{i=1}^{n} (d_i - d)^2}{n-1}} \quad (2)$$

Freedom v=n-1

$$t = \frac{d-u}{s_d/\sqrt{n}} \quad (3)$$

Under the action of the catalyst, the t-value of the Tar mass ratio is about 9.223, and the p-value is about 0.00003, which is much less than 0.05. The original hypothesis cannot be rejected, so the difference is significant. Therefore, it is speculated that the catalyst is more important in the generation of Tar.

The same method can be used to calculate that the p-values of Water and Syngas are both less than 0.05, while the p-value of Char is only slightly greater than 0.05 with a p-value of 0.07. Therefore, it can be analyzed that the differences generated by the catalyst in the pyrolysis reaction of CS are significant, indicating that the catalyst plays an important role in the pyrolysis reaction of CS.

Similarly, integrate other reaction data into the following table:

Table 3: Paired Sample T test for different chemical reaction

	CS	CE	LG
Tar yield (t)	9.22E+00	-1.00E+01	-2.99E+01
Water yield (t)	-5.22E+00	1.26E+01	-9.83E+00
Char yield (t)	-2.11E+00	-1.80E+01	1.46E+01
Syngas yield (t)	-1.00E+01	6.43E+00	-1.18E+01
Tar yield (p)	3.64E-05	5.72E-05	9.23E-08
Water yield (p)	1.23E-03	1.50E-05	6.40E-05
Char yield (p)	7.27E-02	1.91E-06	6.46E-06
Syngas yield (p)	2.13E-05	6.67E-04	2.29E-05

5. Solution to problem two

5.1 Descriptives

5.1.1 Analysis using CS as reactant

Visualize the data in Annex II using CS as the reactant to obtain the following figure:

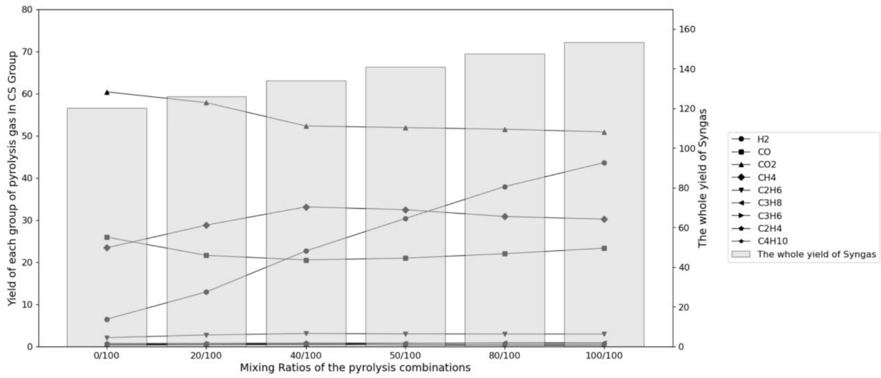


Figure 5: Total mass and respective yield of the gas in CS group

From the graph, it can be seen that the main components of the pyrolysis gas are H2, CO, CO2, CH4, and C2H6. As the mixing ratio of desulfurization ash increases, CO production shows a slight downward trend, while CO2 production shows a relatively obvious downward trend. Therefore, it can be inferred that the catalyst has an inhibitory effect on the generation of CO and CO2; On the contrary, the production of H2 has significantly increased, and the H2 produced when the mixing ratio of desulfurization ash and CE is 100/100 is 6.73 times higher than the H2 production when CE is pyrolysis alone; As the mixing ratio of the catalyst gradually increases, the yields of CH4 and C2H6 show a trend of first increasing and then decreasing, and both reach their maximum values at a mixing ratio of 40/100. At the same time, it can be seen from the column chart that as the desulfurization ash mixing ratio increases, the total amount of pyrolysis gas gradually increases.

In order to compare the changes in the proportion of pyrolysis gases under the action of catalysts, this article also drew a stack diagram of the generation amount of each gas, and the results are as follows:

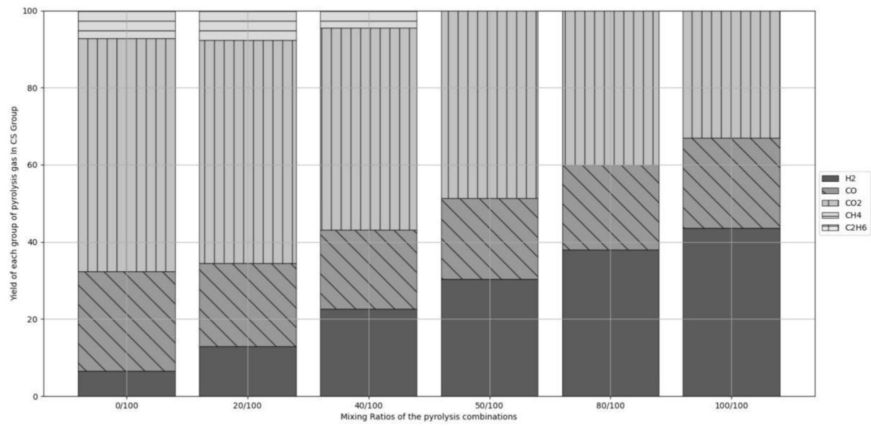


Figure 6: Mass percentage of each gas in CS group

From the graph, it can be seen more intuitively that the proportion of H2 in the generated gas increases significantly with the increase of catalyst mixing ratio, while the proportion of CO and CO2 decreases slightly, while the proportion of CH4 decreases significantly until it is almost negligible.

Summary: Desulfurization ash has a significant catalytic effect on the pyrolysis of CS. It not only increases the production of pyrolysis gas, but also significantly changes the production of different gases in the pyrolysis gas. Specifically, the production of H2 increases significantly, while the production of CO and CO2 is inhibited to a certain extent, and it promotes the production of CH4 and C2H6 within a certain range; At the same time, desulfurization ash also significantly changed the proportion of different gas production in the pyrolysis gas, with the most significant increase being the proportion of H2 production. (Others can be seen in Annex)

Summary: The catalytic effect of desulfurization ash on the pyrolysis reaction with LG as reactant is not significant. Although the total generation of gases has increased, the proportion between the generation of each gas and its ratio remains almost unchanged.

5.2 normal distribution test

To further investigate the significance of the relationship between the mixing ratios of various gases and catalysts, the gas generated during CS pyrolysis reaction was subjected to normal distribution testing to obtain the following table:

Table 4: Shapiro-Wilk Test for syngas

Name	Skewness	Kurtosis	Shapiro-Wilk Test
H2	-0.142	-1.522	0.964(0.852)
CO	1.352	1.624	0.884(0.287)
CO2	1.086	-0.831	0.798(0.056*)
CH4	-1.448	2.381	0.877(0.257)
C2H6	-1.958	3.945	0.757(0.023**)
C3H8	0.454	-1.96	0.875(0.249)
C3H6	0.333	0.516	0.975(0.926)
C2H4	-0.086	-0.641	0.99(0.988)
C4H10	0.706	-0.99	0.926(0.550)

From it, it can be seen that the significance P-values of each gas do not show significance, and the original hypothesis cannot be rejected. Therefore, the data satisfies a normal distribution, so the next Pearson correlation coefficient analysis can be performed on it.

5.3 Pearson correlation coefficient analysis

Calculate the Pearson correlation coefficient between the yield and mixing ratio of each gas in the pyrolysis reaction with CE as the reactant using the same solution as Problem 1, and obtain the following table:

Table 5: Pearson correlation coefficient of syngas

	H2	CO	CO2	CH4	C2H6	C3H8	C3H6	C2H4	C4H10
CS	(0.000***)	(0.552)	(0.014**)	(0.205)	(0.115)	(0.003***)	(0.509)	(0.431)	(0.307)
CE	(0.066*)	(0.003***)	(0.018**)	(0.021**)	(0.027**)	/	/	/	/
LG	(0.035**)	(0.002***)	(0.051*)	(0.889)	(0.391)	/	/	/	/

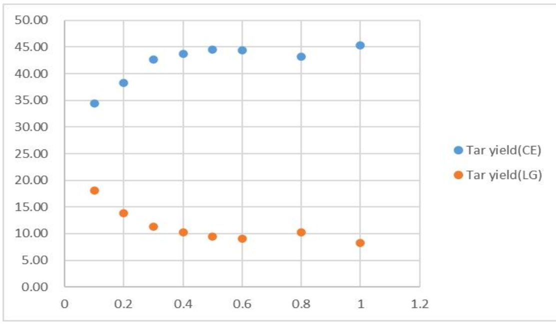
From the table, it can be seen that in the pyrolysis reaction using CS as the reactant, the relationship between the mixing ratio and H2, C3H8 is the most significant and shows a positive correlation trend. This indicates that with the increase of catalyst, the production of H2 and C3H8 gradually increases, and the catalyst plays a promoting role in the generation of H2; The mixing ratio shows a significant negative correlation with CO2 production, indicating that the catalyst has a significant inhibitory effect on CO2 generation. In the pyrolysis reaction using CE as the reactant, the catalyst has a significant relationship with H2, CO, CO2, CH4, C2H6, and has a significant positive correlation with H2. That is, as the catalyst increases, the production of H2 also increases; The rest shows a significant negative correlation with the mixing ratio of the catalyst, which means that as the catalyst increases, its production decreases;
In the pyrolysis reaction using LG as the reactant, the relationship between the catalyst and H2, CO, and CO2 shows a significant positive correlation. It can be inferred that the catalyst has a promoting effect on its production, while it shows a negative correlation with C2H6. It can be inferred that it has a slight inhibitory effect on the production of C2H6, but no significant effect on CH4.

6. Solution to question three

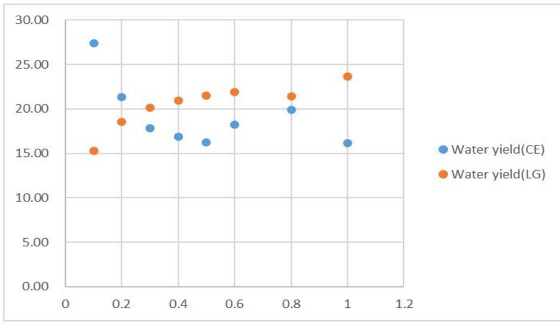
6.1 Yield of pyrolysis products

6.11 Descriptive Statistical Analysis

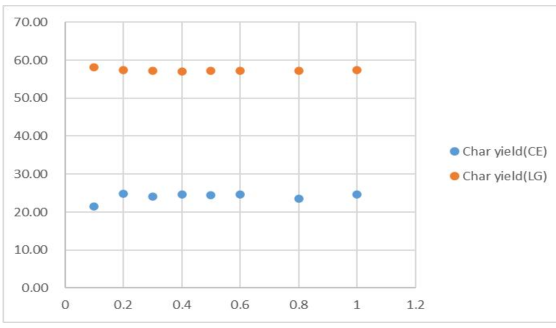
To compare the differences between CE and LG pyrolysis products under the same desulfurization ash mixture ratio, this article first integrates the data and draws charts to visualize the results for easy observation and analysis.



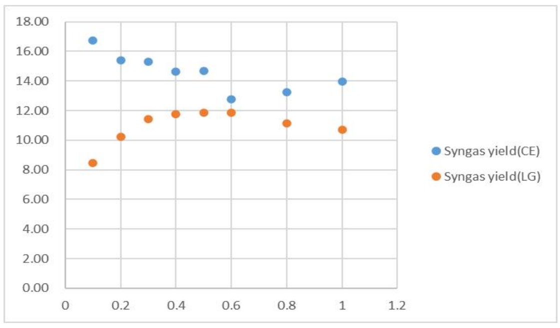
Yield of Tar



Yield of Water



Yield of Char



Yield of Syngas

Figure 7: Yields of pyrolysis products in CE and LG group

From the graph, it can be seen that for the pyrolysis product Tar, there is generally a significant difference in the mass ratio of CE as the reactant and LG as the reactant under all mixing ratios, and the degree of difference increases with the increase of mixing ratio. The maximum increase is observed when the mixing ratio is 0.1 to 0.4, and it stabilizes at the maximum difference after 0.5. It can be understood that under the same mixing ratio, the Tar yield of CE and LG varies greatly, And the desulfurization ash catalyst promotes CE and inhibits LG during the pyrolysis reaction to generate Tar products; For the pyrolysis product Water, the difference in mass ratio between CE as the reactant and LG as the reactant is significant, with a phenomenon of repeated fluctuations of decrease and increase. This is related to the fluctuation and high symmetry of the mass ratio curve between CE and LG. It is speculated that the final product in the pyrolysis reaction of CE and LG is highly similar to water, but the degree of catalyst action is opposite; For the pyrolysis product Char, the difference in mass ratio between CE as the reactant and LG as the reactant shows a stable trend overall, but the absolute difference is significant. This indicates that there is generally a significant difference in Char production under various mixing ratios, but it is not significantly related to the proportion of catalyst; For the pyrolysis product Syngas, the initial difference between CE and LG is relatively large, but as the mixing ratio increases, the difference gradually decreases and then increases, and there is no significant difference under the same mixing ratio.

6.1.2 Two factor analysis of variance

From question one, it can be seen that the mass ratios of each product follow a normal distribution trend when CE and LS are reactants. Therefore, a bivariate analysis of variance can be performed on the data with CE and LG as reactants. As the two experiments are independent, there is no interaction between them.

This article takes a mixture ratio of 10/100 as an example, and integrates the data under this condition to obtain the following table:

Table 6: Yields of pyrolysis product under 10/100 combination

	1	2	3	4
CE	34.42	27.42	21.43	16.73
LG	18.06	15.3	58.17	8.47

Record all sample observations as x_ Ij (i=1,2, j=1,2,3,4), the average value of the overall sample is x ， The sum of squares of errors generated by row factors is SSR, the sum of squares of errors generated by column factors CE and LG is SSC, and the sum of squares of errors generated by residual factors other than row and column factors (sum of squares of random error terms) is SSE:

$$\bar{\bar{x}} = \frac{\sum_{i=1}^{2}\sum_{j=4}^{4} x_{ij}}{8} \tag{7}$$

$$SSR = \sum_{i=1}^{2}\sum_{j=4}^{4} (\bar{x}_{ig} - \bar{\bar{x}})^2 \tag{8}$$

$$SSC = \sum_{i=1}^{2}\sum_{j=4}^{4} (\bar{x}_{gj} - \bar{\bar{x}})^2 \tag{9}$$

$$SSE = \sum_{i=1}^{2}\sum_{j=4}^{4} (x_{ij} - \bar{x}_{jg} - \bar{x}_{gj} + \bar{\bar{x}})^2 \tag{10}$$

From this, the mean square error (MSR) of the travel factor, the mean square error

(MSC) of the column factor, and the mean square error (MSE) of the random error term can be calculated:

$$\mathrm{MSR} = \frac{\mathrm{SSR}}{2-1} \tag{11}$$

$$\mathrm{MSE} = \frac{\mathrm{SSC}}{4-1} \tag{12}$$

$$\mathrm{MSE} = \frac{\mathrm{SSE}}{(2-1)(4-1)} \tag{13}$$

Convert statistic F_R、F_C and the given significance level quantile F_α Relative ratio can determine whether row and column factors have a significant impact on the observed values.

$$F_R = \frac{MSR}{MSE} \sim F[2-1,(2-1)(4-1)] \tag{14}$$

$$F_c = \frac{MSC}{MSE} \sim F[4-1,(2-1)(4-1)] \tag{15}$$

After calculation, it can be concluded that $F_C > F_\alpha$, The p-value is 0.034, rejecting the original hypothesis, indicating significant differences between column vectors, i.e. CE and LG have a significant impact on the yield of pyrolysis products.

Calculate using the same method and organize the F values for each mixing ratio as follows:

Table 7: the significance of catalyst for pyrolysis products in CE/LG reaction

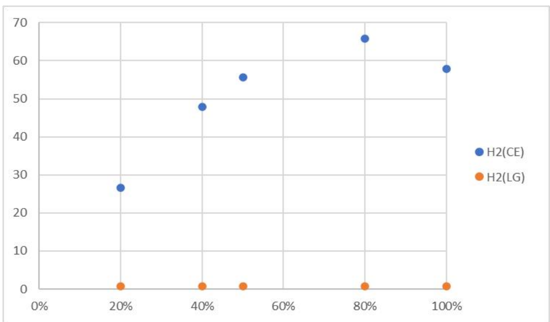
The ratio	10/100	20/100	30/100	40/100	50/100	60/100	80/100	100/100
p	0.034	0.143	0.045	0.039	0.026	0.047	0.053	0.009

From the table, it can be seen that in most mixing ratios, the difference in the mass ratio of desulfurization ash to CE and LG pyrolysis reaction products is significant, and the difference in desulfurization ash to CE and LG pyrolysis reaction is most significant when the mixing ratio is 100/100.

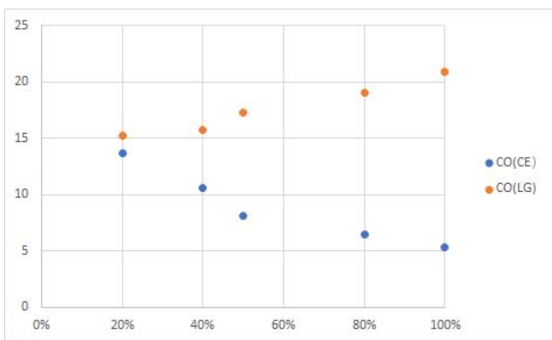
6.12 Yield of pyrolysis gas

6.12.1 Descriptive Statistical Analysis

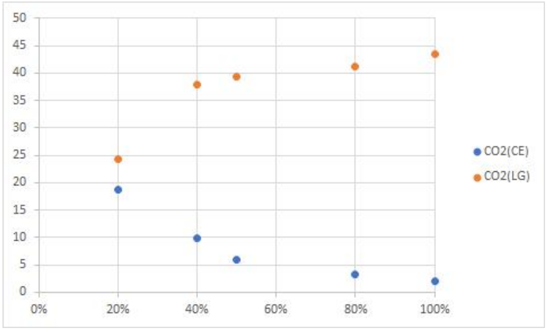
To compare the differences in CE and LG pyrolysis gases under the same desulfurization ash mixture ratio, the data was first integrated and plotted as before, to visualize the results and obtain the following figure:



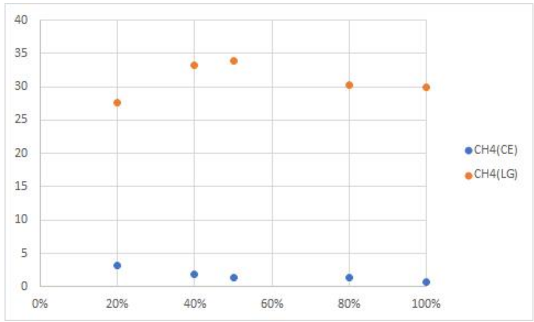
Yield of H2



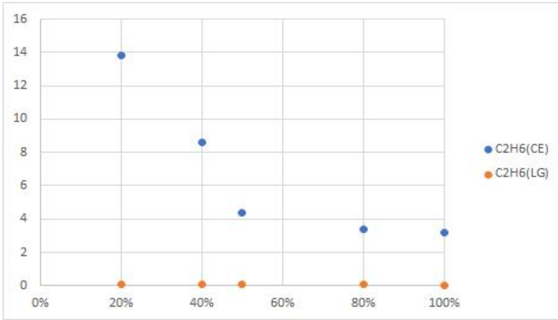
Yield of CO



Yield of CO2



Yield of CH4



Yield of C2H6

Figure 8: Yields of pyrolysis syngas in CE and LG group

6.2.2 Two-way analysis of variance

The following table can be obtained by synchronizing with the previous operation:

Table 8: the significance of catalyst for pyrolysis syngas in CE/LG reaction

The ratio	20/100	40/100	50/100	80/100	100/100
p	0.037	0.013	0.033	0.007	0.005

From the table, it can be seen that under various mixing ratios, the difference in the mass ratio of desulfurization ash to the pyrolysis reaction products of CE and LG is significant, and at a mixing ratio of 100/100, the difference in desulfurization ash to the pyrolysis reaction of CE and LG is the most significant.

7.Solution to question four

7.1 Overview of Reaction Kinetic Equations

In order to quantitatively study the pyrolysis reaction of cotton straw, this article describes the rate law in chemical reactions through mathematical formulas, establishes chemical reaction kinetics equations, and can provide reliable data for future pyrolysis reaction research through parameter adjustment.

7.2 Data organization and preprocessing

For the data in Attachment 1 and Attachment 2, outlier data cleaning and missing value testing have been carried out in Question 1. Present important products and their yields in the form of scatter plots and line plots, and conduct preliminary analysis to infer the stage at which the products are inhibited by the catalyst and the effects occur. The following figure shows the mixing ratio range when the product is inhibited, which is the turning point at which the yield begins to be inhibited or promoted

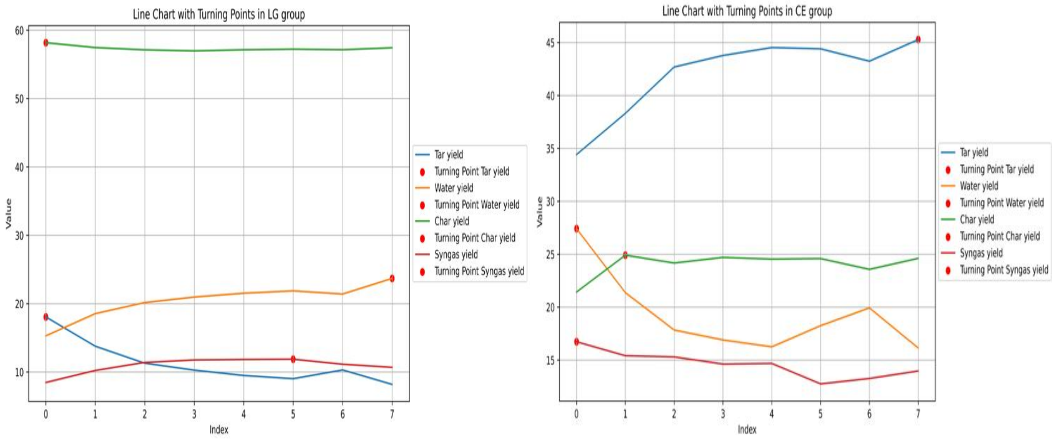


Figure 9: Yield of pyrolysis production in CE and LG group

From the graph, it can be seen that in the CE group Syngas, there was a turning point with an opening downwards in 50/100, while the remaining ones did not show a significant turning trend. The quality score of Char yield in the LG group has reached a turning point of decline.

From the figure, it can be seen that under different mixing ratios, most of the products with increased content are products, while the decrease in content can be understood as intermediate products (as shown in the flowchart) participating in the reaction process midway, serving as new reactants, thereby reducing the proportion of reactant concentration.

7.3 Study on the Mechanism of Straw Pyrolysis Reaction

This article will establish a mechanism model around three stages of straw pyrolysis reaction. The first stage is the dehydration stage. Taking the CE group as an example, at 150 degrees Celsius, straw and catalytic substances undergo dehydration reactions, which is consistent with the increase in water content. At this time, there is no obvious coking reaction or gas generation; The second stage is carbonization and gasification, during which important components of synthetic gas (such as CO, CO2, CH4) will be released, and a large amount of volatile organic compounds will also be emitted from the CE/DSA mixture, and the gas will also exist in the mixture as liquid hydrocarbons; The third stage is the coking reaction, where important products (Tar tar, Char coke) are generated. The following figure shows the flowchart of the pyrolysis reaction

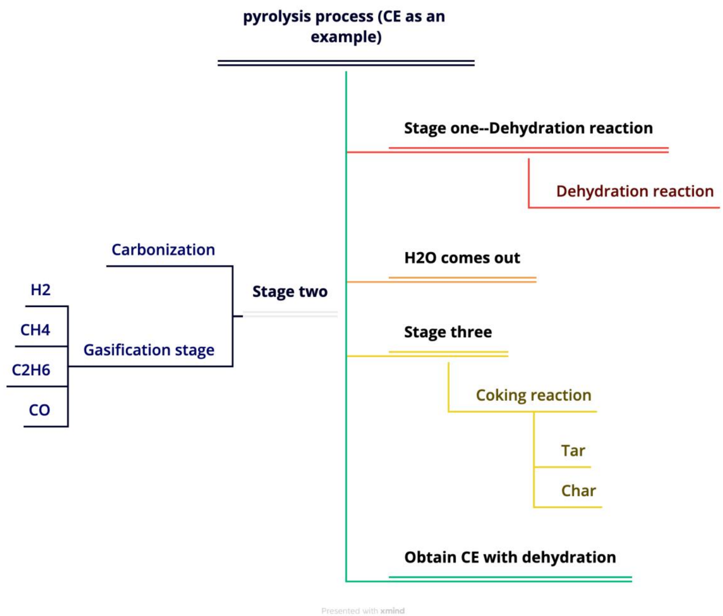


Figure 10: flow chart of question 4

7.4 Establishment and Solution of Reaction Kinetic Model

In constructing a reaction kinetics model in this article, it is first necessary to obtain the concentration and reaction time of the mixture of CE and DSA, in order to establish the relevant rate equation.
Assuming that the reaction of CE conforms to the first-order reaction kinetics model, it can be expressed as:

$$\frac{d[A]}{dt} =- k[A]$$

Among them, [A] is the concentration of reactants, k is the reaction rate coefficient.
Establish a reaction kinetics equation with exponential decline and fit it with the data provided in the appendix. Adjust the parameters and evaluate the fitting to calculate the residual value. Finally, determine whether to retain the reaction kinetics equation based on the residual value.

7.5 Fitting and Solving Reaction Kinetic Equations

7.5.1Polynomial Nonlinear Regression Model

This article uses polynomial linear regression to predict the regression equation between the mixing ratio and various mass fractions under different catalyst and CE, LG mixing ratios. Based on the regression equation, further solve to obtain the reaction kinetics equation.
The regression equation and its image are shown in the following

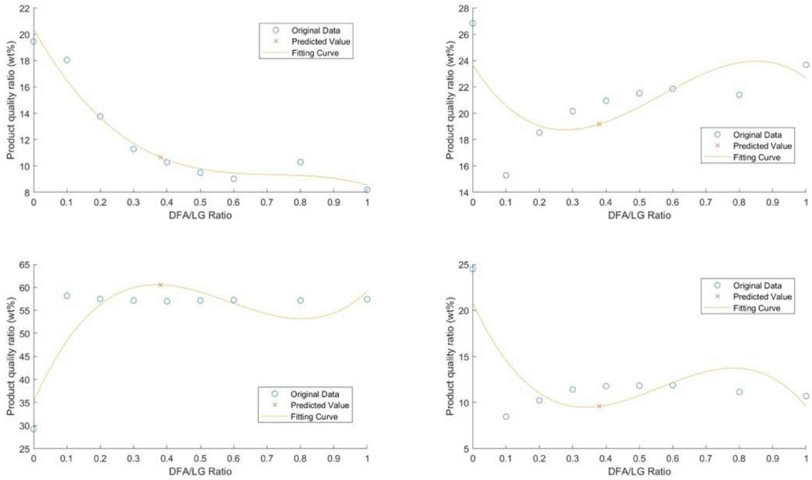


figure:

Figure 12: Quality ratio prediction function by nonlinear regression

The fitting curve results in CE are as follows:

Tar yield fitting curve: -15.9094 + 34.3544 x + -25.7899 x^2 + 19.4409x^3

Char yield fitting curve: -0.038392 + 0.80927 x + -0.08787x^2 + 29.196x^3

Syngas yield fitting curve: 19.1608 + -38.9646 x + 22.4247x^2 + 24.3258x^3

The final fitted curve equation for CE is：$e^{-1.03435323}$

The curve image is

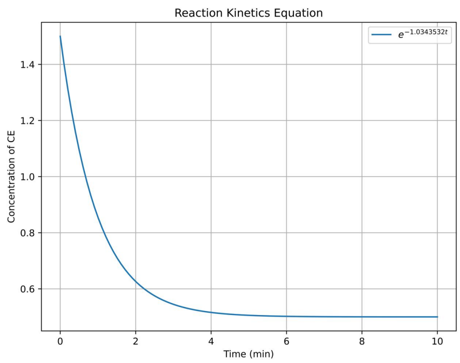


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Figure 12: Reaction kinetics equation after adjustment

8. Solution to question five

8.1 Linear regression model prediction

As can be seen from the previous text, there is a certain relationship between the mixing ratio of pyrolysis products, reactants, and catalysts. This article first predicts them using linear regression:

This article takes the pyrolysis reaction of CS as an example. If the product mass ratio is set to F and the mixing ratio is set to s, the linear relationship is:

$$F=\beta_0 + \beta_1 s + \varepsilon \tag{1}$$

among ε Is the error term.

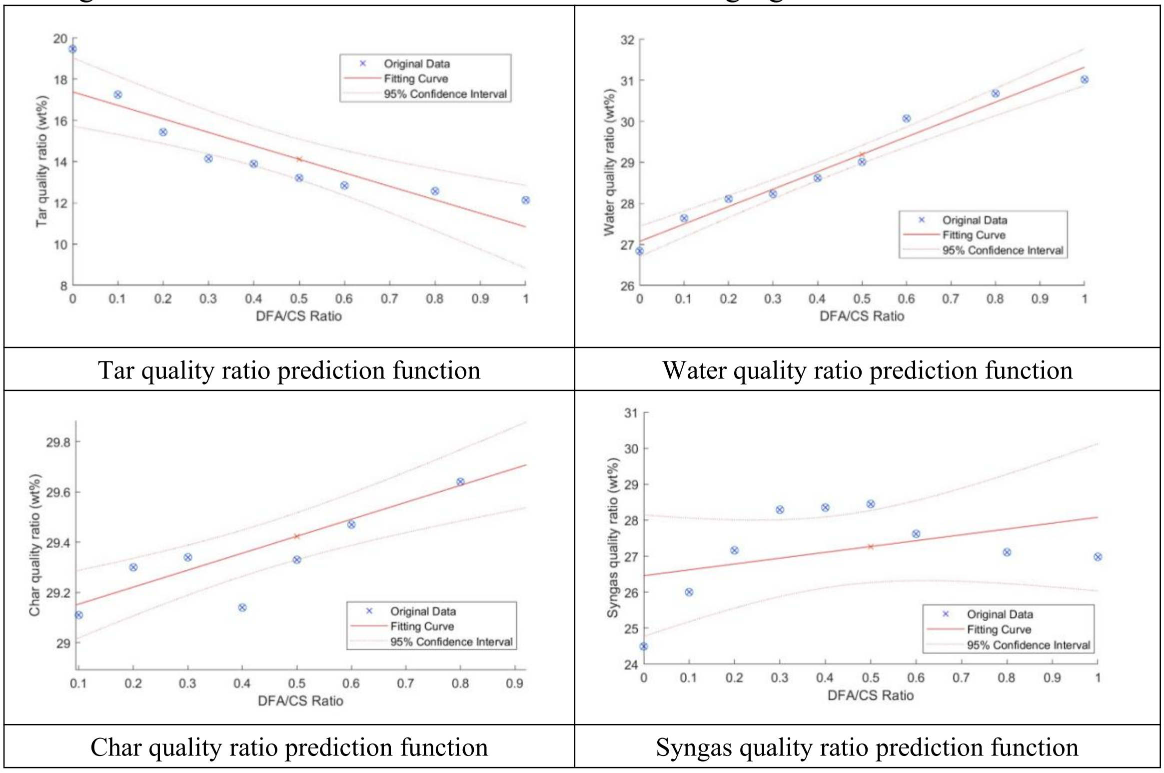
Calculate using the least squares method:

$$\beta_1 = \frac{\sum Fs - n\overline{Fs}}{\sum x^2 - n\bar{x}^2} \tag{2}$$

The final fitting curve obtained is as follows:

$$F_{Tar} = -6.5442s + 17.3825 \tag{3}$$
$$F_{Water} = 4.2465x + 27.0732 \tag{4}$$
$$F_{Char} = 0.67481x + 29.0864 \tag{5}$$
$$F_{Syngas} = 1.6229x + 26.4579 \tag{6}$$

Setting a 95% confidence interval can draw the following figure:



Tar quality ratio prediction function | Water quality ratio prediction function

Char quality ratio prediction function | Syngas quality ratio prediction function

Figure 13: Quality ratio prediction function by linear regression

From the figure, it can be seen that in linear regression, the fitting curves of Tar and Water are relatively close to the input values, but the input values of Char and Syngas show significant fluctuations in the fitting curves, and their accuracy is not significant at a 95% confidence interval. Therefore, this article speculates that the mass ratio and mixing ratio of pyrolysis reaction products exhibit a nonlinear relationship and uses nonlinear inertia to make new predictions.

8.2 Nonlinear regression model prediction

This article sets the product mass ratio to F and the mixing ratio to s. To establish a model using nonlinear regression analysis, a formula is obtained as follows:

$$F = a_0 s^n + a_1 s^{n-1} + \dots + a_{n-1} s + a_n \tag{1}$$

To obtain the coefficients and fit the curve, this article uses polynomial fitting method to estimate them. To obtain a more accurate function and avoid overfitting, this article takes CS as an example and sets the polynomial degree of fitting to 3. The final formula obtained is as follows:

$$F_{Tar} = -15.9094 + 34.3544\,x - 25.7899\,x^2 + 19.4409\,x^3 \tag{2}$$
$$F_{Water} = -3.213\,x + 3.8009x - 3.4531\,x^2 + 27.0737 \tag{3}$$

$$F_{Char} = -0.038391 + 0.80927x - 0.08787x^2 + 29.196x^3 \quad (4)$$
$$F_{Syngas} = 19.1608 - 38.9646x + 22.4247x^2 + 24.3258x^3 \quad (5)$$

To visualize the results more intuitively, this article drew a graph with a confidence interval of 0.95:

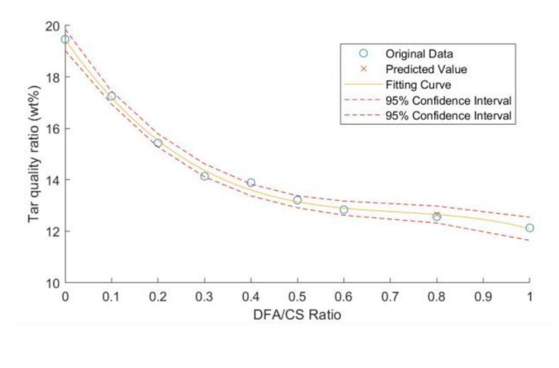
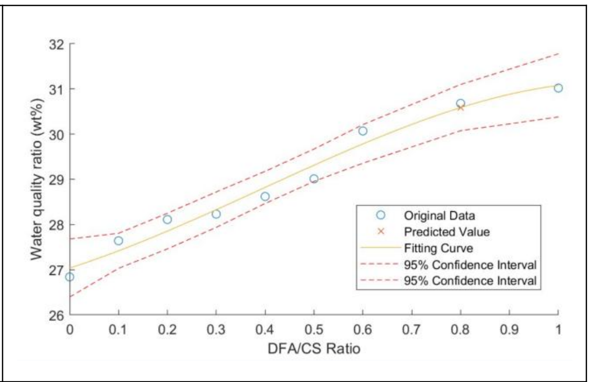
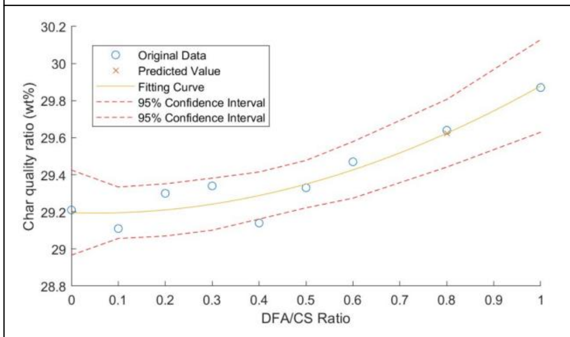
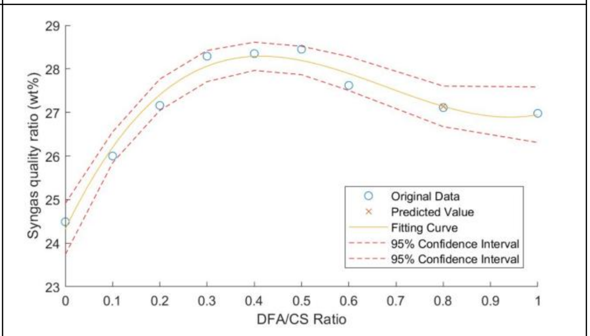
	
Tar quality ratio prediction function	Water quality ratio prediction function
	
Char quality ratio prediction function	Syngas quality ratio prediction function

Figure 14: Quality ratio prediction function by nonlinear regression

From the figure, it can be seen that the fitted prediction curve is almost identical to the training sample, with small errors, and both are within the confidence interval range. The model prediction is more accurate and can be predicted using functions.

To calculate the difference between the observed values and the model values and test the accuracy of the model, this article determines the degree of fitting by calculating its root mean square error (RMSE). The RMSE calculation formula is as follows:

$$\text{RMSE}=\sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i-\hat{y}_i)^2} \quad (6)$$

The root mean square errors of Tar, Water, Char, and Syngas are calculated to be 0.13432, 0.20806, 0.074304, and 0.1897, respectively, which are relatively small, indicating that the model fits the observed data well.

8.3 grey prediction model

To use a grey prediction model, the first step is to perform a quasi-exponential test on the data. This article takes the product Tar in CS pyrolysis reaction as an example and records the mass ratio of Tar as $x^{(0)}$ as the mixing ratio increases. Firstly, accumulate the mass ratios under each mixing ratio to obtain a sequence of r cumulative times $x^{(r)} = (x^{(r)}(1), x^{(r)}(2),\ldots,x^{(r)}(n))$, wherein:

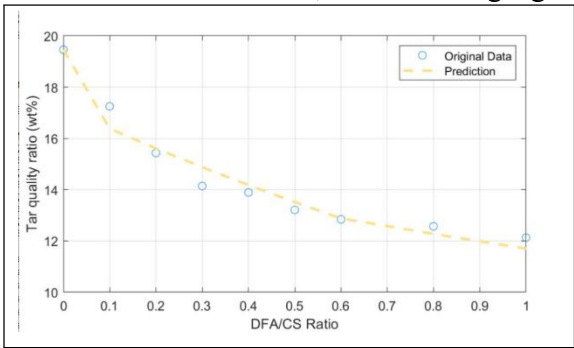
$$x^{(r)}(m) = \sum_{i=1}^{m} x^{(r-1)}(i),\ m = 1,2,\ldots,n \quad (1)$$

Define the level ratio as $\sigma(k) = \frac{x^r(k)}{x^r(k-1)}$, The smoothness ratio of the sequence can be determined based on this $\rho(k)$

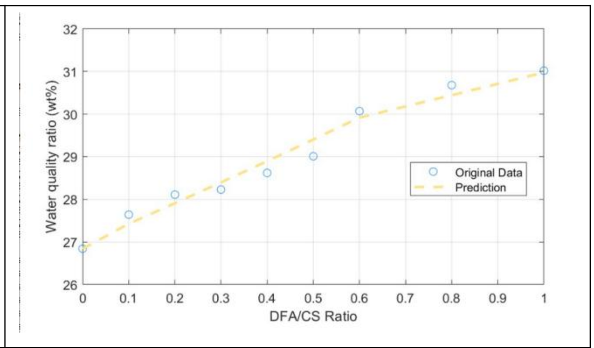
$$\rho(k) = \frac{x^{(0)}(k)}{x^{(0)}(1) + x^{(0)}(2) + \ldots + x^{(0)}(k-1)} \tag{2}$$

Since $x^{(0)}$is a non-negative sequence, as k increases, the smoothness ratio ρ (k) It will gradually approach 0, and after calculation, σ (k) ϵ (0,0.5), so the data of Tar mass ratio has a quasi-exponential law, which can be used for grey prediction.

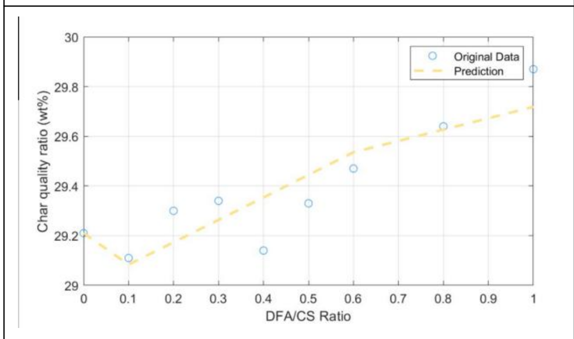
Arrange all the observed data of the pyrolysis product Tar under CS pyrolysis reaction in descending order, and obtain the set {12.13, 12.57, 12.84, 13.21, 13.89, 14.14, 15.43, 17.25, 19.46}. Calculate the difference (range) between the maximum and minimum values as 7.33, and perform a rank comparison test on them. Then, through continuous modification, the following figure can be obtained:



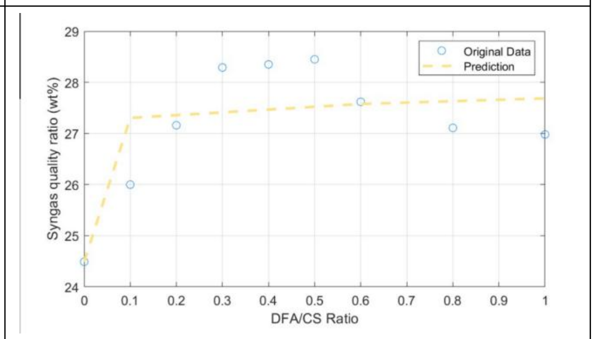
Tar quality ratio prediction function



Water quality ratio prediction function



Char quality ratio prediction function



Syngas quality ratio prediction function

Figure 15: Quality ratio prediction function by gray prediction model

Observing the graph, it can be seen that the quality of Tar and Water is more accurate than the predicted results, and similar to the nonlinear regression prediction results mentioned above. However, the fitting curves of Char and Syngas have significant differences from the original data, far less accurate than the nonlinear prediction. To improve the prediction accuracy, this article also established an AI model for prediction.

8.4 Neural network prediction

Neural network prediction can learn a certain rule through self-training without knowing the input output mapping relationship, and continuously adjust it to achieve a result close to the expected output value after reaching the given input value

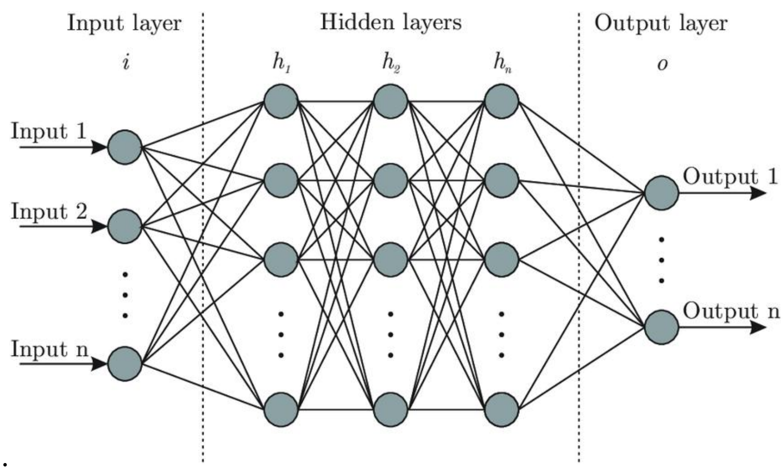


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Figure 16: Diagram of the operation of artificial Neural Network

As shown in the figure, this article adopts the "Feed Forward Neural Network" with "adaptwb" as the fitness function, and sets different mixing ratios as the input layer input vector $X =（x_1, x_2, , , x_m）$, and different product mass ratios as the output layer output vector $Y =（y_1, y_2, , , y_n）$. The number of nodes in the middle hidden layer is set to 5, and the hidden layer vector is set to $H^l = (h_1^l, h_2^l, \ldots, h_j^l, \ldots, h_{sl}^l)$ (l=1,2,...,L-1,j=1,2,..., s_l), combining them linearly or nonlinearly, And set the Input Weights between the input layer and the next layer to {2 ×1 cell}, the Layer Weights between each layer are {2 of contain 1 layer × 2 cells}, bias value is{2×1 cell}（w_{ij}^l） is the connection weight between the i-th neuron in layer l-1 and the jth neuron in layer l, and bj ^ l is the bias of the jth neuron in layer l), from which h can be obtained $h_j^l = f(net_j^l) = f(\sum_{j=1}^{s_{l-1}} w_{ij}^l + b_j^l)$, and then continuously substitute the training samples for error adjustment to achieve the ideal output.

This article takes Tar in the mixed reaction of CS and desulfurization ash as an example (see the attachment for the rest), with input vectors of (0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.8, 1), randomly generating connection weights, and randomly selecting training samples from the training set (0, 19.46), (0.1, 17.25), (0.2, 15.43), (0.3, 14.14), (0.4,13.89), (0.5, 13.21), (0.6, 12.84), (0.8, 15,57), (1, 12.13)). The function of error function E is as follows:

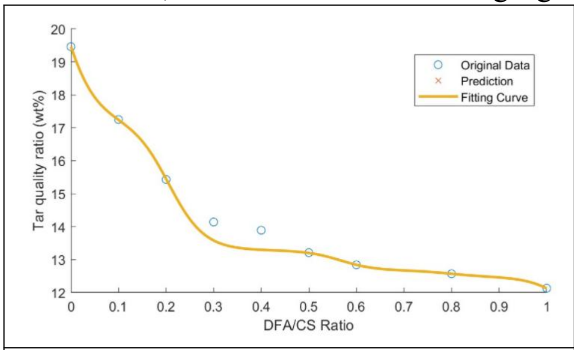
$$E = \frac{1}{2p}\sum_{i=1}^{p}\sum_{k=1}^{n}(d_k(i) - y_k(i))^2 \quad (14)$$

Subsequently, the gradient descent method is used to adjust the weight and bias based on the error, and this article sets the learning efficiency α= 0.15, calculate it using the following formula:

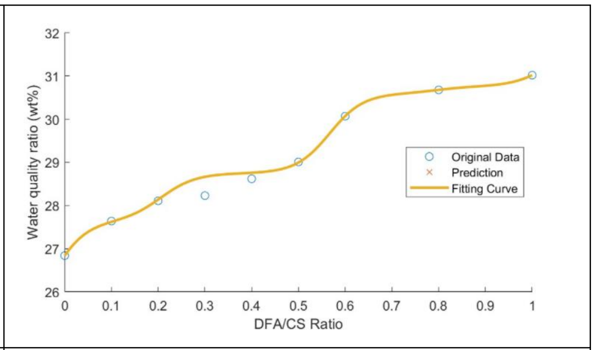
$$w_{ij}^{l} = w_{ij}^{l} - \alpha \frac{\partial E}{\partial w_{ij}^{l}} \tag{14}$$

$$b_{j}^{l} = b_{j}^{l} - \alpha \frac{\partial E}{\partial b_{j}^{l}} \tag{14}$$

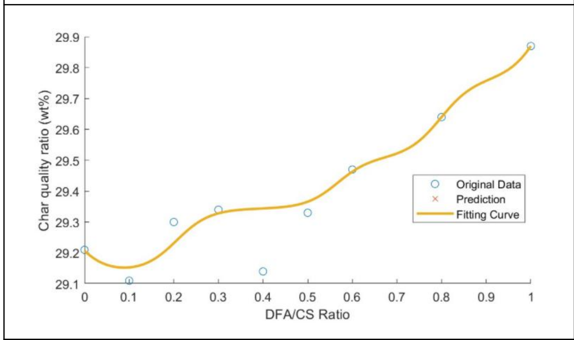
After 100 training iterations, the mean square error of the obtained model is generally less than 0.1, as shown in the following figure:



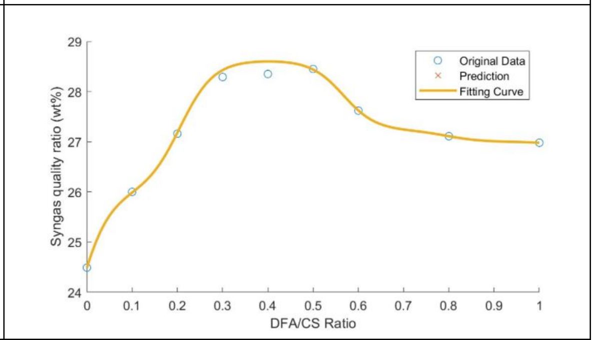
Tar quality ratio prediction function



Water quality ratio prediction function



Char quality ratio prediction function



Syngas quality ratio prediction function

Figure 17: Quality ratio prediction function by artificial neural network

Observing the graph, it can be seen that the fitted prediction curve is almost identical to the training sample, with a small error. By inputting the desired pyrolysis product ratio into the corresponding mixture ratio, a neural network can be used to predict the product mass ratio with a small error.

9. Test the Models

In addition to the previous test of the model during question answering and model establishment, this article also calculated the goodness of fit of each curve of the non-linear regression model in question 5 to further test its accuracy. This article calculates the residual sum of squares (SSR) and total sum of squares (SST) to obtain their goodness of fit. If the product mass ratio of Tar in the pyrolysis reaction with reactant CS is set to F, the specific calculation process of goodness of fit is as follows:

$$SSR = \sum_{i=1}^{n} (\widehat{F}_i - \overline{F})^2 = 47.1102 \tag{1}$$

$$SST = \sum_{i=1}^{n} (F_i - \overline{F})^2 = 47.2726 \tag{2}$$

$$R^2 = 1 - \frac{SSR}{SST} = 0.99657 \tag{3}$$

Similarly, the goodness of fit of the fitting curve for the mass ratio of each product in CS pyrolysis reaction obtained from nonlinear programming is shown in the table below:

Table 9: Goodness of fit of quality ratio prediction function by nonlinear regression

Name	Tar yield	Water yield	Char yield	Syngas yield
R^2	0.99657	0.97569	0.89769	0.97523

Based on the above analysis, our model has good goodness of fit to some extent, but there is still room for improvement. In practical applications, it is necessary to evaluate the applicability of the model based on specific circumstances and may further optimize the model to improve its performance.

10. Strengths and Weakness

10.1 Strengths

• Normal distribution tests and Pearson correlation coefficient analysis were generally conducted on the data, and the relationship between the data was not generalized but specifically analyzed for significance.

• A comprehensive descriptive statistical analysis was conducted on the data, and various charts such as scatter plots, line plots, and stacked plots were drawn to visualize the data and make it easier to observe; And data cleaning was carried out, abnormal values were detected, ensuring the quality and applicability of the data.

• This article uses various prediction methods such as linear regression, nonlinear regression, grey prediction, and neural network to continuously optimize the model from multiple perspectives to make the prediction of pyrolysis product yield more accurate.

• This article uses multiple variance tests such as relative sample T-test and multivariate analysis of variance to provide a more comprehensive and accurate analysis of the differences between data.

• When solving problems, multiple model combinations are applied to avoid the limitations of single model modeling, maximize the richness of the article, meet the needs of multiple limitations of the topic, and make the solution more substantial and complete.

10.2 Weakness

• Some of the models in this article need to be used when the data follows a normal distribution, while the normal distribution of some data is not significant and is not very suitable for individual models.

• The prediction model was not dynamically adjusted by fully considering the interrelationships between reactants, catalysts, and products in the first three questions.

11. Conclusion

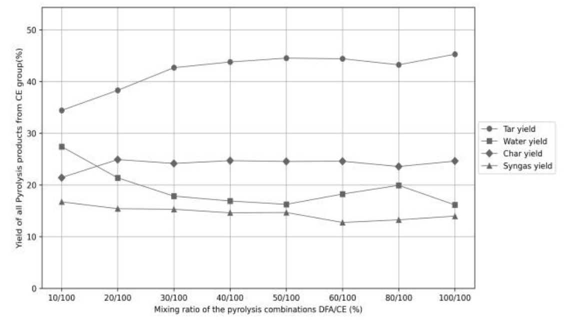
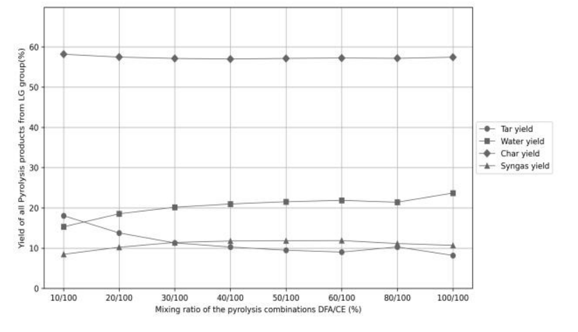
This article delves into the conversion of cotton straw biomass energy under the action of catalyst desulfurization ash, and predicts the pyrolysis products and specific pyrolysis gases under different mixing ratios of catalyst and reactants. Combining multiple sum model methods, it has significant practical significance and can be attempted in the practical application of cotton straw pyrolysis reaction.

References

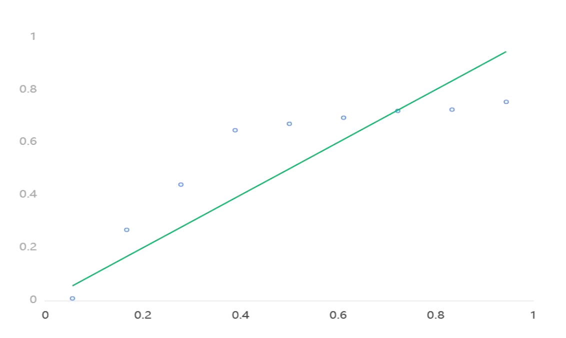
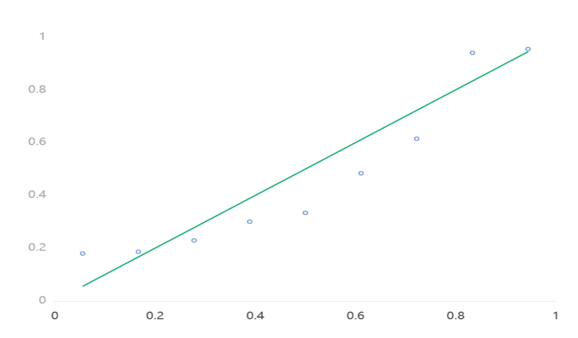
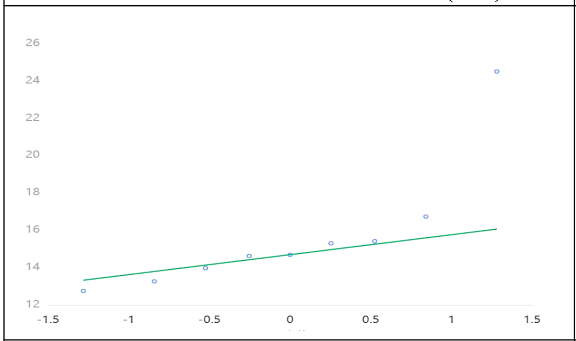
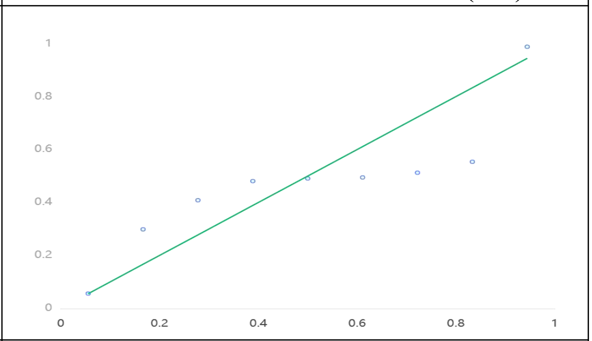
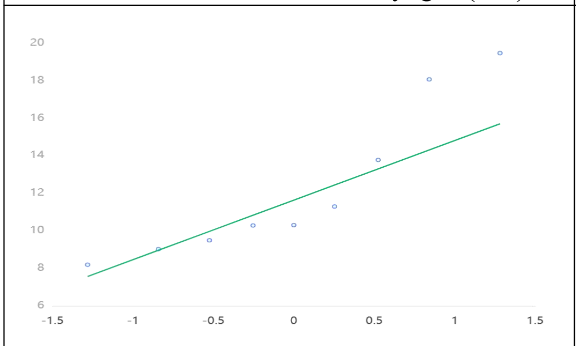
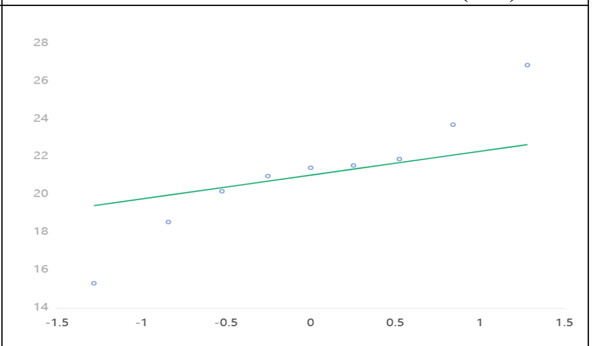
[1] Kataria, G. and Sharma, A. (2022) Materialstoday *A system level analysis of pyrolysis of cotton stalk biomass*: pp.1528-1532
[2] Qi Du (Ed.) (2023) Study on biomass pyrolysis gas extraction by desulfurization ash based on model compound
[3] Scientific Platform Serving for Statistics Professional [onnline].
[4] Weichao Xu (2012) Review of the correlation coefficient studies

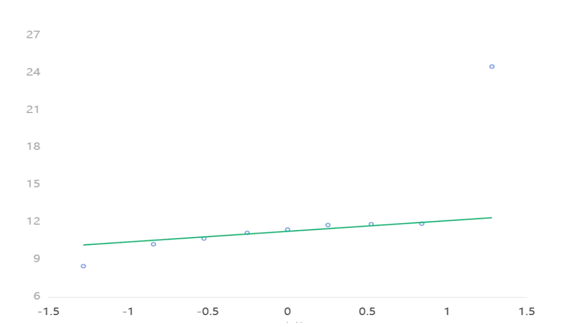
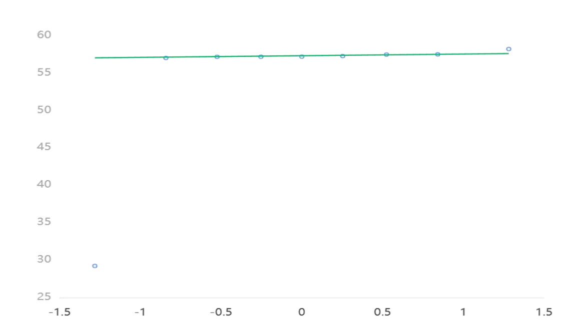
Appendix

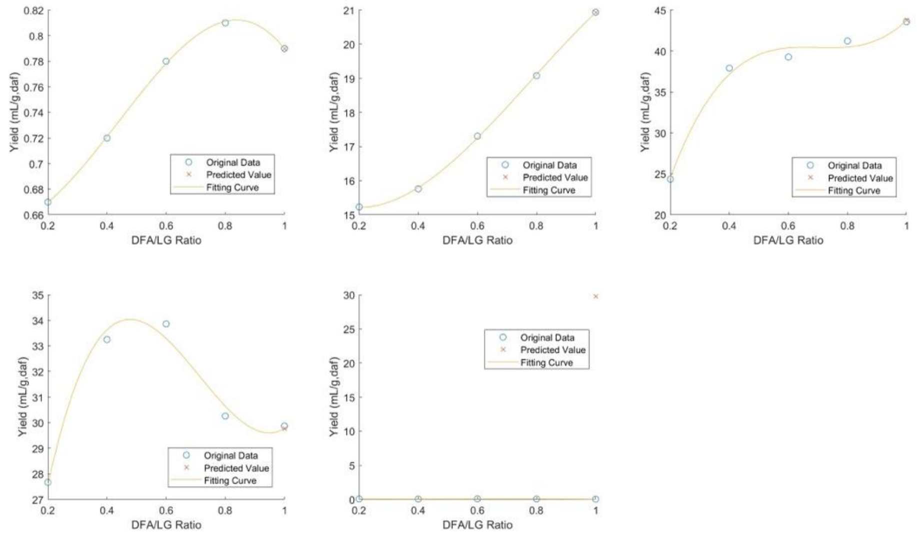
Question 1

	
Normal distribution test of Tar (CE)	Normal distribution test of Water (CE)

Quantile Quantile Plot of pyrolysis products

	
Normal distribution test of Tar (CE)	Normal distribution test of Water (CE)
	
Normal distribution test of Syngas (CE)	Normal distribution test of Char (CE)
	
Normal distribution test of Tar (LG)	Normal distribution test of Water (LG)

	
Normal distribution test of Syngas (LG)	Normal distribution test of Char (LG)



5.1.2 Analysis using CE as reactant

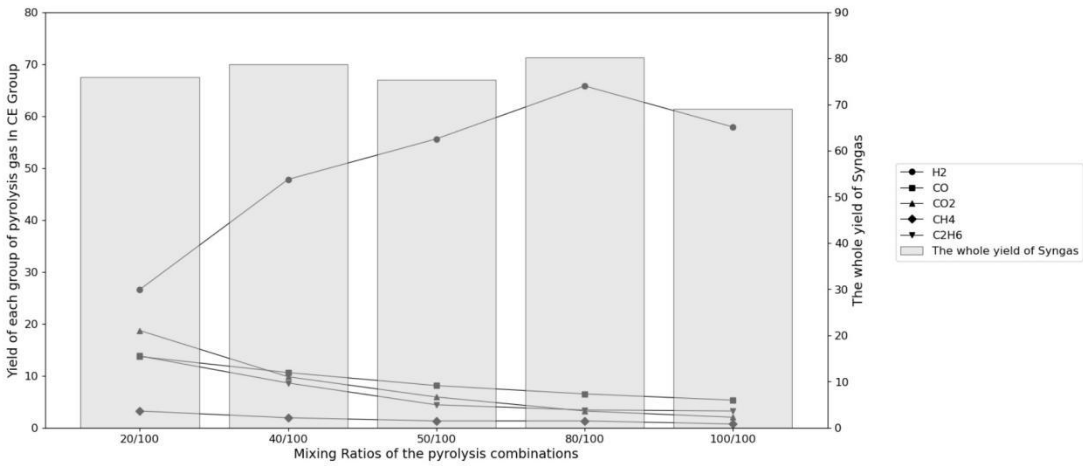


Figure 7: Total mass and respective yield of the gas in CE group

From the graph, it can be seen that the components of the pyrolysis gas are H2, CO, CO2, CH4, and C2H6. As the mixing ratio of desulfurization ash increases, CO, CO2, CH4, and C2H6 all show a significant downward trend. Therefore, it can be inferred that the catalyst has an inhibitory effect on the generation of CO, CO2, CH4, and

C2H6. On the contrary, the production of H2 shows a trend of first increasing and then decreasing with the increase of desulfurization ash mixing ratio, and the maximum value of the channel is reached at a mixing ratio of 80/100, The yield is 2.47 times that of a mixture ratio of 20/100. Unlike the reaction when desulfurization ash is mixed with CS, the total production of pyrolysis gas shows a fluctuating trend and is not stable when desulfurization ash is mixed with CE.

Similarly, this article also drew a stack diagram of the gas generation amounts, and the results are as
follows:

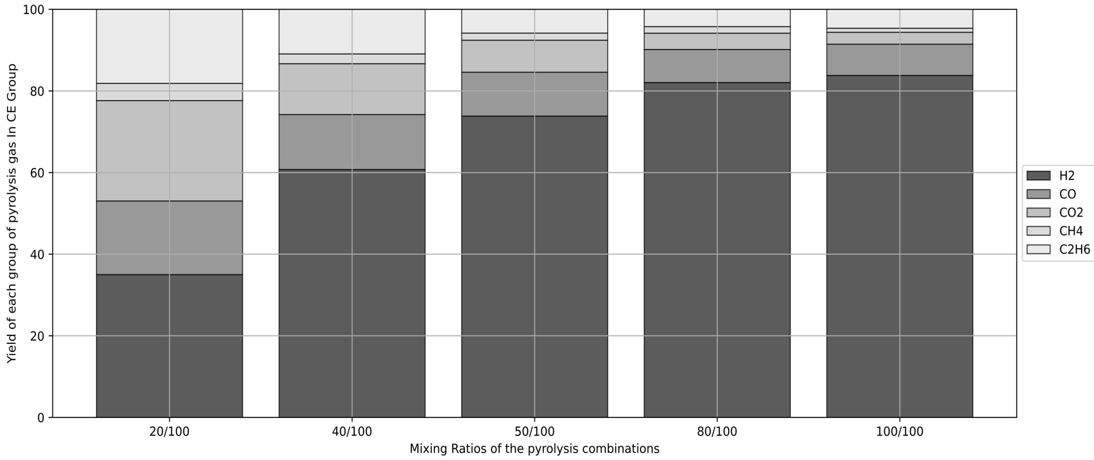


Figure 8: Mass percentage of each gas in CE group

From the graph, it can be seen more intuitively that when the reactant is a mixture of CE and desulfurization ash, the trend of the proportion of H2 in the generated gas is almost the same as that of CS, both of which significantly increase with the increase of catalyst mixing ratio. The proportion of CO, CO2, and C2H6 all decrease, and the decrease of CO2 and C2H6 is very significant, while the proportion of CH4 remains relatively small.

Summary: Desulfurization ash has a significant catalytic effect on CE pyrolysis, significantly changing the production and proportion of different gases in the pyrolysis gas. Its specific manifestation is a significant increase in H2 production, while the production of CO, CO2, and C2H6 is inhibited to a certain extent.**5.1.3 以 LG 为反应物的分析**

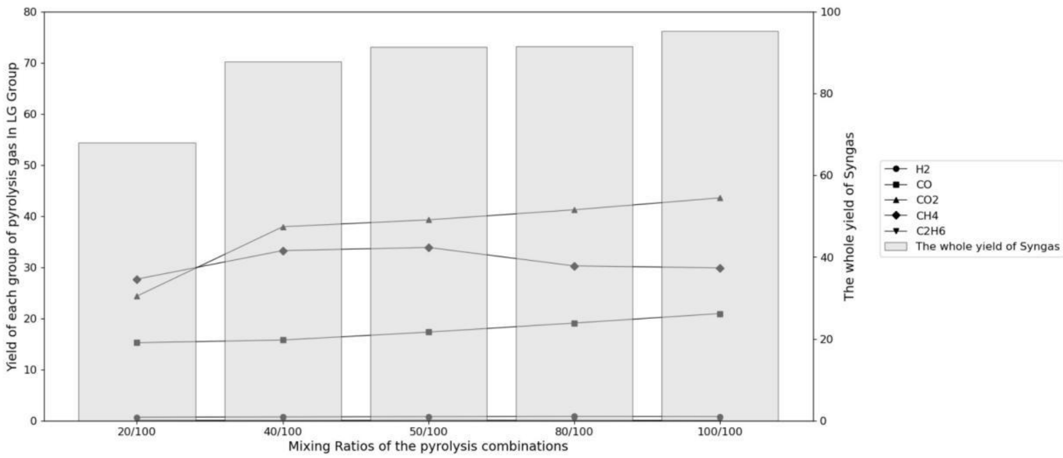


Figure 9: Total mass and respective yield of the gas in LG group

From the graph, it can be seen that the composition of the pyrolysis gas is H2, CO, CO2, CH4, and C2H6, and the change in gas production with the increase of desulfurization ash is relatively small compared to the previous two experiments. CO2 and CO show a slight upward trend with the increase of mixing ratio, with CO2 production increasing significantly at the initial stage, while CO production fluctuates slightly when the mixing ratio is high. It can be inferred that the catalyst has a promoting effect on its production; The production of C2H6 and H2 is extremely small, and the effect of catalysts on them is almost invisible; The production of CH4 first increases and then decreases with the increase of desulfurization ash, indicating that the catalyst has a promoting effect on it within a certain range and a inhibiting effect within a certain range.

Similarly, this article also drew a stack diagram of the gas generation amounts, and the results are as
follows:

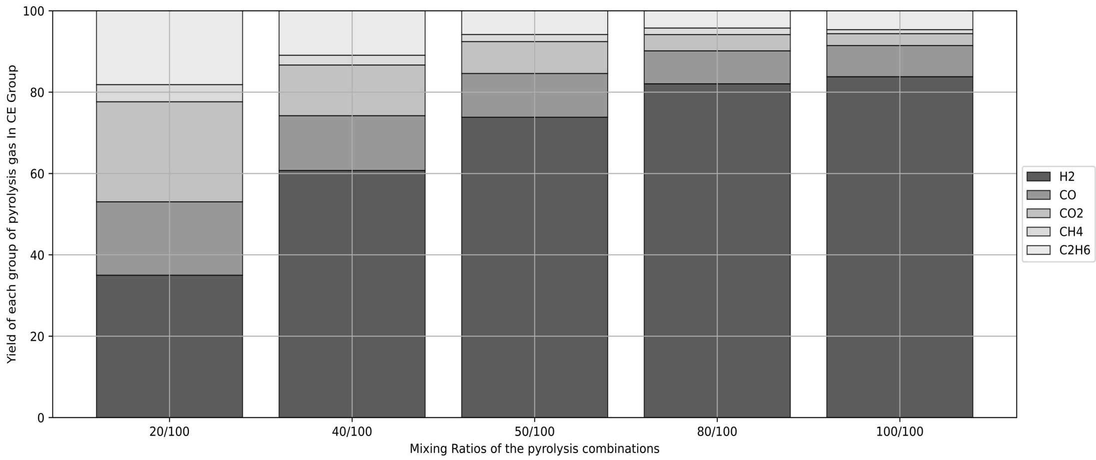


Figure 10: Mass percentage of each gas in LG group

From the graph, it can be seen more intuitively that when the reactant is a mixture of LG and desulfurization ash, the proportion of H2 in the generated gas remains almost constant and always small, while C2H6 is so small that it cannot be observed. CO, CO2, and CH4 have small fluctuations in different trends.

附录
线性回归代码

```
% 读取 Excel 文件
data = xlsread('draft_1.xlsx');

% 提取数据
ratio = data(:, 1);
Tar_yield = data(:, 2);
Water_yield = data(:, 3);
Char_yield = data(:, 4);
Syngas_yield = data(:, 5);
```

```
% 输入 ratio
user_ratio = inputdlg('请输入 0 到 1 之间的数代表 ratio: ', '输入', 1);
user_ratio = str2double(user_ratio);

% 选择模型类型，这里选择线性回归模型
model_Tar = fitlm(ratio, Tar_yield);
model_Water = fitlm(ratio, Water_yield);
model_Char = fitlm(ratio, Char_yield);
model_Syngas = fitlm(ratio, Syngas_yield);

% 展示预测值
disp(['输入的 ratio 值: ', num2str(user_ratio)]);
disp(['Tar yield 预测值: ', num2str(predict(model_Tar, user_ratio))]);
disp(['Water yield 预测值: ', num2str(predict(model_Water, user_ratio))]);
disp(['Char yield 预测值: ', num2str(predict(model_Char, user_ratio))]);
disp(['Syngas yield 预测值: ', num2str(predict(model_Syngas, user_ratio))]);

% 画图
figure;

subplot(2, 2, 1);
scatter(ratio, Tar_yield, 'o', 'DisplayName', 'Original Data');
hold on;
scatter(user_ratio, predict(model_Tar, user_ratio), 'x', 'DisplayName',
'Predicted Value');
h = plot(model_Tar, 'DisplayName', 'Fitted Curve');
xlabel('DFA/CS Ratio');
ylabel('Product quality ratio (wt%)');

subplot(2, 2, 2);
scatter(ratio, Water_yield, 'o', 'DisplayName', 'Original Data');
hold on;
scatter(user_ratio, predict(model_Water, user_ratio), 'x', 'DisplayName',
'Predicted Value');
plot(model_Water);
xlabel('DFA/CS Ratio');
ylabel('Product quality ratio (wt%)');
legend('Location', 'best');

subplot(2, 2, 3);
scatter(ratio, Char_yield, 'o', 'DisplayName', 'Original Data');
hold on;
scatter(user_ratio, predict(model_Char, user_ratio), 'x', 'DisplayName',
```

```
'Predicted Value');
plot(model_Char);
xlabel('DFA/CS Ratio');
ylabel('Product quality ratio (wt%)');
legend('Location', 'best');

subplot(2, 2, 4);
scatter(ratio, Syngas_yield, 'o', 'DisplayName', 'Original Data');
hold on;
scatter(user_ratio, predict(model_Syngas, user_ratio), 'x', 'DisplayName',
'Predicted Value');
plot(model_Syngas);
xlabel('DFA/CS Ratio');
ylabel('Product quality ratio (wt%)');
legend('Location', 'best');

% 展示拟合曲线的函数表达式
disp(['Tar yield 拟合曲线: ', num2str(model_Tar.Coefficients.Estimate(2)), ' *
x + ', num2str(model_Tar.Coefficients.Estimate(1))]);
disp(['Water yield 拟合曲线: ',
num2str(model_Water.Coefficients.Estimate(2)), ' * x + ',
num2str(model_Water.Coefficients.Estimate(1))]);
disp(['Char yield 拟合曲线: ', num2str(model_Char.Coefficients.Estimate(2)), '
* x + ', num2str(model_Char.Coefficients.Estimate(1))]);
disp(['Syngas yield 拟合曲线: ',
num2str(model_Syngas.Coefficients.Estimate(2)), ' * x + ',
num2str(model_Syngas.Coefficients.Estimate(1))]);

% 计算模型准确度
Tar_rmse = sqrt(mean((Tar_yield - predict(model_Tar, ratio)).^2));
Water_rmse = sqrt(mean((Water_yield - predict(model_Water, ratio)).^2));
Char_rmse = sqrt(mean((Char_yield - predict(model_Char, ratio)).^2));
Syngas_rmse = sqrt(mean((Syngas_yield - predict(model_Syngas, ratio)).^2));

disp(['Tar yield 模型准确度 (RMSE): ', num2str(Tar_rmse)]);
disp(['Water yield 模型准确度 (RMSE): ', num2str(Water_rmse)]);
disp(['Char yield 模型准确度 (RMSE): ', num2str(Char_rmse)]);
disp(['Syngas yield 模型准确度 (RMSE): ', num2str(Syngas_rmse)]);
% 计算 SSR 和 SST
SSR_Tar = sum((predict(model_Tar, ratio) - mean(Tar_yield)).^2);
SSR_Water = sum((predict(model_Water, ratio) - mean(Water_yield)).^2);
SSR_Char = sum((predict(model_Char, ratio) - mean(Char_yield)).^2);
SSR_Syngas = sum((predict(model_Syngas, ratio) - mean(Syngas_yield)).^2);
```

```
SST_Tar = sum((Tar_yield - mean(Tar_yield)).^2);
SST_Water = sum((Water_yield - mean(Water_yield)).^2);
SST_Char = sum((Char_yield - mean(Char_yield)).^2);
SST_Syngas = sum((Syngas_yield - mean(Syngas_yield)).^2);

% 计算拟合优度
R_squared_Tar = SSR_Tar / SST_Tar;
R_squared_Water = SSR_Water / SST_Water;
R_squared_Char = SSR_Char / SST_Char;
R_squared_Syngas = SSR_Syngas / SST_Syngas;

disp(['Tar yield 拟合优度 (R-squared): ', num2str(R_squared_Tar)]);
disp(['Water yield 拟合优度 (R-squared): ', num2str(R_squared_Water)]);
disp(['Char yield 拟合优度 (R-squared): ', num2str(R_squared_Char)]);
disp(['Syngas yield 拟合优度 (R-squared): ', num2str(R_squared_Syngas)]);
```

附录

灰色预测代码

```
clear;clc

% 读取 Excel 文件
data = xlsread('draft_1.xlsx');

for o = 2:5

% 提取数据
ratio = data(:, 1);
A1 = data(:, o);


% 原始数据长度
n1=length(A1);


% 原始数据累加
B1=cumsum(A1);


% 数列 B 做紧邻均值生成
for i = 2:n1
C1(i) = (B1(i)+B1(i-1))/2;
end
C1(1)=[];
```

```
%建立符号变量 a(发展系数)和 b(灰作用量)
syms a1 b1;
c1 = [a1 b1]';

%构造数据矩阵
B1 = [-C1;ones(1,n1-1)];
Y1 = A1; Y1(1) = [];

%使用最小二乘法计算参数 a(发展系数)和 b(灰作用量)
c1 = inv(B1*B1')*B1*Y1;
c1 = c1';
a1 = c1(1); b1 = c1(2);



%预测后续数据
F1 = []; F1(1) = A1(1);
for i = 2:(n1)
    F1(i) = (A1(1)-b1/a1)/exp(a1*(i-1))+ b1/a1  ;
end

%对数列 F 累减还原,得到预测出的数据
G1 = []; G1(1) = A1(1);
for i = 2:(n1)
    G1(i) = F1(i) - F1(i-1); %得到预测出来的数据
end

%绘制曲线图
subplot(2,2,o-1)

t1 = [0,0.1,0.2,0.3,0.4,0.5,0.6,0.8,1];
t2 = [0,0.1,0.2,0.3,0.4,0.5,0.6,0.8,1];

plot(t1, A1,'o','Color',[0.12 0.56 1]); hold on;
plot(t2, G1, '--','Color',[1 0.89 0.52],'linewidth',2);
xlabel('DFA/CS Ratio'); ylabel('Product quality ratio (wt%)');
legend('Original Data','Prediction');

grid on;

%模型检验
```

```
H1 = G1(1:9);
%计算残差序列
epsilon = A1 - H1;

%法一：相对残差Q检验
%计算相对误差序列
delta1 = abs(epsilon./A1);
%计算相对误差Q
disp('相对残差Q检验：')
Q1 = mean(delta1)

end
```

附录
非线性回归代码

```
% 读取 Excel 文件
data = xlsread('draft_1.xlsx');

% 提取数据
ratio = data(:, 1);
Tar_yield = data(:, 2);
Water_yield = data(:, 3);
Char_yield = data(:, 4);
Syngas_yield = data(:, 5);

% 输入 ratio
user_ratio = inputdlg('请输入0到1之间的数代表ratio：', '输入', 1);
user_ratio = str2double(user_ratio);

% 高阶多项式拟合
degree = 3; % 可以尝试不同的多项式次数
model_Tar = fitnlm(ratio, Tar_yield, @(p, x) polyval(p, x), zeros(1, degree+1));
model_Water = fitnlm(ratio, Water_yield, @(p, x) polyval(p, x), zeros(1,
degree+1));
model_Char = fitnlm(ratio, Char_yield, @(p, x) polyval(p, x), zeros(1,
degree+1));
model_Syngas = fitnlm(ratio, Syngas_yield, @(p, x) polyval(p, x), zeros(1,
degree+1));

% 展示预测值
disp(['输入的ratio值：', num2str(user_ratio)]);
disp(['Tar yield 预测值：', num2str(predict(model_Tar, user_ratio))]);
disp(['Water yield 预测值：', num2str(predict(model_Water, user_ratio))]);
```

```
disp(['Char yield 预测值: ', num2str(predict(model_Char, user_ratio))]);
disp(['Syngas yield 预测值: ', num2str(predict(model_Syngas, user_ratio))]);

% 画图
figure;

subplot(2, 2, 1);
scatter(ratio, Tar_yield, 'o', 'DisplayName', 'Original Data');
hold on;
scatter(user_ratio, predict(model_Tar, user_ratio), 'x', 'DisplayName',
'Predicted Value');
fplot(@(x) polyval(model_Tar.Coefficients.Estimate, x), [min(ratio),
max(ratio)]);
legend('Location', 'best');
xlabel('DFA/CS Ratio');
ylabel('Product quality ratio (wt%)');

subplot(2, 2, 2);
scatter(ratio, Water_yield, 'o', 'DisplayName', 'Original Data');
hold on;
scatter(user_ratio, predict(model_Water, user_ratio), 'x', 'DisplayName',
'Predicted Value');
fplot(@(x) polyval(model_Water.Coefficients.Estimate, x), [min(ratio),
max(ratio)]);

legend('Location', 'best');
xlabel('DFA/CS Ratio');
ylabel('Product quality ratio (wt%)');

subplot(2, 2, 3);
scatter(ratio, Char_yield, 'o', 'DisplayName', 'Original Data');
hold on;
scatter(user_ratio, predict(model_Char, user_ratio), 'x', 'DisplayName',
'Predicted Value');
fplot(@(x) polyval(model_Char.Coefficients.Estimate, x), [min(ratio),
max(ratio)]);

legend('Location', 'best');
xlabel('DFA/CS Ratio');
ylabel('Product quality ratio (wt%)');

subplot(2, 2, 4);
scatter(ratio, Syngas_yield, 'o', 'DisplayName', 'Original Data');
hold on;
```

```
scatter(user_ratio, predict(model_Syngas, user_ratio), 'x', 'DisplayName',
'Predicted Value');
fplot(@(x) polyval(model_Syngas.Coefficients.Estimate, x), [min(ratio),
max(ratio)]);

legend('Location', 'best');
xlabel('DFA/CS Ratio');
ylabel('Product quality ratio (wt%)');

% 展示拟合曲线的函数表达式
disp(['Tar yield 拟合曲线: ', num2str(model_Tar.Coefficients.Estimate(1)), ' +
', ...
    num2str(model_Tar.Coefficients.Estimate(2)), ' * x + ', ...
    num2str(model_Tar.Coefficients.Estimate(3)), ' * x^2 + ', ...
    num2str(model_Tar.Coefficients.Estimate(4)), ' * x^3']);
disp(['Water yield 拟合曲线: ',
num2str(model_Water.Coefficients.Estimate(1)), ' + ', ...
    num2str(model_Water.Coefficients.Estimate(2)), ' * x + ', ...
    num2str(model_Water.Coefficients.Estimate(3)), ' * x^2 + ', ...
    num2str(model_Water.Coefficients.Estimate(4)), ' * x^3']);
disp(['Char yield 拟合曲线: ', num2str(model_Char.Coefficients.Estimate(1)), '
+ ', ...
    num2str(model_Char.Coefficients.Estimate(2)), ' * x + ', ...
    num2str(model_Char.Coefficients.Estimate(3)), ' * x^2 + ', ...
    num2str(model_Char.Coefficients.Estimate(4)), ' * x^3']);
disp(['Syngas yield 拟合曲线: ',
num2str(model_Syngas.Coefficients.Estimate(1)), ' + ', ...
    num2str(model_Syngas.Coefficients.Estimate(2)), ' * x + ', ...
    num2str(model_Syngas.Coefficients.Estimate(3)), ' * x^2 + ', ...
    num2str(model_Syngas.Coefficients.Estimate(4)), ' * x^3']);

% 计算模型准确度
Tar_rmse = sqrt(mean((Tar_yield - predict(model_Tar, ratio)).^2));
Water_rmse = sqrt(mean((Water_yield - predict(model_Water, ratio)).^2));
Char_rmse = sqrt(mean((Char_yield - predict(model_Char, ratio)).^2));
Syngas_rmse = sqrt(mean((Syngas_yield - predict(model_Syngas, ratio)).^2));

disp(['Tar yield 模型准确度 (RMSE): ', num2str(Tar_rmse)]);
disp(['Water yield 模型准确度 (RMSE): ', num2str(Water_rmse)]);
disp(['Char yield 模型准确度 (RMSE): ', num2str(Char_rmse)]);
disp(['Syngas yield 模型准确度 (RMSE): ', num2str(Syngas_rmse)]);
% ... (Previous code remains unchanged)

% 计算模型准确度
```

```
Tar_rmse = sqrt(mean((Tar_yield - predict(model_Tar, ratio)).^2));
Water_rmse = sqrt(mean((Water_yield - predict(model_Water, ratio)).^2));
Char_rmse = sqrt(mean((Char_yield - predict(model_Char, ratio)).^2));
Syngas_rmse = sqrt(mean((Syngas_yield - predict(model_Syngas, ratio)).^2));

disp(['Tar yield 模型准确度 (RMSE): ', num2str(Tar_rmse)]);
disp(['Water yield 模型准确度 (RMSE): ', num2str(Water_rmse)]);
disp(['Char yield 模型准确度 (RMSE): ', num2str(Char_rmse)]);
disp(['Syngas yield 模型准确度 (RMSE): ', num2str(Syngas_rmse)]);

% 计算 SSR 和 SST
SSR_Tar = sum((predict(model_Tar, ratio) - mean(Tar_yield)).^2);
SSR_Water = sum((predict(model_Water, ratio) - mean(Water_yield)).^2);
SSR_Char = sum((predict(model_Char, ratio) - mean(Char_yield)).^2);
SSR_Syngas = sum((predict(model_Syngas, ratio) - mean(Syngas_yield)).^2);

SST_Tar = sum((Tar_yield - mean(Tar_yield)).^2);
SST_Water = sum((Water_yield - mean(Water_yield)).^2);
SST_Char = sum((Char_yield - mean(Char_yield)).^2);
SST_Syngas = sum((Syngas_yield - mean(Syngas_yield)).^2);

disp(['Tar yield SSR: ', num2str(SSR_Tar)]);
disp(['Tar yield SST: ', num2str(SST_Tar)]);
disp(['Water yield SSR: ', num2str(SSR_Water)]);
disp(['Water yield SST: ', num2str(SST_Water)]);
disp(['Char yield SSR: ', num2str(SSR_Char)]);
disp(['Char yield SST: ', num2str(SST_Char)]);
disp(['Syngas yield SSR: ', num2str(SSR_Syngas)]);
disp(['Syngas yield SST: ', num2str(SST_Syngas)]);

% 显示拟合优度
disp(['Tar yield 拟合优度 (R-squared): ', num2str(SSR_Tar / SST_Tar)]);
disp(['Water yield 拟合优度 (R-squared): ', num2str(SSR_Water / SST_Water)]);
disp(['Char yield 拟合优度 (R-squared): ', num2str(SSR_Char / SST_Char)]);
disp(['Syngas yield 拟合优度 (R-squared): ', num2str(SSR_Syngas /
SST_Syngas)]);
```

附录

神经网络预测代码

```
clear;clc
% 读取 Excel 文件
data = xlsread('draft_1.xlsx');

% 提取输入和输出数据
input_data = data(:, 1);  % 输入数据，即 ratio
output_data = data(:, 2:5);  % 输出数据，四个产物的产量质量比

% 创建并训练神经网络模型
input_layer_size = size(input_data, 2);  % 或者直接指定为 1，取决于你的实际情况
hidden_layer_size = 5;  % 隐藏层节点数
output_layer_size = 4;  % 输出层节点数

% 构建神经网络模型
net = feedforwardnet(hidden_layer_size);

% 设置训练参数
net.trainParam.epochs = 100;  % 设置训练迭代次数
net.trainParam.lr = 0.15;  % 设置学习率

% 训练神经网络
net = train(net, input_data', output_data');

% 1. 输入对话框，获取用户输入的 ratio
ratio_input = inputdlg('请输入 ratio（0 到 1 之间的数）：', '输入', 1, {'0.5'});
ratio_input = str2double(ratio_input);

% 用神经网络模型进行预测
predicted_output = net(ratio_input);

% 显示预测结果
disp('预测值：');
disp(predicted_output');
disp(['输入的 ratio 值：', num2str(ratio_input)]);

% 2. 画出四个图，标出原数据点和神经网络模型拟合曲线
figure;

for i = 1:4
    subplot(2, 2, i);
    scatter(input_data, output_data(:, i), 'o', 'DisplayName', 'Original
Data');
```

```
    hold on;
    scatter(ratio_input, predicted_output(i), 'x', 'DisplayName',
'Prediction');

    % 画出拟合曲线
    x_vals = linspace(min(input_data), max(input_data), 100);
    y_vals = net(x_vals);
    plot(x_vals, y_vals(i, :), 'LineWidth', 2, 'DisplayName', 'Fitting Curve');


    xlabel('DFA/CS Ratio');
    ylabel('Product quality ratio (wt%)');
    legend;
end

% 3. 显示拟合曲线的函数
disp('拟合曲线的函数：');
disp(net);

% 4. 检验模型准确度
performance = perform(net, output_data', net(input_data'));
disp(['均方误差：', num2str(performance)]);
disp(net(input_data'))
```