Problem Chosen	2023 ShuWei Cup Summary Sheet	Team Control Number
B		2023081819323

Abstract

With the increasing global demand for renewable energy, cotton stalk, as an important biomass resource, has attracted much attention recently. Based on the data of pyrolysis products and pyrolysis gas products under different catalytic pyrolysis reactions, the effective utilization and sustainable development of cotton stalk are studied in this paper.

Data preprocessing. For the data given by the question, firstly, the scatterplot is drawn to roughly analyze the given data set. Then using the data set to draw q-q graph and carry out Shapiro-Wilk test, the data set given by the question is judged to obey the normal distribution.

For the first problem, in order to analyze the relationship between the yield of pyrolysis products of each pyrolysis combination and the mixture ratio of the corresponding pyrolysis combination. Firstly, the line graphs of thermal valence products under different mixing ratios are drawn and discussed. Then we introduced person correlation analysis to conduct correlation analysis on the yields of different products under different mixing ratios. For example, the correlation coefficient between tar yield and DFA/CS ratio was -0.8827, which showed a strong negative correlation. Then polynomial regression fitting was carried out, and the scatter plot trend was fitted by using second-order polynomial curve. Finally, the relationship between pyrolysis products and mixing ratio was judged by functional relationship. In order to verify the importance of desulfurization ash as catalyst, the reaction results were compared separately under the condition of desulfurization ash as catalyst.

For the second problem, the line diagram of each of the three pyrolysis combinations was drawn by matlab, and the function relationship was obtained by using the second-order polynomial curve fitting method of the first problem. The image and function relationship were used for discussion and analysis, and the change process under different mixing ratios was explained, and the different results of each group of pyrolysis gases were explained. For example, we can find that the yield of H2 increases significantly with the increase of DFA/CS ratio. This may indicate that desulfurization ash promotes the release of H2 in the catalytic reaction, possibly because it affects the pyrolysis reaction during the pyrolysis process and enhances the generation of H2.

For the third problem, for the situation with the same mixing ratio, the rank sum test method was used for significance analysis. For example, the analysis results of the yield difference of CE and LG pyrolysis products were observed, and the relationship between P-value and 0.05 was compared to determine whether there was a significant difference. The P-values for both Tar , Char and Syngas yields are very small (near zero) at about 0.0002, well below the standard significance level of 0.05, indicating a statistically significant difference between tar yields at DFA/CE and DFA/LG ratios.

For the fourth problem, we demonstrated the reaction mechanism through the pyrolysis reaction process, and queried relevant parameters according to the characteristics of the reaction path and the Arrhenius equation to establish the reaction kinetics model.

For the fifth problem, we use BP neural network to make prediction, specify input index and output index, divide training set and test set, adjust and train the model parameters, and then predict the data of the test set and finally conduct error analysis. In this paper, according to the BP neural network prediction model, the data in DAF/CS group in Annex 1 is selected as the training set, the prediction model is trained and the test results of the test set are predicted. The fitting coefficient R is 0.9993 and the relative error is very small, which indicating that the fitting effect is very good.

Keywords: person correlation analysis，person correlation analysis，BP neural network，regression analysis， reaction kinetics model

Content

1. Introduction

1.1 Background

With the increasing global demand for renewable energy, cotton stalk is rich in cellulose, lignin and other biomass components, which is regarded as an important biomass resource and has attracted much attention recently. The quality and yield of cotton straw pyrolysis products are affected by various temperatures such as pyrolysis temperature and catalyst. Based on the data of pyrolysis products and pyrolysis gas products under different catalytic pyrolysis reactions, this paper will study the mechanism and properties of cotton straw pyrolysis products as well as the mechanism and function of catalysts in the pyrolysis process, so as to promote the effective utilization and sustainable development of cotton stalk.

1.2 Work

For the first problem, in order to analyze the relationship between the yield of pyrolysis products of each pyrolysis combination and the mixture ratio of the corresponding pyrolysis combination. Taking DFA/CS combination as an example, the line graphs of thermal valence products under different mixing ratios are drawn first, and the line graphs are discussed. In order to further obtain the exact relationship, person correlation analysis was introduced to conduct correlation analysis on the yields of different products under different mixing ratios. Then a polynomial regression model was established to solve the relationship between the mixing ratio of different pyrolysis combinations and the yield of pyrolysis products. In order to verify whether desulfurization ash as catalyst can promote the pyrolysis of cotton stalk, cellulose and lignin, the first derivative of each function is obtained, and the influence of catalyst on the pyrolysis is analyzed and explained.

For the second problem, images of each of the three pyrolysis combinations is drawn by using matlab. The function relationship is obtained by using the second-order polynomial curve fitting method of problem 1, and the image and function relationship are discussed and analyzed, and the variation process under different mixing ratios is explained, and the different results of each group of pyrolysis gases are explained.

For the third problem, For the same mixed ratio, we use the rank sum test method for significance analysis and observe the results of significance difference analysis.

For the fourth problem, we demonstrated the reaction mechanism through the pyrolysis reaction process, and queried relevant parameters according to the characteristics of the reaction path and the Arrhenius equation to establish the reaction kinetics model.

For the fifth problem, We used BP neural network to predict, then input index and output index are specified, training set and test set are divided, model parameters are adjusted and trained, and then data of test set are predicted and error analysis is carried out.

2. Problem analysis

2.1 Data analysis

The question gives us two attachments.

Annex I is Annex I- Pyrolysis Product Yields of Three Pyrolysis Combinations, it contains three tables： Yield of Decomposition Products from DA/CS Pyrolysis wt.%(daf), Yield of Decomposition Products from DFA/CE Pyrolysis wt.%(daf), Yield of Decomposition Products from DFA/LG Pyrolysis wt.%(daf).

Tab 1 Yield of Decomposition Products from DA/CS Pyrolysis wt.%(daf)

DFA/CS	0/100	10/100	20/100	30/100	40/100	50/100	60/100	80/100	100/100
Tar yield	19.46	17.25	15.43	14.14	13.89	13.21	12.84	12.57	12.13
Water yield	26.84	27.64	28.11	28.23	28.62	29.01	30.07	30.68	31.02
Char yield	29.21	29.11	29.3	29.34	29.14	29.33	29.47	29.64	29.87
Syngas yield	24.49	26	27.16	28.29	28.35	28.45	27.62	27.11	26.98

Tab 2 Yield of Decomposition Products from DFA/CE Pyrolysis wt.%(daf)

DFA/CE	10/100	20/100	30/100	40/100	50/100	60/100	80/100	100/100
Tar yield	34.42	38.31	42.69	43.78	44.53	44.41	43.24	45.28
Water yield	27.42	21.37	17.84	16.9	16.25	18.25	19.93	16.14
Char yield	21.43	24.91	24.17	24.7	24.54	24.59	23.57	24.61
Syngas yield	16.73	15.41	15.3	14.62	14.68	12.75	13.26	13.97

Tab 3 Yield of Decomposition Products from DFA/LG Pyrolysis wt.%(daf)

DFA/LG	10/100	20/100	30/100	40/100	50/100	60/100	80/100	100/100
Tar yield	18.06	13.77	11.29	10.28	9.49	9.02	10.3	8.19
Water yield	15.3	18.54	20.17	20.97	21.53	21.87	21.41	23.69
Char yield	58.17	57.46	57.13	56.98	57.14	57.23	57.15	57.43
Syngas yield	8.47	10.23	11.41	11.77	11.84	11.88	11.14	10.69

Fig.1. Screenshot of Annex I

Annex II is Annex II-Pyrolysis Gas Yields of Three Pyrolysis Combinations, it contains three tables: Yield of Gaseous Components from DFA/CS Pyrolysis (mL/g,daf), Yield of Gaseous Components from DFA/CE Pyrolysis (mL/g,daf), Yield of Gaseous Components from DFA/LG Pyrolysis (mL/g,daf).

Tab 1 Yield of Gaseous Components from DFA/CS Pyrolysis (mL/g,daf)

DFA/CS	H2	CO	CO2	CH4	C2H6	C3H8	C3H6	C2H4	C4H10
0/100	6.48	25.93	60.4	23.41	2.09	0.55	0.35	0.71	0.32
20/100	12.94	21.61	57.84	28.79	2.73	0.61	0.37	0.74	0.48
40/100	22.65	20.53	52.31	33.11	3.08	0.62	0.41	0.81	0.56
50/100	30.35	20.95	51.92	32.45	2.99	0.71	0.39	0.79	0.37
80/100	37.93	22	51.53	30.83	2.96	0.88	0.37	0.77	0.28
100/100	43.62	23.32	50.91	30.21	2.94	0.87	0.38	0.75	0.25

Tab 2 Yield of Gaseous Components from DFA/CE Pyrolysis (mL/g,daf)

DFA/CE	H2	CO	CO2	CH4	C2H6
20/100	26.6	13.7	18.7	3.2	13.8
40/100	47.8	10.6	9.8	1.9	8.6
50/100	55.6	8.1	5.9	1.3	4.4
80/100	65.8	6.5	3.2	1.3	3.4
100/100	57.9	5.3	2	0.7	3.2

Tab 3 Yield of Gaseous Components from DFA/LG Pyrolysis (mL/g,daf)

DFA/LG	H2	CO	CO2	CH4	C2H6
20/100	0.67	15.23	24.35	27.67	0.08
40/100	0.72	15.76	37.91	33.25	0.06
50/100	0.78	17.305	39.26	33.86	0.09
80/100	0.81	19.075	41.23	30.26	0.07
100/100	0.79	20.935	43.56	29.87	0.05

Fig.2. Screenshot of Annex II

Data preprocessing. Drawing q-q graph for the given data set and carrying out

Shapiro-Wilk test to determine that the data set given by the question is subject to normal distribution.

2.2 Analysis of question one

To solve problem 1, in order to analyze the relationship between the yield of pyrolysis products of each pyrolysis combination and the mixing ratio of the corresponding pyrolysis combination, the line graph of the yield of pyrolysis products under different mixing ratios was first drawn, and the general relationship was obtained by analyzing the line graph. Then Pearson correlation analysis was used to analyze the yield of different products at different mixing ratios. After correlation analysis, we establish a regression analysis model, where the mixing ratio is the independent variable and the output of the product is the dependent variable. In order to verify whether desulfurization ash as catalyst can promote the pyrolysis of cotton stalk, cellulose and lignin, the first derivative of each function is obtained, and the influence of catalyst on the pyrolysis is analyzed and explained.

2.3 Analysis of question two

To solve problem 2, images of each of the three pyrolysis combinations is drawn by using matlab. The function relationship is obtained by using the second-order polynomial curve fitting method of problem 1, and the image and function relationship are discussed and analyzed, and the variation process under different mixing ratios is explained, and the different results of each group of pyrolysis gases are explained.

2.4 Analysis of question three

To solve problem 3, For the same mixed ratio, we use the rank sum test method for significance analysis and observe the results of significance difference analysis.

2.5 Analysis of question four

To solve problem 4, we demonstrated the reaction mechanism through the pyrolysis reaction process, and queried relevant parameters according to the characteristics of the reaction path and the Arrhenius equation to establish the reaction kinetics model.

2.6 Analysis of question five

To solve problem 5,BP neural network is used for prediction, input index and output index are specified, training set and test set are divided, model parameters are adjusted and trained, and then data of test set are predicted and error analysis is carried out.

3. Symbol and Assumptions

3. 1 Symbol Description

variable	description	dimension
cov (X,Y)	**the covariance of X multiplied by the covariance of Y**	**-**
σX and σY	**the standard deviations of X and Y respectively**	**-**
E_i	**chemical reaction activation energy**	**KJ/mol^{-1}**
A	**frequency factors**	**min^{-1}**
T	**ambient temperature**	**℃**
R_C	**gas constant**	**-**
k_i	**parameter**	**-**

3.2 Fundamental assumptions

1. Assume that the data given by the title is true and reliable, and does not contain any missing values or error records;

2. The data preprocessing method is reasonable and has no great impact on the results;

3. It is assumed that desulfurization ash, as a catalyst, has the same catalytic effect on all samples, that is, it is not affected by the characteristics of samples (such as the origin and type of cotton stalk);

4. It is assumed that the data set accurately reflects various conditions of the catalytic reaction of cotton stalk pyrolysis, including changes under different conditions.

4. Model

4.1Data preprocessing

Using the data set to draw the QQ map and carry out Shapiro-Wilk test, the judgment problem shows that there is no anomaly in the data set and all obey normal distribution.

Shapiro-Wilk test

Shapiro-Wilk test is a statistical test used to test whether a sample data set is derived from a normal distribution. Especially suitable for small and medium sample size. The null hypothesis (H0) of the SW test is that the sample data comes from a normal distribution. If the P-value is less than the significance level (0.05 is usually chosen), the null hypothesis can be rejected, indicating that the sample data is not from a normal distribution. The figure is the result of the SW test. Since the P-values are all much higher than 0.05, the null hypothesis of the test, that is, the data come from the normal distribution, cannot be rejected. So this sample of data might come from a normal distribution.

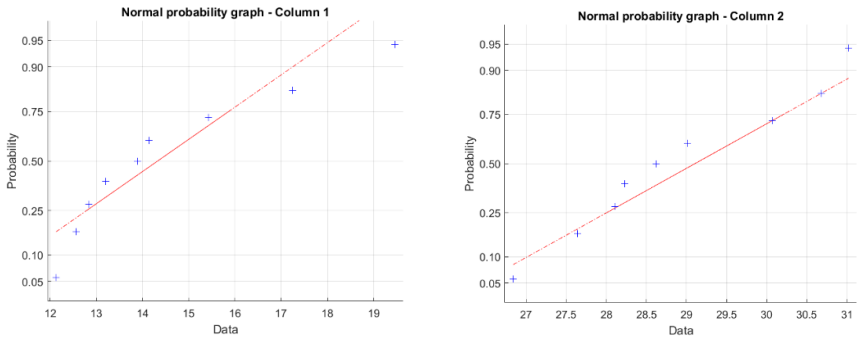
```
>> dl_shujuchuli
Column 1 data follows a normal distribution (p-value = 0.09748)
Warning: P is greater than the largest tabulated value, returning 0.5.
> In jbtest (line 133)
In dl_shujuchuli (line 15)
Column 2 data follows a normal distribution (p-value = 0.50000)
Column 3 data follows a normal distribution (p-value = 0.16242)
Column 4 data follows a normal distribution (p-value = 0.11361)
>>
```

Fig.3. p-value

QQ map drawing

The QQ (Quantile-Quantile) graph is used to test whether a sample data set conforms to a particular theoretical distribution, most commonly to test whether it conforms to a normal distribution.

QQ plots evaluate the consistency between the quantiles of the sample data by comparing them to the quantiles of the theoretical distribution. In the QQ plot, the horizontal axis represents the quantile of the theoretical distribution, while the vertical axis represents the quantile of the sample data. If the sample data agrees with the theoretical distribution, then the points on the QQ plot will approximately fall on a straight line, usually a 45-degree diagonal. If the scatter plot deviates from the diagonal, it may indicate that the distribution of the sample data is inconsistent with the chosen theoretical distribution.



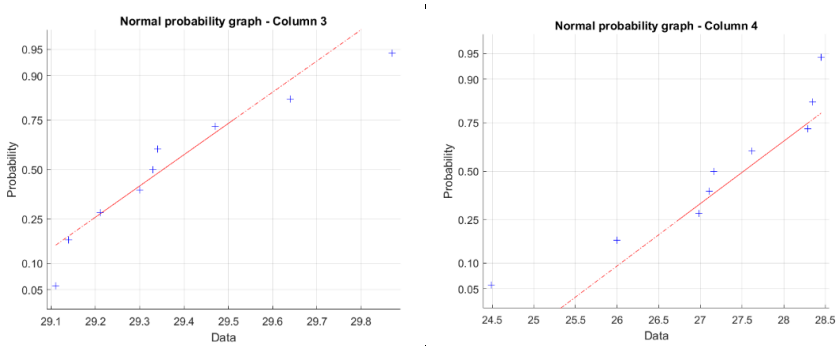


Fig.4. QQ map

As shown in the figure above, the points on the QQ chart will approximately fall on a straight line, so that this set of sample data comes from a normal distribution. Therefore, we can conclude that there are no abnormal data in this dataset and all of them obey normal distribution.

4.2Establishment and solution of problem 1 model

Data visualization

In order to explore the relationship between the yield of pyrolysis products (Tar, Water, Char, Syngas) and the ratio of pyrolysis combination under the condition of different proportions of pyrolysis combination, the data of DFA/CS group was first taken as an example, and the relationship between them was visually demonstrated by drawing line charts.

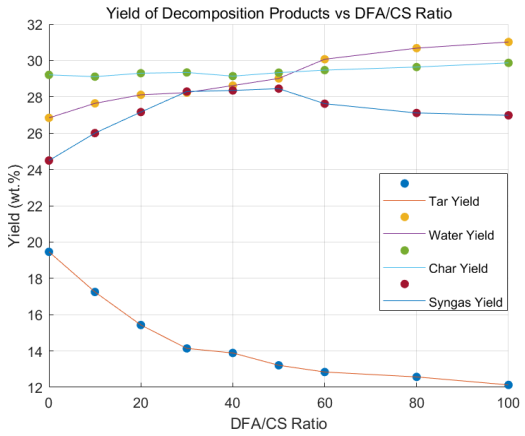


Fig.5. Yield of Decomposition Products vs DFA/CS Ratio

According to the above line chart, taking Tar as an example, we can see that as the proportion increases, Tar production gradually decreases.

Person correlation analysis

The person correlation coefficient between two variables is defined as the quotient of the covariance of the two variables and the standard deviation product of both, which defines the overall correlation coefficient, expressed in ρ :

$$\rho_{XY} = \frac{cov(x,Y)}{\sigma_X \sigma_Y} = \frac{E(X-\mu_X)(Y-\mu_Y)}{\sigma_X \sigma_Y}$$

If the covariance and standard deviation calculated by the sample are replaced by the covariance and standard deviation of the population, it is the sample correlation coefficient, which is usually expressed as follows:

$$r = \frac{\sum_{i=1}^{n}(X_i - \overline{X})(Y_i - \overline{Y})}{\sqrt{\sum_{i=1}^{n}(X_i - \overline{X})^2}\sqrt{\sum_{i=1}^{n}(Y_i - \overline{Y})^2}}$$

Where, cov (X,Y) is the covariance of X multiplied by the covariance of Y, σX and σY are the standard deviations of X and Y respectively, $\overline{X}$ and $\overline{Y}$ are the sample means of X and Y respectively.

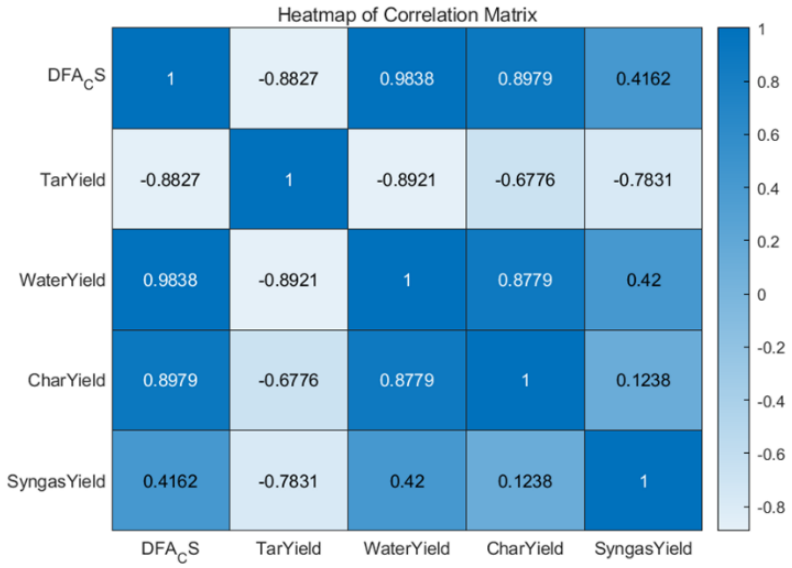


Fig.6. Thermal map of correlation coefficient

Based on the person correlation analysis, we can make a thermal map of the correlation coefficient, which clearly shows the correlation between the yield of each pyrolysis product and the ratio of DFA/CS. As can be seen from the figure:

There is a strong negative correlation between Tar yield and DFA/CS ratio, and the correlation coefficient is -0.8827, which indicates that with the increase of DFA/CS ratio, Tar yield has a significant downward trend.

There is a very strong positive correlation between Water yield and DFA/CS ratio, and the correlation coefficient is 0.9838, which indicates that with the increase of DFA/CS ratio, Water yield has a significant upward trend.

There is a very strong positive correlation between Char yield and DFA/CS ratio, and the correlation coefficient is 0.8979, which indicates that with the increase of DFA/CS ratio, Char yield has a significant upward trend.

There is no strong correlation between Syngas yield and DFA/CS ratio, and the correlation coefficient is 0.4162, which indicates that with the increase of DFA/CS ratio, there is no significant trend of increase or decrease of Syngas yield.

Regression analysis

In order to get the exact functional relationship between the two, we take DFA/CS

and Tar yield as examples, and use their data to judge the reaction mechanism.

Assume that the relationship between Tar yield and combination ratio is:

$$y=a_nx^n+a_{n-1}x^{n-1}+...+a_0$$

Where y represents the tar yield, x represents the combination ratio, and ai represents the coefficient. The ai is then solved using the least square method.

$$y=0.0011x^2-0.1710x+18.9240$$

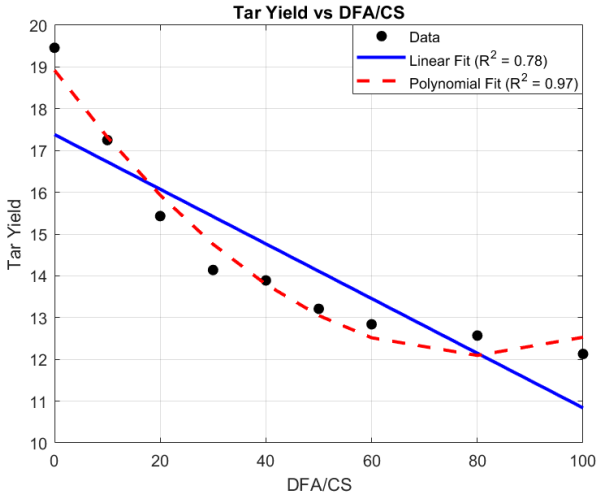


Fig.7. Tar Yield vs DFA/CS

Where R2=0.96936, the correlation coefficient obtained from the above calculation is close to 1, indicating a high degree of fitting. The above formula can be used to describe the relationship between tar yield and combination ratio.

The relationship between Water yield and combination ratio:

Through matlab software to solve the relationship:

$$y=-0.0001x^2+0.0521x+26.9329$$

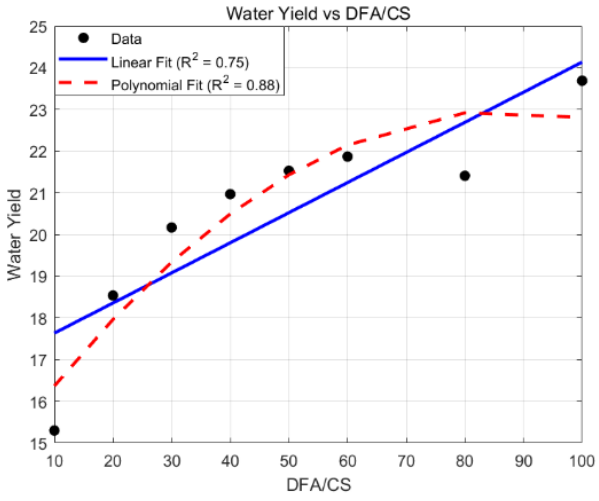


Fig.8. Water Yield vs DFA/CS

The relationship between Char yield and combination ratio:

Through matlab software to solve the relationship:

$$y=0.0001x^2-0.0007x+29.1948$$

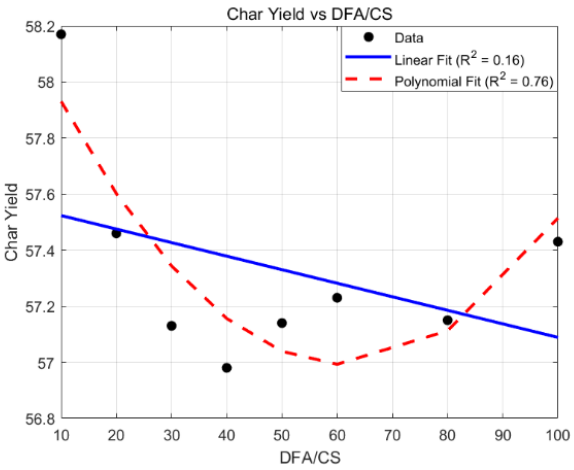


Fig.9. Char Yield vs DFA/CS

The relationship between Char yield and combination ratio:

Through matlab software to solve the relationship:

$$y=-0.0010x^2+0.1196x+24.9498$$

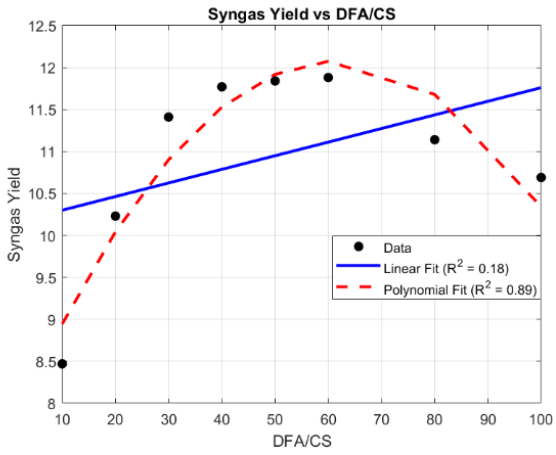


Fig.10. Syngas Yield vs DFA/CS

Similarly, the proportional relationship between pyrolysis products and combinations can be obtained by using the above method for other combinations, as shown in the following table.

Table 2 proportional relationship between pyrolysis products and combinations.

Pyrolysis combinition	Pyrolysis product	Relational expression
DFA/CS	Tar yield	$y=0.0011x^2-0.1710x+18.9240$
	Water yield	$y=-0.0001x^2+0.0521x+26.9329$
	Char yield	$y=0.0001x^2-0.0007x+29.1948$
	Syngas yield	$y=-0.0010x^2+0.1196x+24.9498$
DFA/CE	Tar yield	$y=-0.0025x^2+0.3633x+32.2226$
	Water yield	$y=0.0024x^2-0.3369x+28.0436$
	Char yield	$y=-0.0007x^2+0.0879x+21.9392$
	Syngas yield	$y=0.0007x^2-0.1144x+17.7945$
DFA/LG	Tar yield	$y=0.0019x^2-0.2940x+19.5045$

	Water yield	$y=-0.0011x^2+0.1926x+14.5517$
	Char yield	$y=0.0004x^2-0.0435x+58.3300$
	Syngas yield	$y=-0.0012x^2+0.1449x+7.6138$

Differentiate the four functional relations in the DFA/CS combination respectively.
Tar：

$$y' = 0.0022x - 0.1710$$

By analyzing the above first-order derivative function, we can see that in the DFA/CS group, with the increase of catalyst proportion, the increase of Tar yield becomes larger, and the catalyst can promote the production of Tar.
Water：

$$y' = -0.0002x + 0.0521$$

By analyzing the first derivative function above, we can see that in the DFA/CS group, with the increase of catalyst proportion, the increase of Water yield becomes smaller, and the catalyst has an inhibitory effect on the production of Water.
Char：

$$y' = 0.0002x - 0.0007$$

By analyzing the above first-order derivative function, we can see that in the DFA/CS group, the Char yield increases with the increase of catalyst proportion, and the catalyst can promote the Char production.
Syngas：

$$y' = -0.0020x + 0.1196$$

By analyzing the first derivative function above, we can see that in the DFA/CS group, with the increase of catalyst proportion, the growth of Syngas yield becomes smaller, and the catalyst has an inhibitory effect on Syngas production.

4.3Establishment and solution of problem 2 model

Through the classification and discussion of the three combinations, we explore the influence of different mixing ratios on the gas yield under different combinations.

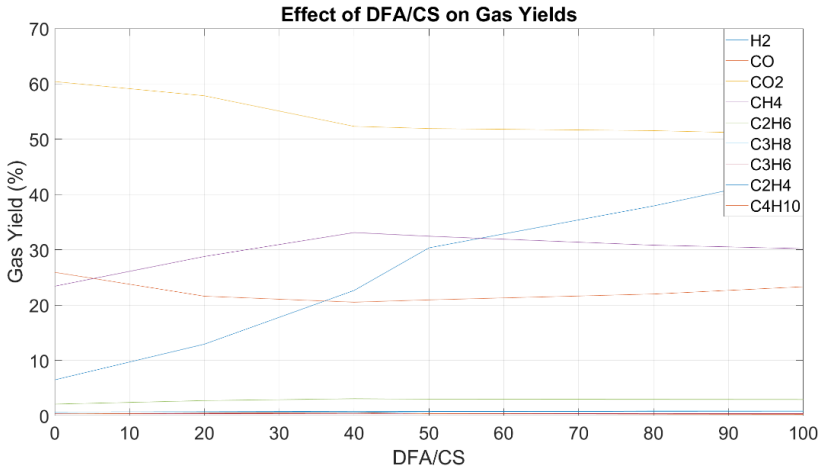


Fig.11. Effect of DFA/CS Gas Yield (all)

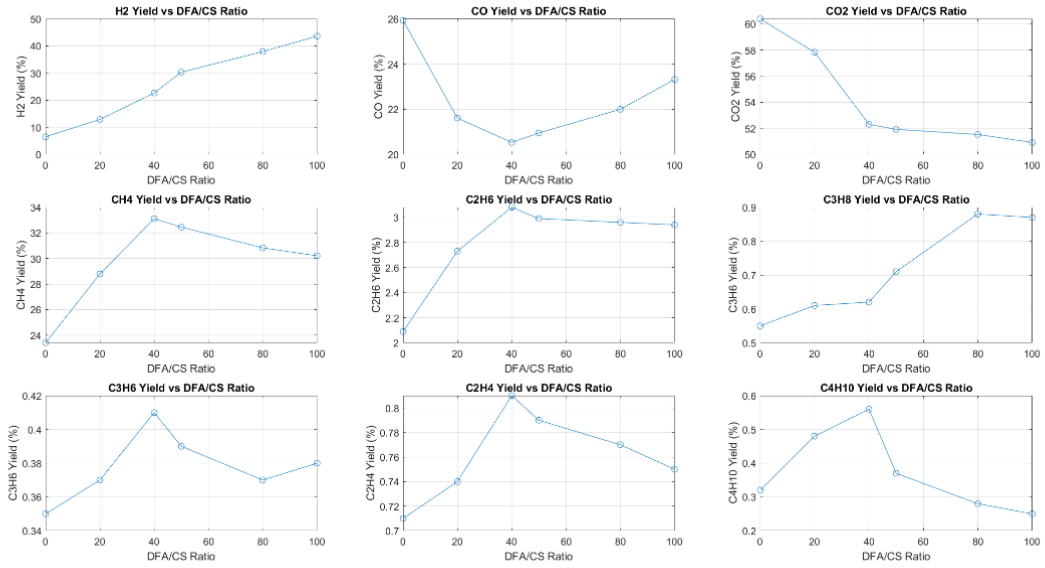


Fig.12. Line chart of DFA/CS

According to problem-1 regression analysis model, the relationship between different mixing ratios and yields under this combination condition is as follows:

Table 3 the relationship between different mixing ratios and yields under this combination condition(DFA/CS)

Products	Functional relationship
H2	$y = -0.0013x^2 + 0.5111x + 5.3516$
CO	$y = 0.0016x^2 - 0.1803x + 25.418$
CO2	$y = 0.0015x^2 - 0.2462x + 60.821$
CH4	$y = -0.0025x^2 + 0.3026x + 23.722$
C2H6	$y = -0.0002x^2 + 0.0294x + 2.1543$
C3H8	$y = 6E\text{-}06x^2 + 0.003x + 0.5403$
C3H6	$y = -1E\text{-}05x^2 + 0.0015x + 0.3515$
C2H4	$y = -1E\text{-}05x^2 + 0.0015x + 0.3515$
C4H10	$y = -7E\text{-}05x^2 + 0.0052x + 0.3602$

Below are the four main products affected by the DFA/CS mixture ratio. Because the proportion of the five secondary products is very small, only about 6% at most, and their changes are very small for the whole, so the analysis of their changes is almost not practical significance, only the analysis of the four main products.

H2：

We can find that the hydrogen yield increases significantly with the increase of DFA/CS ratio. This may indicate that desulfurization ash promotes the release of H2 in the catalytic reaction, possibly because it affects the pyrolysis reaction during the pyrolysis process and enhances the generation of H2.

CO：

We can find that the CO yield initially decreased with the increase of DFA/CS ratio, and then stabilized. This may indicate that desulfurization ash has an inhibitory

effect on CO production at a lower DFA/CS ratio, but this effect is weakened with the increase of catalyst proportion.

CO2：

We can find that the overall CO2 yield shows a downward trend. This may mean that desulphurized ash promotes partial oxidation of carbon rather than complete oxidation, resulting in lower CO2 yield.

CH4：

The CH4 yield decreased after peaking at a moderate DFA/CS ratio, which may indicate that the moderate desulfurization ash concentration is the most favorable condition for CH4 production.

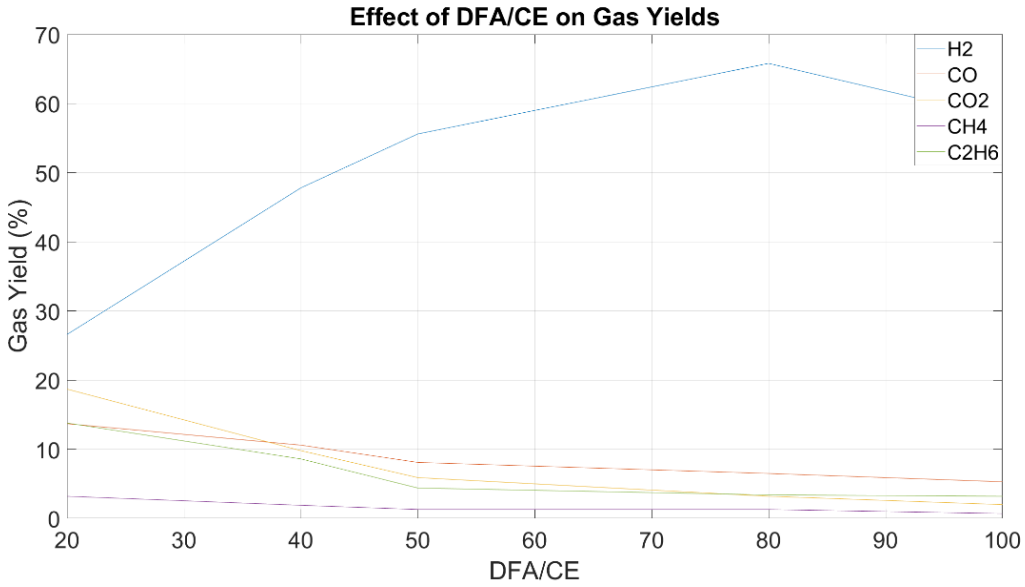


Fig.13. Effect of DFA/CE on Gas Yield

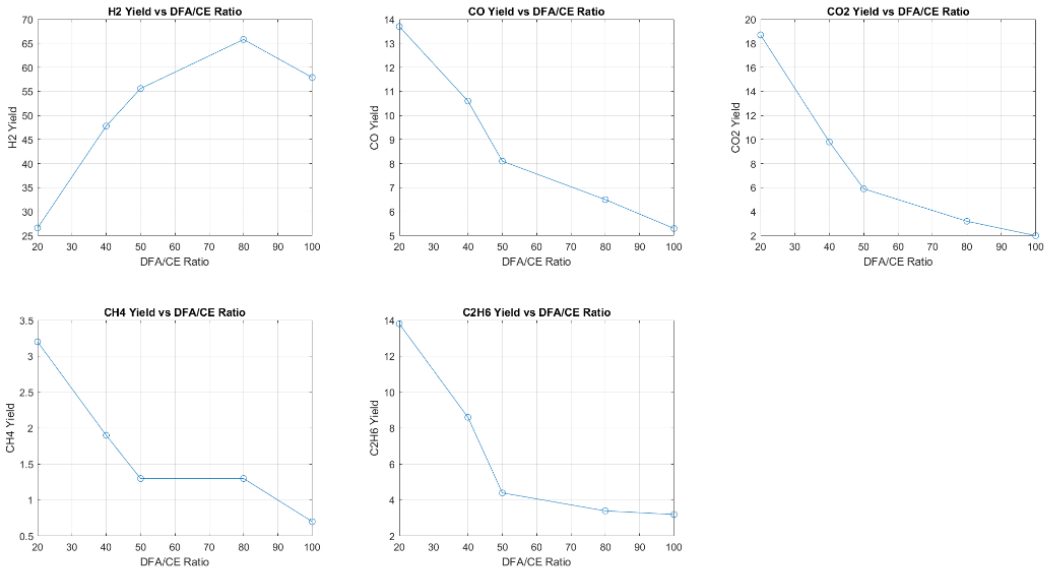


Fig.14. Line chart of DFA/CE

According to problem-1 regression analysis model, the relationship between

different mixing ratios and yields under this combination condition is as follows:

Table 4 the relationship between different mixing ratios and yields under this combination condition(DFA/CE)

Products	Functional relationship
H2	$y = -0.0119x^2 + 1.8261x - 5.6417$
CO	$y = 0.0012x^2 - 0.2491x + 18.192$
CO2	$y = 0.0038x^2 - 0.6496x + 29.858$
CH4	$y = 0.0005x^2 - 0.0824x + 4.5417$
C2H6	$y = 0.0029x^2 - 0.4726x + 22.117$

H2:

The H2 yield generally increased with the increase of DFA/CE ratio, but decreased slightly at 100/100. This may indicate that the catalyst is more effective at promoting H2 production at higher concentrations, but at some point its efficiency is slightly reduced, perhaps because an equilibrium or other limitation of the reaction has been reached.

CO:

The CO yield continued to decrease with the increase of DFA/CE ratio. This suggests that the addition of desulfurized ash may inhibit the formation of CO or promote the conversion of CO to CO2.

CO2:

The CO2 yield decreased significantly with the increase of DFA/CE ratio, which may be due to the presence of desulfurization ash to promote partial oxidation of carbon, resulting in more CO and H2 than CO2.

CH4:

The CH4 yield continued to decrease with the increase of DFA/CE ratio, which indicated that the addition of desulphurized ash may inhibit the formation of CH4 or promote the conversion of CH4.

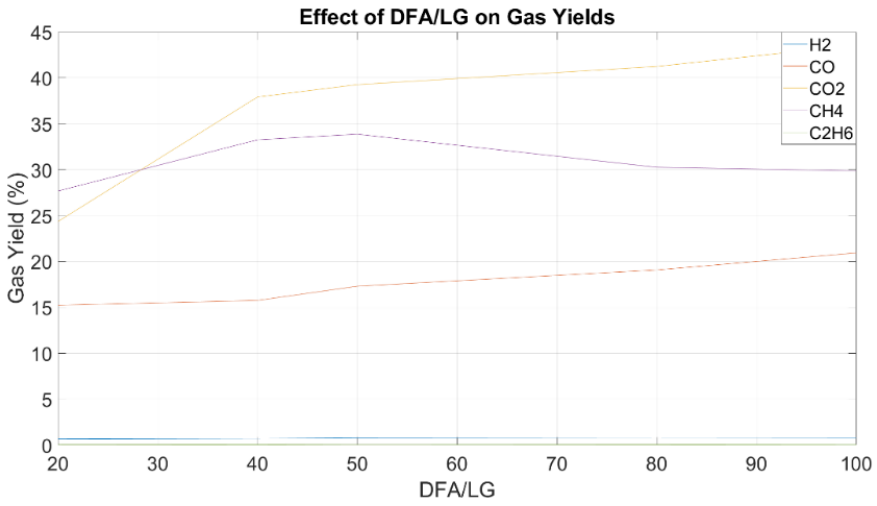


Fig.15. Effect of DFA/LG on Gas Yields

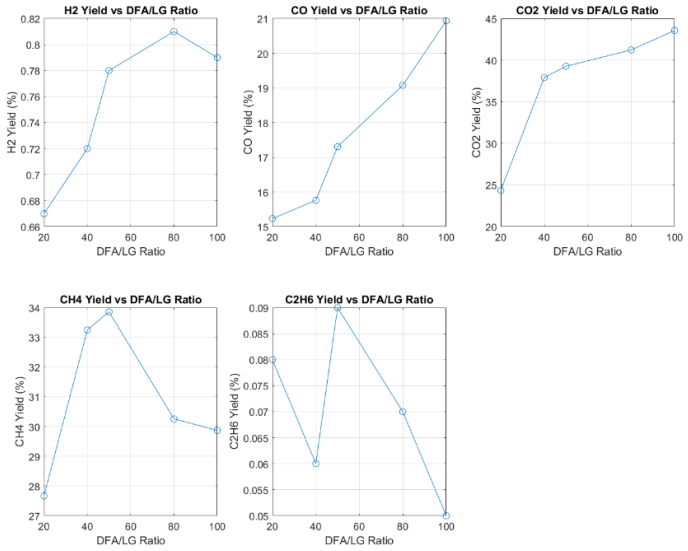


Fig.16. Line chart of DFA/LG

According to problem-1 regression analysis model, the relationship between different mixing ratios and yields under this combination condition is as follows:

Table 4 the relationship between different mixing ratios and yields under this combination condition(DFA/LG)

Products	Functional relationship
H2	$y = -4E\text{-}05x^2 + 0.006x + 0.5575$
CO	$y = 0.0003x^2 + 0.0383x + 14.247$
CO2	$y = -0.0048x^2 + 0.7849x + 11.826$
CH4	$y = -0.003x^2 + 0.3619x + 22.419$
C2H6	$y = -8E\text{-}06x^2 + 0.0006x + 0.065$

H2:

H2 yield increases with the increase of DFA/LG ratio, but decreases slightly at 100/100. This indicates that with the increase of the ratio of DFA to LG, the hydrogen production first increases and then decreases, possibly because the catalytic efficiency reaches its peak.

CO:

The CO yield continues to rise with the increase of DFA/LG ratio. This may indicate that the increase in desulphurized ash is beneficial for the production of CO, which may be related to the promotion of oxidation reactions.

CO2:

The CO2 yield increased significantly with the increase of DFA/LG ratio. This may mean that the desulfurization ash promotes the complete oxidation of the lignin components.

CH4:

The CH4 yield peaked at a DFA/LG ratio of 50/100 and then declined. This may indicate that a moderate desulfurization ash concentration is the most favorable

condition for CH4 formation.

4.4Establishment and solution of problem 3 model

Due to the small amount of data in this paper, methods such as T test are excluded, and rank sum test is chosen instead. Its principle is to assign rank after sorting continuous data, which is used to compare the distribution difference between two groups of independent samples. The process is as follows :

1. Set hypothesis null hypothesis (H0): The distribution of the two groups of samples is the same; Alternative hypothesis (H1): There is a significant difference in the distribution of the two groups of samples.
2. Collect data Merge the data of the two samples and label each data point with the group it belongs to. Assign rank to each data point: The combined data is sorted by size, and the rank is assigned to each data point, and the average rank is taken for data of the same value.
3. Calculate the rank sum For each group, calculate the rank sum of all its data points.
4. Calculate the U statistic using the smaller sum of ranks as the U statistic. Since the sample size in this paper is small, the exact calculation method is used, that is, U= small rank sum.

The calculation formula is:

$$Z = \frac{U - \frac{n_1 n_2}{2}}{\sqrt{\frac{n_1 n_2 (n_1 + n_2 + 1)}{12}}}$$

5. Compare the U statistic with the critical value: Compare the calculated U statistic with the critical value, and reject the null hypothesis if the U statistic is less than or equal to the critical value of 0.05.

In this paper, MALTAB was used for calculation and bar chart was drawn to analyze the differences.

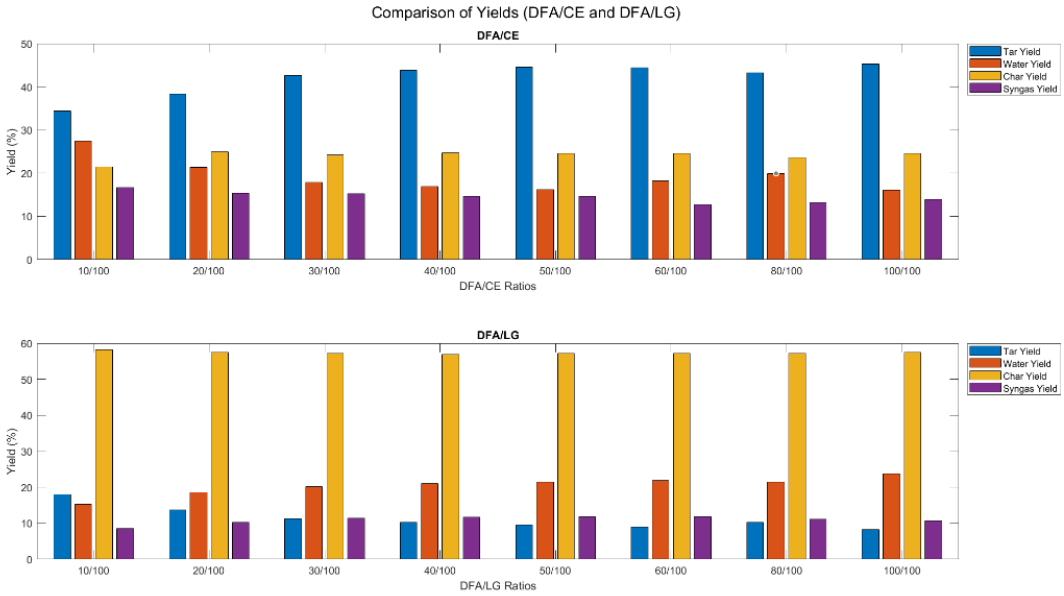


Fig.17. Comparison of Yeild

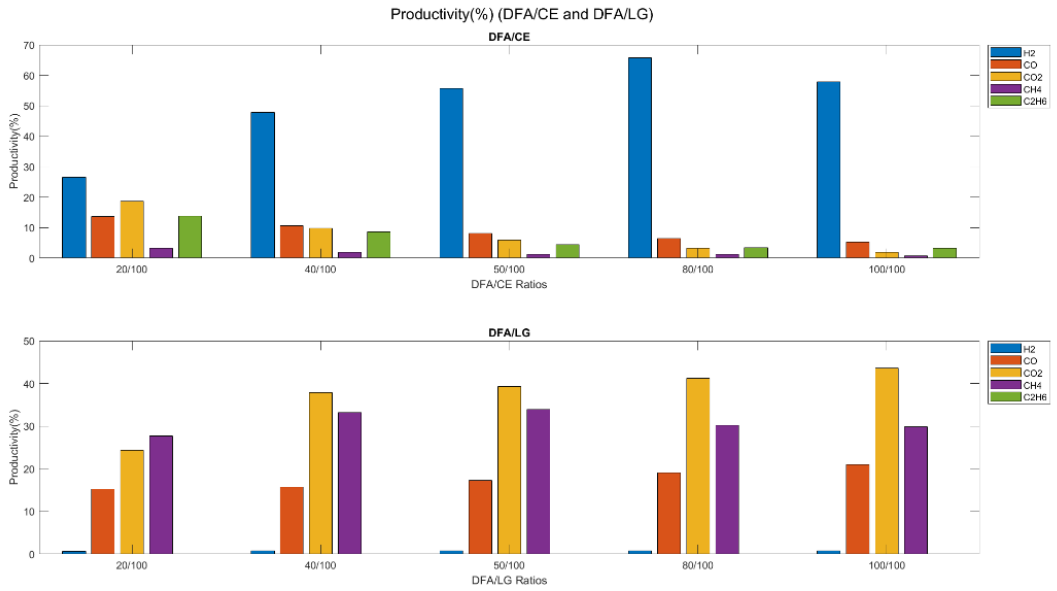


Fig.18. Productivity

The analysis results of the significant difference in yield of CE and LG pyrolysis products are shown in the figure below.

```
Rank Sum Test (Mann Whitney U Test)
Tar yield P Value: 0.0002
Water yield P Value: 0.1949
Char yield P Value: 0.0002
Syngas yield P Value: 0.0002
Refusing the null hypothesis, there is a significant difference
```

Fig.19. analysis results of the significant difference in yield of CE and LG pyrolysis products

Through analysis, we can see that the P-value of Tar, Char and Syngas yield: both about 0.0002 is very small(near to 0), Well below the standard significance level of 0.05, indicating a statistically significant difference between tar yields at DFA/CE and DFA/LG ratios. This means that we have very strong evidence that the change in tar yield under both conditions is not accidental. That is, there is a significant difference in the yield of Tar, Char and Syngas compared with that of LG.

The p value of Water yield, 0.1949, was higher than the standard significance level of 0.05, indicating that there was no statistically significant difference between water yield at the DFA/CE and DFA/LG ratios. This means that we do not have sufficient evidence to conclude that the variation in water yield under the two conditions is due to the different conditions rather than chance factors, that is, there is no significant difference in water yield between CE and LG.

Similarly, we can know whether there are significant differences in pyrolysis gases under different pyrolysis ratios. P-values for each gas yield: all about 0.0079, very small (near zero), well below the standard significance level of 0.05, indicating a statistically significant difference between tar yields at the DFA/CE and DFA/LG ratios. This means that we have very strong evidence that the change in tar yield under both conditions is not accidental. That is, there are significant differences in the yield of CE and LG pyrolysis gas components.

4.5Establishment and solution of problem 4 model

4.5.1Reaction mechanism

By analyzing the question, we can conclude that the decomposition path of CE under catalytic action is assumed as follows:

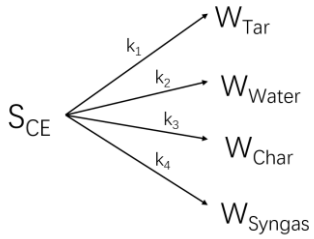


Fig.20. Reaction mechanism

4.5.2Reaction kinetics model

According to the reaction path characteristics and the Arrhenius equation, taking the combination DFA/CE as an example without considering the catalyst mixing ratio, the generation rate of the four products generated by the pyrolysis reaction meets the following formula:

$$\frac{dS_{CE}}{dt} = -A_1 \exp\left[-\frac{E_1}{R_C T}\right] - A_2 \exp\left[-\frac{E_2}{R_C T}\right] - A_3 \exp\left[-\frac{E_3}{R_C T}\right] - A_4 \exp\left[-\frac{E_4}{R_C T}\right]$$

Where, E_1 represents the chemical reaction activation energy of tar; E_2 is the activation energy of chemical reaction of water. E_3 represents the activation energy of chemical reaction of coke residue. E_4 represents the chemical reaction activation energy of gas; A_1,A_2,A_3,A_4 are frequency factors. R_C is the gas constant; T is the experimental temperature.

When the pyrolysis combination is the same, different mixing ratios will affect the generation rate of various pyrolysis products. Therefore, we assume that ρ_i is the influencing factor of the generation rate of pyrolysis products.

$$\rho_i = k_i \exp\left[f_i(x)\right]$$

Where, k_i represents the parameter; $f_i(x)$ is the relationship between the yield of pyrolysis products and the mixing ratio. x represents the corresponding mixture ratio.

In summary, the reaction kinetics equation of DFA/CE combination under different mixing ratios can be written as

$$\frac{dS_{CE}}{dt} = -\sum_{i=1}^{4} k_i A_i \exp\left[\frac{E_i}{R_C T}\right] \cdot exp[f_i(x)]$$

Where,

$f_1(x) = -0.0025x^2 + 0.3633x + 32.2226$

$f_2(x) = 0.0024x^2 - 0.3369x + 28.0436$

$f_3(x) = -0.0007x^2 + 0.0879x + 21.9392$

$f_4(x) = 0.0007x^2 - 0.1144x + 17.7945$

According to the data query[1], the kinetic parameters of the pyrolysis products are shown as follows:

Table 5 the kinetic parameters of the pyrolysis products

Products	A_i/min^{-1}	E_i/(kJ·mol^{-1})
Tar	1.5	39.5
Water	9	27
Char	7	19
Syngas	6	22

同理可知 DFA/LG 组合在不同混合比例的情况下的反应动力学方程

$$\frac{dS_{LG}}{dt} = -\sum_{i=1}^{4} k_i A_i \exp\left[\frac{E_i}{R_C T}\right] \cdot exp[f_i(x)]$$

其中

$f_1(x) = 0.0019x^2 - 0.2940x + 19.5045$

$f_2(x) = -0.0011x^2 + 0.1926x + 14.5517$

$f_3(x) = 0.0004x^2 - 0.0435x + 58.3300$

$f_4(x) = -0.0012x^2 + 0.1449x + 7.6138$

4.6Establishment and solution of problem 5 model

4.6.1Data selection

Among the three sets of data, DFA/ CS, DFA/CE and DFA/LG, DFA/ CS has the largest amount of data, which is more conducive to the training of training sets and improve the accuracy of model prediction results. Therefore, we selected the yield data of pyrolysis products at different DFA/CS ratios to predict the yield data through BP neural network

4.6.2Model selection

BP neural network

Back Propagation Network is called BP neural network for short. The theory of neural network has proved that BP network has powerful nonlinear mapping ability and generalization function, and any continuous function or mapping can be implemented by three-layer network [2]. Taking a three-layer BP network as an example, the network can be described as follows: the input layer neurons are numbered by i, the hidden layer neurons are numbered by j, and the output layer neurons are numbered by k. The prediction model is established by using a BP neural network containing a hidden layer. The structure is shown in the figure[3].

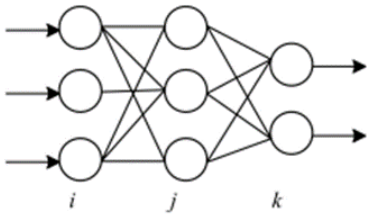


Fig.21. BP neural network(3 layers)

4.6.3 Model use

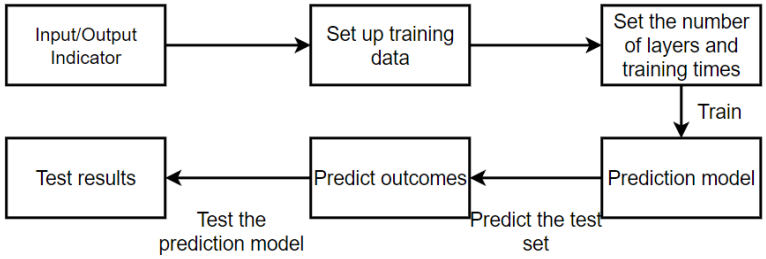


Fig.22. BP neural network model prediction flowchart

In this paper, the mixing ratio of different combinations is used as input index, while the pyrolysis products (Tar, Water, Char, Syngas) are used as output index. Set the data in Attachment 1 as training data, set the appropriate number of layers and training times. The predictive model can then be trained to predict the test results of the test set.

According to the BP neural network prediction model, the data in DAF/CS group in Annex 1 is selected as the training set, wherein, set the mixing ratio as $P_{训练集}$ and the corresponding thermal engine product yield as $T_{训练集}$. Then set various training index data to obtain the BP neural network prediction model, set $P_{测试集}=P_{训练集}$, The predicted value of the product $T_{预测}$ can be obtained by using the BP neural network prediction model.

$$\omega = \frac{|T_{预测} - T_{训练集}|}{T_{训练集}} \times 100\%$$

Where, ω represents the prediction error of BP neural network.

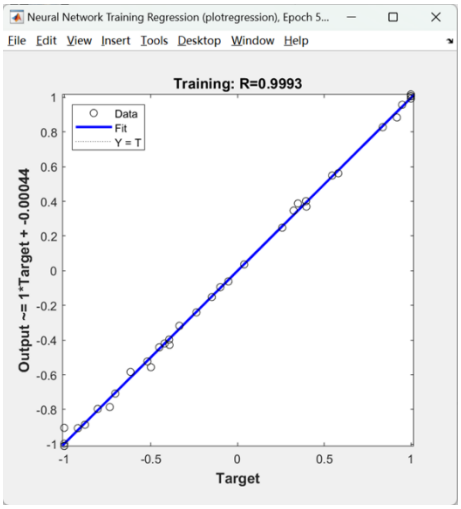


Fig.23. R

We can draw from the figure above that the fitting coefficient R=0.9993 indicates that the fitting effect is very good.

The predicted values and errors obtained by substituding DFA/CS group data in Annex 1 are shown in the following table:

Table 6 The predicted values and errors obtained by substituding DFA/CS group data in Annex 1

DFA/CS	0/100	10/100	20/100	30/100	40/100	50/100	60/100	80/100	100/100
Tar yield	19.4600	17.2500	15.4300	14.1400	13.8900	13.2100	12.8400	12.5700	12.1300
Water yield	26.8400	27.6400	28.1100	28.2300	28.6200	29.0100	30.0700	30.6800	31.0200
Char yield	29.2100	29.1100	29.3000	29.3400	29.1400	29.3300	29.4700	29.6400	29.8700
Syngas yield	24.4900	26.0000	27.1600	28.2900	28.3500	28.4500	27.6200	27.1100	26.9800
Predicted value of Tar yield	19.5228	17.1497	15.4484	14.1756	13.8783	13.1988	12.8735	12.5404	12.1386
Predicted value of Water yield	26.8182	27.7103	28.0355	28.2660	28.6121	29.0062	30.0781	30.6605	31.0327
Predicted value of Char yield	29.1912	29.1457	29.2786	29.3390	19.1450	29.3305	29.4666	29.6425	29.8673
Predicted value of Syngas yield	24.4678	25.9943	27.2375	28.2194	28.3647	28.4645	27.5818	27.1566	26.9615
Error of Tar yield	0.0032	0.0058	0.0012	0.0025	0.0008	0.0008	0.0026	0.0024	0.0007
Error of Water yield	0.0008	0.0025	0.0027	0.0013	0.0003	0.0001	0.0003	0.0006	0.0004
Error of Char yield	0.0006	0.0012	0.0007	0.0000	0.0002	0.0000	0.0001	0.0001	0.0001
Error of Syngas yield	0.0009	0.0002	0.0029	0.0025	0.0005	0.0005	0.0014	0.0017	0.0007

In the above table, we summarized the true value, predicted value and predicted value error of Tar, Water, Char and Syngas production in one table. According to the fact that all errors are far less than 1%, and the average variance of the training results is less than or equal to the negative third power of 10, the relative error of training and prediction using BP neural network model is small, so this model can be used to predict the yield of pyrolysis products.

5.Error Analysis

For the second-order polynomial curves fitted by regression in problem 1 and problem 2, a few curves have low fitting degree, which may not accurately reflect the changing trend of pyrolysis product yield. For example, in the DFA/CE combination, the R2 of the fitting curve of Char yield is only 0.37426, and the curve fitting degree is low. Therefore, the regression model used in this paper needs to be improved to improve the fitting accuracy to reflect the changing trend more accurately.

6.Strengths and Weakness

6.1Strengths

6.1.1 We first conducted data preprocessing, which can eliminate some biased, incomplete or wrong data and improve the quality of data. After data preprocessing, the subsequent fitting and prediction will be more accurate.

6.1.2 As for the correlation analysis, we combine the person correlation analysis and polynomial regression fitting from the simple to the deep, which is conducive to obtaining more accurate correlation. Person correlation analysis is an intuitive and easy to understand analysis method that can help people quickly understand the degree of relationship between variables.

6.1.3 We use BP neural network for prediction. This method has strong fitting ability and can perform well when dealing with complex data patterns and prediction tasks. It is suitable for various types of data.

6.2Weakness

6.2.1 The validity and accuracy of the model are strongly dependent on the quality of the data. If the quality of the data is poor, the prediction results may be affected.

6.2.2 We use person correlation analysis to analyze the correlation, but this method usually only considers the relationship between two variables, without considering other possible influencing factors, which may lead to the limitation of the results. Sample size has an impact on the results of correlation analysis, and small samples tend to produce unstable correlation estimation.

6.2.2 We used BP neural network for prediction, which may fall into local optimal solution, resulting in the model performance failing to reach global optimal. For large-scale neural networks and complex tasks, training times of BP neural network can be long, especially with limited computing resources. In addition, BP neural network has many hyperparameters that need to be tuned, such as learning rate, number of hidden layer nodes, etc., so it takes a certain amount of time and energy to tune.

7.Conclusion

This article investigates the relationship between catalyst mixing ratio and product yield, establishes reaction mechanism and reaction kinetics models, and uses BP neural network to predict yield. The model in this article has significant advantages in achieving its goals efficiently and accurately.

References

[1] 沈力. 木质素热解反应动力学与模型研究[D].厦门学,2021
[2] 夏玫.BP神经网络泛化能力改进研究[D].太原，2009
[3] 李锋,田霞,宋文渊.基于BP神经网络的设备维修人员训练数量预测方法研究[J].计算机与数字工程,2017,45(07)

Appendix

```
function [RMSE, MAPE, R2] = calculate_metrics(actual, predicted)
    % Calculate root mean square error (RMSE)
    RMSE = sqrt(mean((actual - predicted).^2));

    % Calculate Average Absolute Percentage Error (MAPE)
    MAPE = mean(abs((actual - predicted) ./ actual)) * 100;

    % Calculate the coefficient of determination (R2)
    ssRes = sum((actual - predicted).^2);
    ssTot = sum((actual - mean(actual)).^2);
    R2 = 1 - (ssRes / ssTot);
End

function eq = generateFitEquation(coeffs, modelType)
    if startsWith(modelType, 'poly')
        % for polynomial models
        degree = str2double(extractAfter(modelType, 'poly')) - 1;
        terms = cell(1, length(coeffs));

        % Constructing polynomial equations item by item
        for idx = 1:length(coeffs)
            coeff = coeffs(idx);
            power = degree - idx + 1;

            if power == 0
                terms{idx} = sprintf('%f', coeff);
            elseif power == 1
                terms{idx} = sprintf('%f*x', coeff);
            else
                terms{idx} = sprintf('%f*x^%d', coeff, power);
            end
        end

        eq = strjoin(terms, ' + ');
    elseif any(strcmp(modelType, {'exp1', 'exp2'}))
        % For exponential models, add equation generation logic for exponential models
        eq = 'exp model equation here...';
    else
        eq = 'Other model equation here...';
    end
end
```

```
data=[19.46    26.84      29.21      24.49
17.25      27.64      29.11      26
15.43      28.11      29.3 27.16
14.14      28.23      29.34      28.29
13.89      28.62      29.14      28.35
13.21      29.01      29.33      28.45
12.84      30.07      29.47      27.62
12.57      30.68      29.64      27.11
12.13      31.02      29.87      26.98
];
numCols = size(data, 2);

% Go through each column and perform the Jarque-Bera test
for i = 1:numCols
    [h, p] = jbtest(data(:, i));
    if h == 0
        fprintf('Column %d data follows a normal distribution (p-value = %.5f)\n', i, p);
    else
        fprintf('Column %d data does not follow a normal distribution (p-value = %.5f)\n', i, p);
    end
end
% Select the column for which you want to plot a normal probability graph
selectedColumns = [1, 2, 3,4];

% Plot a normal probability plot for each column
for i = selectedColumns
    figure;
    normplot(data(:, i));
    hold on;
    h = probplot(gca,'normal');
    set(h,'marker','*');
    title(sprintf('Normal probability graph - Column %d', i));
    hold off;
end

DFA_CS = [0, 10, 20, 30, 40, 50, 60, 80, 100]; % Due to the naming requirements of the matlab language, DFA CS is used instead of DFA/CS
TarYield = [19.46, 17.25, 15.43, 14.14, 13.89, 13.21, 12.84, 12.57, 12.13];
WaterYield = [26.84, 27.64, 28.11, 28.23, 28.62, 29.01, 30.07, 30.68, 31.02];
CharYield = [29.21, 29.11, 29.3, 29.34, 29.14, 29.33, 29.47, 29.64, 29.87];
SyngasYield = [24.49, 26, 27.16, 28.29, 28.35, 28.45, 27.62, 27.11, 26.98];

%   Create a graphics window，Draw scatter line plots
```

```
figure;
hold on; %Make the graphics appear on a picture

% Scatter plot and line plot of yield of four kinds of products were drawn
scatter(DFA_CS, TarYield, 'filled');
plot(DFA_CS, TarYield, 'DisplayName', 'Tar Yield');

scatter(DFA_CS, WaterYield, 'filled');
plot(DFA_CS, WaterYield, 'DisplayName', 'Water Yield');

scatter(DFA_CS, CharYield, 'filled');
plot(DFA_CS, CharYield, 'DisplayName', 'Char Yield');

scatter(DFA_CS, SyngasYield, 'filled');
plot(DFA_CS, SyngasYield, 'DisplayName', 'Syngas Yield');

% add legend
legend show;

%Add title and axis labels
title('Yield of Decomposition Products vs DFA/CS Ratio');
xlabel('DFA/CS Ratio');
ylabel('Yield (wt.%)');

% Display grid
grid on;

% end
hold off;

DFA_CE = [10, 20, 30, 40, 50, 60, 80, 100];
TarYield = [34.42   38.31      42.69      43.78      44.53      44.41      43.24      45.28
];
WaterYield = [27.42      21.37      17.84      16.9 16.25      18.25      19.93      16.14
];
CharYield = [21.43 24.91      24.17      24.7 24.54      24.59      23.57      24.61
];
SyngasYield = [16.73     15.41      15.3 14.62      14.68      12.75      13.26      13.97
];

Yields = {TarYield, WaterYield, CharYield, SyngasYield};
YieldNames = {'Tar Yield', 'Water Yield', 'Char Yield', 'Syngas Yield'};

% Loop through each yield type and perform linear and polynomial fitting
```

```
for i = 1:length(Yields)
    y = Yields{i};

    % Linear fit
    [p_lin, S_lin] = polyfit(DFA_CE, y, 1);
    y_lin_fit = polyval(p_lin, DFA_CE);

    % Polynomial fit (2nd degree)
    [p_poly, S_poly] = polyfit(DFA_CE, y, 2);
    y_poly_fit = polyval(p_poly, DFA_CE);

    % Calculate R-squared for linear and polynomial fits
    y_mean = mean(y);
    SS_tot = sum((y - y_mean).^2);
    SS_res_lin = sum((y - y_lin_fit).^2);
    SS_res_poly = sum((y - y_poly_fit).^2);
    R2_lin = 1 - SS_res_lin/SS_tot;
    R2_poly = 1 - SS_res_poly/SS_tot;

    % Plotting the results
    figure;
    plot(DFA_CE, y, 'ko', 'MarkerFaceColor', 'k'); % Original Data
    hold on;
    plot(DFA_CE, y_lin_fit, 'b-', 'LineWidth', 2); % Linear Fit
    plot(DFA_CE, y_poly_fit, 'r--', 'LineWidth', 2); % Polynomial Fit
    hold off;

    title([YieldNames{i} ' vs DFA/CE']);
    xlabel('DFA/CE');
    ylabel(YieldNames{i});
    legend('Data', ['Linear Fit (R^2 = ' num2str(R2_lin, '%.4f') ')'], ...
        ['Polynomial Fit (R^2 = ' num2str(R2_poly, '%.4f') ')']);
    grid on;

    % Display the fitting equations and R-squared values in the command window
    lin_eq = ['Linear Fit: y = ' num2str(p_lin(1), '%.4f') '*x + ' num2str(p_lin(2), '%.4f')];
    poly_eq = ['Polynomial Fit: y = ' num2str(p_poly(1), '%.4f') '*x^2 + ' ...
                num2str(p_poly(2), '%.4f') '*x + ' num2str(p_poly(3), '%.4f')];

    disp([YieldNames{i} ':']);
    disp(lin_eq);
    disp(['R-squared for Linear Fit: ' num2str(R2_lin)]);
    disp(poly_eq);
    disp(['R-squared for Polynomial Fit: ' num2str(R2_poly)]);
```

```
    disp(' ');
end

DFA_CS = [0, 10, 20, 30, 40, 50, 60, 80, 100];
TarYield = [19.46, 17.25, 15.43, 14.14, 13.89, 13.21, 12.84, 12.57, 12.13];

% linear fitting
fit_lin = polyfit(DFA_CS, TarYield, 1);
lin_y = polyval(fit_lin, DFA_CS);

% Draw a fitting graph
figure;
plot(DFA_CS, TarYield, 'o'); % data point
hold on;
plot(DFA_CS, lin_y, '-'); % fit line
title('Linear Fit of Tar Yield vs DFA/CS');
xlabel('DFA/CS');
ylabel('Tar Yield');
legend('Data Points', 'Linear Fit');
hold off;
% The fitting coefficients are converted to symbolic polynomials and displayed
syms x
lin_poly = poly2sym(fit_lin, x);
fprintf('Linear fit equation: y = %s\n', char(lin_poly));



% Polynomial fitting, select the appropriate polynomial order, this time using 2 order polynomial
fit_poly = polyfit(DFA_CS, TarYield, 2);
poly_y = polyval(fit_poly, DFA_CS);

%Plot the fitted curve and data points
figure;
plot(DFA_CS, TarYield, 'o'); % data point
hold on;
plot(DFA_CS, poly_y, '-'); % fitted curve
title('Polynomial Fit of Tar Yield vs DFA/CS');
xlabel('DFA/CS');
ylabel('Tar Yield');
legend('Data Points', 'Polynomial Fit');
hold off;

% The fitting coefficients are converted to symbolic polynomials and displayed
poly_poly = poly2sym(fit_poly, x);
```

```
fprintf('Polynomial fit equation: y = %s\n', char(poly_poly));

DFA_LG = [10, 20, 30, 40, 50, 60, 80, 100];
TarYield = [18.06    13.77       11.29       10.28       9.49 9.02 10.3 8.19

];
WaterYield = [15.3 18.54       20.17       20.97       21.53       21.87       21.41       23.69

];
CharYield = [58.17 57.46       57.13       56.98       57.14       57.23       57.15       57.43

];
SyngasYield = [8.47       10.23       11.41       11.77       11.84       11.88       11.14       10.69

];

Yields = {TarYield, WaterYield, CharYield, SyngasYield};
YieldNames = {'Tar Yield', 'Water Yield', 'Char Yield', 'Syngas Yield'};

% Loop through each yield type and perform linear and polynomial fitting
for i = 1:length(Yields)
    y = Yields{i};

    % Linear fit
    [p_lin, S_lin] = polyfit(DFA_LG, y, 1);
    y_lin_fit = polyval(p_lin, DFA_LG);

    % Polynomial fit (2nd degree)
    [p_poly, S_poly] = polyfit(DFA_LG, y, 2);
    y_poly_fit = polyval(p_poly, DFA_LG);

    % Calculate R-squared for linear and polynomial fits
    y_mean = mean(y);
    SS_tot = sum((y - y_mean).^2);
    SS_res_lin = sum((y - y_lin_fit).^2);
    SS_res_poly = sum((y - y_poly_fit).^2);
    R2_lin = 1 - SS_res_lin/SS_tot;
    R2_poly = 1 - SS_res_poly/SS_tot;

    % Plotting the results
    figure;
    plot(DFA_LG, y, 'ko', 'MarkerFaceColor', 'k'); % Original Data
    hold on;
    plot(DFA_LG, y_lin_fit, 'b-', 'LineWidth', 2); % Linear Fit
```

```
    plot(DFA_LG, y_poly_fit, 'r--', 'LineWidth', 2); % Polynomial Fit
    hold off;

    title([YieldNames{i} ' vs DFA/LG']);
    xlabel('DFA/LG');
    ylabel(YieldNames{i});
    legend('Data', ['Linear Fit (R^2 = ' num2str(R2_lin, '%.4f') ')'], ...
        ['Polynomial Fit (R^2 = ' num2str(R2_poly, '%.4f') ')']);
    grid on;

    % Display the fitting equations and R-squared values in the command window
    lin_eq = ['Linear Fit: y = ' num2str(p_lin(1), '%.4f') '*x + ' num2str(p_lin(2), '%.4f')];
    poly_eq = ['Polynomial Fit: y = ' num2str(p_poly(1), '%.4f') '*x^2 + ' ...
                num2str(p_poly(2), '%.4f') '*x + ' num2str(p_poly(3), '%.4f')];

    disp([YieldNames{i} ':']);
    disp(lin_eq);
    disp(['R-squared for Linear Fit: ' num2str(R2_lin)]);
    disp(poly_eq);
    disp(['R-squared for Polynomial Fit: ' num2str(R2_poly)]);
    disp(' ');
end

DFA_CS = [0, 10, 20, 30, 40, 50, 60, 80, 100]';
TarYield = [19.46, 17.25, 15.43, 14.14, 13.89, 13.21, 12.84, 12.57, 12.13]';
WaterYield = [26.84, 27.64, 28.11, 28.23, 28.62, 29.01, 30.07, 30.68, 31.02]';
CharYield = [29.21, 29.11, 29.3, 29.34, 29.14, 29.33, 29.47, 29.64, 29.87]';
SyngasYield = [24.49, 26, 27.16, 28.29, 28.35, 28.45, 27.62, 27.11, 26.98]';

% Creating a table from the data
data = table(DFA_CS, TarYield, WaterYield, CharYield, SyngasYield);

% Calculating the correlation matrix
corrMatrix = corr(data{:,:});

% Plotting the heatmap of the correlation matrix
figure;
heatmap(data.Properties.VariableNames, data.Properties.VariableNames, corrMatrix);
title('Heatmap of Correlation Matrix');
colorbar;

DFA_CS = [0, 10, 20, 30, 40, 50, 60, 80, 100];
TarYield = [19.46, 17.25, 15.43, 14.14, 13.89, 13.21, 12.84, 12.57, 12.13];
```

```
% linear fitting
fit_lin = polyfit(DFA_CS, TarYield, 1);
lin_y = polyval(fit_lin, DFA_CS);

% Draw a fitting graph
figure;
plot(DFA_CS, TarYield, 'o'); % data point
hold on;
plot(DFA_CS, lin_y, '-'); % fit line
title('Linear Fit of Tar Yield vs DFA/CS');
xlabel('DFA/CS');
ylabel('Tar Yield');
legend('Data Points', 'Linear Fit');
hold off;
% The fitting coefficients are converted to symbolic polynomials and displayed
syms x
lin_poly = poly2sym(fit_lin, x);
fprintf('Linear fit equation: y = %s\n', char(lin_poly));



% Polynomial fitting, select the appropriate polynomial order, this time using 2 order polynomial
fit_poly = polyfit(DFA_CS, TarYield, 2);
poly_y = polyval(fit_poly, DFA_CS);

%Plot the fitted curve and data points
figure;
plot(DFA_CS, TarYield, 'o'); % data point
hold on;
plot(DFA_CS, poly_y, '-'); % fitted curve
title('Polynomial Fit of Tar Yield vs DFA/CS');
xlabel('DFA/CS');
ylabel('Tar Yield');
legend('Data Points', 'Polynomial Fit');
hold off;

% The fitting coefficients are converted to symbolic polynomials and displayed
poly_poly = poly2sym(fit_poly, x);
fprintf('Polynomial fit equation: y = %s\n', char(poly_poly));

DFA_CE = [20, 40, 50, 80, 100];
H2 = [26.6, 47.8, 55.6, 65.8, 57.9];
CO = [13.7, 10.6, 8.1, 6.5, 5.3];
CO2 = [18.7, 9.8, 5.9, 3.2, 2];
```

```
CH4 = [3.2, 1.9, 1.3, 1.3, 0.7];
C2H6 = [13.8, 8.6, 4.4, 3.4, 3.2];

% Create a new graphics window
figure;

% Draw a scatter line plot of H2 yield
subplot(2,3,1);
plot(DFA_CE, H2, 'o-');
title('H2 Yield vs DFA/CE Ratio');
xlabel('DFA/CE Ratio');
ylabel('H2 Yield');
grid on;

% Draw a scatter line plot of CO yield
subplot(2,3,2);
plot(DFA_CE, CO, 'o-');
title('CO Yield vs DFA/CE Ratio');
xlabel('DFA/CE Ratio');
ylabel('CO Yield');
grid on;

% Draw a scatter line plot of CO2 yield
subplot(2,3,3);
plot(DFA_CE, CO2, 'o-');
title('CO2 Yield vs DFA/CE Ratio');
xlabel('DFA/CE Ratio');
ylabel('CO2 Yield');
grid on;

% Draw a scatter line plot of CH4 yield
subplot(2,3,4);
plot(DFA_CE, CH4, 'o-');
title('CH4 Yield vs DFA/CE Ratio');
xlabel('DFA/CE Ratio');
ylabel('CH4 Yield');
grid on;

% Draw a scatter line plot of C2H6 yield
subplot(2,3,5);
plot(DFA_CE,C2H6,    'o-');
title('C2H6 Yield vs DFA/CE Ratio');
xlabel('DFA/CE Ratio');
ylabel('C2H6 Yield');
```

```
grid on;


tight_layout();
set(gcf, 'Position', [100, 100, 1024, 768]); % Set graphic size
saveas(gcf, 'Pyrolysis_Yields_vs_DFACERatio.png');

DFA_CS = [0, 20, 40, 50, 80, 100];
H2 = [6.48, 12.94, 22.65, 30.35, 37.93, 43.62];
CO = [25.93, 21.61, 20.53, 20.95, 22, 23.32];
CO2 = [60.4, 57.84, 52.31, 51.92, 51.53, 50.91];
CH4 = [23.41, 28.79, 33.11, 32.45, 30.83, 30.21];
C2H6 = [2.09, 2.73, 3.08, 2.99, 2.96, 2.94];
C3H8 = [0.55, 0.61, 0.62, 0.71, 0.88, 0.87];
C3H6 = [0.35, 0.37, 0.41, 0.39, 0.37, 0.38];
C2H4 = [0.71, 0.74, 0.81, 0.79, 0.77, 0.75];
C4H10 = [0.32, 0.48, 0.56, 0.37, 0.28, 0.25];

% Create a new graphics window
figure;

% Plot a scatter line plot of H2 yield
subplot(3, 3, 1);
plot(DFA_CS, H2, '-o');
title('H2 Yield vs DFA/CS Ratio');
xlabel('DFA/CS Ratio');
ylabel('H2 Yield (%)');
grid on;

% Draw a scatter line plot of CO yield
subplot(3, 3, 2);
plot(DFA_CS, CO, '-o');
title('CO Yield vs DFA/CS Ratio');
xlabel('DFA/CS Ratio');
ylabel('CO Yield (%)');
grid on;

% Draw a scatter line plot of CO2 yield
subplot(3, 3, 3);
plot(DFA_CS, CO2, '-o');
title('CO2 Yield vs DFA/CS Ratio');
xlabel('DFA/CS Ratio');
ylabel('CO2 Yield (%)');
grid on;
```

```
% Draw a scatter line plot of CH4 yield
subplot(3, 3, 4);
plot(DFA_CS, CH4, '-o');
title('CH4 Yield vs DFA/CS Ratio');
xlabel('DFA/CS Ratio');
ylabel('CH4 Yield (%)');
grid on;

% Draw a scatter line plot of C2H6 yield
subplot(3, 3, 5);
plot(DFA_CS, C2H6, '-o');
title('C2H6 Yield vs DFA/CS Ratio');
xlabel('DFA/CS Ratio');
ylabel('C2H6 Yield (%)');
grid on;

%Draw a scatter line plot of C3H8 yield
subplot(3, 3, 6);
plot(DFA_CS, C3H8, '-o');
title('C3H8 Yield vs DFA/CS Ratio');
xlabel('DFA/CS Ratio');
ylabel('C3H6 Yield (%)');
grid on;

%Draw a scatter line plot of C3H6 yield
subplot(3, 3, 7);
plot(DFA_CS, C3H6, '-o');
title('C3H6 Yield vs DFA/CS Ratio');
xlabel('DFA/CS Ratio');
ylabel('C3H6 Yield (%)');
grid on;

%Draw a scatter line plot of C2H4 yield
subplot(3, 3, 8);
plot(DFA_CS, C2H4, '-o');
title('C2H4 Yield vs DFA/CS Ratio');
xlabel('DFA/CS Ratio');
ylabel('C2H4 Yield (%)');
grid on;

%Draw a scatter line plot of C4H10 yield
subplot(3, 3, 9);
plot(DFA_CS, C4H10, '-o');
```

```
title('C4H10 Yield vs DFA/CS Ratio');
xlabel('DFA/CS Ratio');
ylabel('C4H10 Yield (%)');
grid on;

set(gcf, 'Position', [100, 100, 1024, 768]); % Set graphic size
tight_layout();


saveas(gcf, 'Pyrolysis_Gas_Yields_vs_DFACS.png');

DFA_LG = [20, 40, 50, 80, 100];
H2 = [0.67, 0.72, 0.78, 0.81, 0.79];
CO = [15.23, 15.76, 17.305, 19.075, 20.935];
CO2 = [24.35, 37.91, 39.26, 41.23, 43.56];
CH4 = [27.67, 33.25, 33.86, 30.26, 29.87];
C2H6 = [0.08, 0.06, 0.09, 0.07, 0.05];

% Create a new graphics window
figure;

% Set drawing color
colors = lines(5); % 'lines'A is a MATLAB built-in function that generates colors

% Draw a scatter line plot of H2 yield
subplot(2, 3, 1);
plot(DFA_LG, H2, 'o-');
title('H2 Yield vs DFA/LG Ratio');
xlabel('DFA/LG Ratio');
ylabel('H2 Yield (%)');
grid on;

% Draw a scatter line plot of CO yield
subplot(2, 3, 2);
plot(DFA_LG, CO, 'o-');
title('CO Yield vs DFA/LG Ratio');
xlabel('DFA/LG Ratio');
ylabel('CO Yield (%)');
grid on;

% Draw a scatter line plot of CO2 yield
subplot(2, 3, 3);
plot(DFA_LG, CO2, 'o-');
title('CO2 Yield vs DFA/LG Ratio');
```

```
xlabel('DFA/LG Ratio');
ylabel('CO2 Yield (%)');
grid on;

% Draw a scatter line plot of CH4 yield
subplot(2, 3, 4);
plot(DFA_LG, CH4, 'o-');
title('CH4 Yield vs DFA/LG Ratio');
xlabel('DFA/LG Ratio');
ylabel('CH4 Yield (%)');
grid on;

% Draw a scatter line plot of C2H6 yield
subplot(2, 3, 5);
plot(DFA_LG, C2H6,    'o-');
title('C2H6 Yield vs DFA/LG Ratio');
xlabel('DFA/LG Ratio');
ylabel('C2H6 Yield (%)');
grid on;

set(gcf, 'Position', [100, 100, 1024, 768]); % Set graphic size
tight_layout();

saveas(gcf, 'Gas_Yields_vs_DFALG.png');

DFA_CE = [20, 40, 50, 80, 100];
H2 = [26.6, 47.8, 55.6, 65.8, 57.9];
CO = [13.7, 10.6, 8.1, 6.5, 5.3];
CO2 = [18.7, 9.8, 5.9, 3.2, 2];
CH4 = [3.2, 1.9, 1.3, 1.3, 0.7];
C2H6 = [13.8, 8.6, 4.4, 3.4, 3.2];

figure;

plot(DFA_CE, [H2', CO', CO2', CH4', C2H6']);
title('Effect of DFA/CE on Gas Yields');
xlabel('DFA/CE');
ylabel('Gas Yield (%)');
legend('H2', 'CO', 'CO2', 'CH4', 'C2H6');
grid on;

DFA_CS = [0, 20, 40, 50, 80, 100];
H2 = [6.48, 12.94, 22.65, 30.35, 37.93, 43.62];
CO = [25.93, 21.61, 20.53, 20.95, 22, 23.32];
```

```
CO2 = [60.4, 57.84, 52.31, 51.92, 51.53, 50.91];
CH4 = [23.41, 28.79, 33.11, 32.45, 30.83, 30.21];
C2H6 = [2.09, 2.73, 3.08, 2.99, 2.96, 2.94];
C3H8 = [0.55, 0.61, 0.62, 0.71, 0.88, 0.87];
C3H6 = [0.35, 0.37, 0.41, 0.39, 0.37, 0.38];
C2H4 = [0.71, 0.74, 0.81, 0.79, 0.77, 0.75];
C4H10 = [0.32, 0.48, 0.56, 0.37, 0.28, 0.25];

% Plotting
figure;

plot(DFA_CS, [H2', CO', CO2', CH4', C2H6', C3H8', C3H6', C2H4', C4H10']);
title('Effect of DFA/CS on Gas Yields');
xlabel('DFA/CS');
ylabel('Gas Yield (%)');
legend('H2', 'CO', 'CO2', 'CH4', 'C2H6', 'C3H8', 'C3H6', 'C2H4', 'C4H10');
grid on;

DFA_LG = [20, 40, 50, 80, 100];
H2 = [0.67, 0.72, 0.78, 0.81, 0.79];
CO = [15.23, 15.76, 17.305, 19.075, 20.935];
CO2 = [24.35, 37.91, 39.26, 41.23, 43.56];
CH4 = [27.67, 33.25, 33.86, 30.26, 29.87];
C2H6 = [0.08, 0.06, 0.09, 0.07, 0.05];

figure;

plot(DFA_LG, [H2', CO', CO2', CH4', C2H6']);
title('Effect of DFA/LG on Gas Yields');
xlabel('DFA/LG');
ylabel('Gas Yield (%)');
legend('H2', 'CO', 'CO2', 'CH4', 'C2H6');
grid on;

DFA_CS = [0, 20, 40, 50, 80, 100];
H2 = [6.48, 12.94, 22.65, 30.35, 37.93, 43.62];
CO = [25.93, 21.61, 20.53, 20.95, 22, 23.32];
CO2 = [60.4, 57.84, 52.31, 51.92, 51.53, 50.91];
CH4 = [23.41, 28.79, 33.11, 32.45, 30.83, 30.21];
C2H6 = [2.09, 2.73, 3.08, 2.99, 2.96, 2.94];
C3H8 = [0.55, 0.61, 0.62, 0.71, 0.88, 0.87];
C3H6 = [0.35, 0.37, 0.41, 0.39, 0.37, 0.38];
C2H4 = [0.71, 0.74, 0.81, 0.79, 0.77, 0.75];
C4H10 = [0.32, 0.48, 0.56, 0.37, 0.28, 0.25];
```

```
figure;

plot(DFA_CS, [H2', CO', CO2', CH4', C2H6', C3H8']);
title('Major Gas Yields');
xlabel('DFA/CS');
ylabel('Gas Yield (%)');
legend('H2', 'CO', 'CO2', 'CH4', 'C2H6', 'C3H8');
grid on;

H2_CE = [26.6, 47.8, 55.6, 65.8, 57.9];
CO_CE = [13.7, 10.6, 8.1, 6.5, 5.3];
CO2_CE = [18.7, 9.8, 5.9, 3.2, 2];
CH4_CE = [3.2, 1.9, 1.3, 1.3, 0.7];
C2H6_CE = [13.8, 8.6, 4.4, 3.4, 3.2];


H2_LG = [0.67, 0.72, 0.78, 0.81, 0.79];
CO_LG = [15.23, 15.76, 17.305, 19.075, 20.935];
CO2_LG = [24.35, 37.91, 39.26, 41.23, 43.56];
CH4_LG = [27.67, 33.25, 33.86, 30.26, 29.87];
C2H6_LG = [0.08, 0.06, 0.09, 0.07, 0.05];

% Using Rank Sum Test (Mann Whitney U Test)
[p_value_H2, ~, stats_H2] = ranksum(H2_CE, H2_LG);
[p_value_CO, ~, stats_CO] = ranksum(CO_CE, CO_LG);
[p_value_CO2, ~, stats_CO2] = ranksum(CO2_CE, CO2_LG);
[p_value_CH4, ~, CH4_syngas] = ranksum(CH4_CE, CH4_LG);
[p_value_C2H6, ~, C2H6] = ranksum(C2H6_CE, C2H6_LG);
% Output inspection results
fprintf('Rank Sum Test (Mann Whitney U Test)\n');
fprintf('H2 P Value: %.4f\n', p_value_H2);
fprintf('CO P Value: %.4f\n', p_value_CO);
fprintf('CO2 P Value: %.4f\n', p_value_CO2);
fprintf('CH4 P Value: %.4f\n', p_value_CH4);
fprintf('C2H6 P Value: %.4f\n', p_value_C2H6);
% Determine whether to reject the null hypothesis
alpha = 0.05;
if any([p_value_H2, p_value_CO, p_value_CO2, p_value_CH4,p_value_C2H6] < alpha)
    disp('Refusing the null hypothesis, there is a significant difference');
else
    disp('Refusing the null hypothesis, there is a significant difference; rejecting the null hypothesis,
no significant difference found');
```

```
end

tar_yield_CE = [34.42, 38.31, 42.69, 43.78, 44.53, 44.41, 43.24, 45.28];
water_yield_CE = [27.42, 21.37, 17.84, 16.9, 16.25, 18.25, 19.93, 16.14];
char_yield_CE = [21.43, 24.91, 24.17, 24.7, 24.54, 24.59, 23.57, 24.61];
syngas_yield_CE = [16.73, 15.41, 15.3, 14.62, 14.68, 12.75, 13.26, 13.97];

tar_yield_LG = [18.06, 13.77, 11.29, 10.28, 9.49, 9.02, 10.3, 8.19];
water_yield_LG = [15.3, 18.54, 20.17, 20.97, 21.53, 21.87, 21.41, 23.69];
char_yield_LG = [58.17, 57.46, 57.13, 56.98, 57.14, 57.23, 57.15, 57.43];
syngas_yield_LG = [8.47, 10.23, 11.41, 11.77, 11.84, 11.88, 11.14, 10.69];

% Using Rank Sum Test (Mann Whitney U Test)
[p_value_tar, ~, stats_tar] = ranksum(tar_yield_CE, tar_yield_LG);
[p_value_water, ~, stats_water] = ranksum(water_yield_CE, water_yield_LG);
[p_value_char, ~, stats_char] = ranksum(char_yield_CE, char_yield_LG);
[p_value_syngas, ~, stats_syngas] = ranksum(syngas_yield_CE, syngas_yield_LG);

% Output inspection results
fprintf('Rank Sum Test (Mann Whitney U Test)\n');
fprintf('Tar yield P Value: %.4f\n', p_value_tar);
fprintf('Water yield P Value: %.4f\n', p_value_water);
fprintf('Char yield P Value: %.4f\n', p_value_char);
fprintf('Syngas yield P Value: %.4f\n', p_value_syngas);

% Determine whether to reject the null hypothesis
alpha = 0.05;
if any([p_value_tar, p_value_water, p_value_char, p_value_syngas] < alpha)
    disp('Refusing the null hypothesis, there is a significant difference');
else
    disp('Refusing the null hypothesis, there is a significant difference; rejecting the null hypothesis,
no significant difference found');
end

dfa_CE_ratios = {'20/100', '40/100', '50/100',    '80/100', '100/100'};
H2_CE = [26.6, 47.8, 55.6, 65.8, 57.9];
CO_CE = [13.7, 10.6, 8.1, 6.5, 5.3];
CO2_CE = [18.7, 9.8, 5.9, 3.2, 2];
CH4_CE = [3.2, 1.9, 1.3, 1.3, 0.7];
C2H6_CE = [13.8, 8.6, 4.4, 3.4, 3.2];



H2_LG = [0.67, 0.72, 0.78, 0.81, 0.79];
CO_LG = [15.23, 15.76, 17.305, 19.075, 20.935];
```

```
CO2_LG = [24.35, 37.91, 39.26, 41.23, 43.56];
CH4_LG = [27.67, 33.25, 33.86, 30.26, 29.87];
C2H6_LG = [0.08, 0.06, 0.09, 0.07, 0.05];

% Create a drawing
figure;

% Draw a bar chart of DFA/CE
subplot(2, 1, 1);
bar_data_dfa_CE = [H2_CE; CO_CE; CO2_CE; CH4_CE;C2H6_CE];
bar(bar_data_dfa_CE', 'BarWidth', 0.8);
set(gca, 'XTickLabel', dfa_CE_ratios, 'XTick', 1:numel(dfa_CE_ratios));
legend({'H2', 'CO', 'CO2', 'CH4','C2H6'}, 'Location', 'BestOutside');
title('DFA/CE');
xlabel('DFA/CE Ratios');
ylabel('Productivity(%)');

% Draw a bar chart of DFA/LG
subplot(2, 1, 2);
bar_data_dfa_LG = [H2_LG; CO_LG; CO2_LG;CH4_LG;C2H6_LG];
bar(bar_data_dfa_LG', 'BarWidth', 0.8);
set(gca, 'XTickLabel', dfa_CE_ratios, 'XTick', 1:numel(dfa_CE_ratios));
legend({'H2', 'CO', 'CO2', 'CH4','C2H6'}, 'Location', 'BestOutside');
title('DFA/LG');
xlabel('DFA/LG Ratios');
ylabel('Productivity(%)');


sgtitle('Productivity(%) (DFA/CE and DFA/LG)');

dfa_CE_ratios = {'10/100', '20/100', '30/100', '40/100', '50/100', '60/100', '80/100', '100/100'};
tar_yield_dfa_CE = [34.42, 38.31, 42.69, 43.78, 44.53, 44.41, 43.24, 45.28];
water_yield_dfa_CE = [27.42, 21.37, 17.84, 16.9, 16.25, 18.25, 19.93, 16.14];
char_yield_dfa_CE = [21.43, 24.91, 24.17, 24.7, 24.54, 24.59, 23.57, 24.61];
syngas_yield_dfa_CE = [16.73, 15.41, 15.3, 14.62, 14.68, 12.75, 13.26, 13.97];

tar_yield_dfa_LG = [18.06, 13.77, 11.29, 10.28, 9.49, 9.02, 10.3, 8.19];
water_yield_dfa_LG = [15.3, 18.54, 20.17, 20.97, 21.53, 21.87, 21.41, 23.69];
char_yield_dfa_LG = [58.17, 57.46, 57.13, 56.98, 57.14, 57.23, 57.15, 57.43];
syngas_yield_dfa_LG = [8.47, 10.23, 11.41, 11.77, 11.84, 11.88, 11.14, 10.69];

% Create a drawing
figure;
```

```
% Draw a bar chart of DFA/CE
subplot(2, 1, 1);
bar_data_dfa_CE = [tar_yield_dfa_CE; water_yield_dfa_CE; char_yield_dfa_CE; syngas_yield_dfa_CE];
bar(bar_data_dfa_CE', 'BarWidth', 0.8);
set(gca, 'XTickLabel', dfa_CE_ratios, 'XTick', 1:numel(dfa_CE_ratios));
legend({'Tar Yield', 'Water Yield', 'Char Yield', 'Syngas Yield'}, 'Location', 'BestOutside');
title('DFA/CE');
xlabel('DFA/CE Ratios');
ylabel('Yield (%)');

% Draw a bar chart of DFA/LG
subplot(2, 1, 2);
bar_data_dfa_LG = [tar_yield_dfa_LG; water_yield_dfa_LG; char_yield_dfa_LG; syngas_yield_dfa_LG];
bar(bar_data_dfa_LG', 'BarWidth', 0.8);
set(gca, 'XTickLabel', dfa_CE_ratios, 'XTick', 1:numel(dfa_CE_ratios));
legend({'Tar Yield', 'Water Yield', 'Char Yield', 'Syngas Yield'}, 'Location', 'BestOutside');
title('DFA/LG');
xlabel('DFA/LG Ratios');
ylabel('Yield (%)');


sgtitle('Comparison of Yields (DFA/CE and DFA/LG)');

DFA_over_CE = [10, 20, 30, 40, 50, 60, 80, 100];
Tar_yield = [34.42, 38.31, 42.69, 43.78, 44.53, 44.41, 43.24, 45.28];
Water_yield = [27.42, 21.37, 17.84, 16.9, 16.25, 18.25, 19.93, 16.14];
Char_yield = [21.43, 24.91, 24.17, 24.7, 24.54, 24.59, 23.57, 24.61];
Syngas_yield = [16.73, 15.41, 15.3, 14.62, 14.68, 12.75, 13.26, 13.97];

%Set initial guess parameter values
k_Tar_initial = 0.1;
m_Tar_initial = 2;
n_Tar_initial = 1;
k_dec_Tar_initial = 0.01;

k_Water_initial = 0.1;
m_Water_initial = 2;
n_Water_initial = 1;
k_dec_Water_initial = 0.01;

k_Char_initial = 0.1;
m_Char_initial = 2;
```

```
n_Char_initial = 1;
k_dec_Char_initial = 0.01;

k_Syngas_initial = 0.1;
m_Syngas_initial = 2;
n_Syngas_initial = 1;
k_dec_Syngas_initial = 0.01;

% Initial Guess Parameter Values
initial_guess = [k_Tar_initial, m_Tar_initial, n_Tar_initial, k_dec_Tar_initial, ...
                 k_Water_initial, m_Water_initial, n_Water_initial, k_dec_Water_initial, ...
                 k_Char_initial, m_Char_initial, n_Char_initial, k_dec_Char_initial, ...
                 k_Syngas_initial, m_Syngas_initial, n_Syngas_initial,
k_dec_Syngas_initial];

% Fitting using lsqcurvefit
fit_params = lsqcurvefit(@reaction_model, initial_guess, DFA_over_CE, [Tar_yield; Water_yield;
Char_yield; Syngas_yield]);

% Output fitted parameters
disp('Fitted parameters:');
disp(['k_Tar = ', num2str(fit_params(1))]);
disp(['m_Tar = ', num2str(fit_params(2))]);
disp(['n_Tar = ', num2str(fit_params(3))]);
disp(['k_dec_Tar = ', num2str(fit_params(4))]);

disp(['k_Water = ', num2str(fit_params(5))]);
disp(['m_Water = ', num2str(fit_params(6))]);
disp(['n_Water = ', num2str(fit_params(7))]);
disp(['k_dec_Water = ', num2str(fit_params(8))]);

disp(['k_Char = ', num2str(fit_params(9))]);
disp(['m_Char = ', num2str(fit_params(10))]);
disp(['n_Char = ', num2str(fit_params(11))]);
disp(['k_dec_Char = ', num2str(fit_params(12))]);

disp(['k_Syngas = ', num2str(fit_params(13))]);
disp(['m_Syngas = ', num2str(fit_params(14))]);
disp(['n_Syngas = ', num2str(fit_params(15))]);
disp(['k_dec_Syngas = ', num2str(fit_params(16))]);

% Calculate R ² value
y_pred = reaction_model(fit_params, DFA_over_CE);
R2 = 1 - sum((y_pred - [Tar_yield; Water_yield; Char_yield; Syngas_yield]).^2) /
```

```
sum((mean([Tar_yield; Water_yield; Char_yield; Syngas_yield]) - [Tar_yield; Water_yield; Char_yield; Syngas_yield]).^2);

disp(['R² value: ', num2str(R2)]);

% Draw fitting curve
DFA_over_CE_fit = linspace(10, 100, 100);
rates_fit = reaction_model(fit_params, DFA_over_CE_fit);

figure;

subplot(2, 1, 1);
plot(DFA_over_CE, [Tar_yield; Water_yield; Char_yield; Syngas_yield], 'o', 'DisplayName', 'experimental data');
hold on;
plot(DFA_over_CE_fit, rates_fit, '-', 'DisplayName', 'Fit curve');
xlabel('DFA/CE');
ylabel('Product yield');
legend('Location', 'Best');
title('DFA catalytic reaction kinetics fitting');
grid on;

% Draw a schematic diagram of the dynamic model
subplot(2, 1, 2);
DFA_over_CE_model = linspace(10, 100, 100);
rates_model = reaction_model(fit_params, DFA_over_CE_model);

plot(DFA_over_CE_model, rates_model, '-', 'LineWidth', 2);
xlabel('DFA/CE');
ylabel('Product yield');
title('Schematic diagram of dynamic model');
grid on;

function rates = reaction_model(params, DFA_over_LG)
    k1a = params(1);
    k1b = params(2);
    m = params(3);
    n = params(4);
    k2a = params(5);
    p = params(6);
    q = params(7);
    k3 = params(8);
    k4 = params(9);
    k5 = params(10);
```

```
    k6 = params(11);

    %Use the selected dynamic equation
    Rate_LG = k1a * DFA_over_LG.^m + k1b * DFA_over_LG;
    Rate_Syngas = k2a * Rate_LG.^p;
    Rate_Surface = k3 * Rate_Syngas;
    Rate_Tar = k4 * Rate_Syngas;
    Rate_Water = k5 * Rate_Syngas;
    Rate_Char = k6 * Rate_LG;

    % Combine rates into a vector
    rates = [Rate_Tar; Rate_Water; Rate_Char; Rate_Syngas];
end

figure;

%Set coordinate mapping range
x_scale = 5; % Adjust this value to fit the specific situation
y_scale = 5; % Adjust this value to fit the specific situation
% Set the coordinates of reactants and products
LG_x = 1 / x_scale;
Syngas_x = 2 / x_scale;
Tar_x = 2 / x_scale;
Water_x = 2 / x_scale;
Char_x = 2 / x_scale;

LG_y = 2 / y_scale;
Syngas_y = 4 / y_scale;
Tar_y = 3 / y_scale;
Water_y = 2 / y_scale;
Char_y = 1 / y_scale;

% Draw arrows to indicate reactions
annotation('arrow', [LG_x, Syngas_x], [LG_y, Syngas_y], 'HeadWidth', 0.05, 'HeadLength', 0.05);
annotation('arrow', [LG_x, Tar_x], [LG_y, Tar_y], 'HeadWidth', 0.05, 'HeadLength', 0.05);
annotation('arrow', [LG_x, Water_x], [LG_y, Water_y], 'HeadWidth', 0.05, 'HeadLength', 0.05);
annotation('arrow', [LG_x, Char_x], [LG_y, Char_y], 'HeadWidth', 0.05, 'HeadLength', 0.05);

% Add text labels to the diagram
text(LG_x, LG_y, 'LG', 'FontSize', 12, 'HorizontalAlignment', 'right');
text(Syngas_x, Syngas_y, 'Syngas', 'FontSize', 12, 'HorizontalAlignment', 'left');
text(Tar_x, Tar_y, 'Tar', 'FontSize', 12, 'HorizontalAlignment', 'left');
text(Water_x, Water_y, 'Water', 'FontSize', 12, 'HorizontalAlignment', 'left');
text(Char_x, Char_y, 'Char', 'FontSize', 12, 'HorizontalAlignment', 'left');
```

```
% Set axis labels and titles
xlabel('x-axis');
ylabel('Y-axis');
title('Schematic diagram of gasification and cracking reactions');

% show grid
grid on;

A=[0/100
10/100
20/100
30/100
40/100
50/100
60/100
80/100
100/100
];   %The A matrix row represents the number of groups of input data in the training set, and the list shows the number of input indicators;

y=[19.46      26.84     29.21     24.49
17.25     27.64     29.11     26
15.43     28.11     29.3      27.16
14.14     28.23     29.34     28.29
13.89     28.62     29.14     28.35
13.21     29.01     29.33     28.45
12.84     30.07     29.47     27.62
12.57     30.68     29.64     27.11
12.13     31.02     29.87     26.98

]';% The y-matrix row represents the number of groups of input data in the training set, and the list shows the number of input indicators;

[n1,n]=size(A); %%n represents the number of independent variables
[m,m1]=size(y); %m represents the number of dependent variables
p=A';   %Merge all independent variables to obtain the input data matrix
t=y; %Merge all dependent variables into the target data matrix
%Normalizing data using the premnmx function

[pn,minp,maxp,tn,mint,maxt]=premnmx(p,t); % Normalize the input matrix p and output matrix t
u=ones(n,1);
dx=[-1*u,1*u];                    %After normalization, the minimum value is -1 and the maximum value is 1
```

```
%BP network training
net=newff(dx,[n,7,m],{'tansig','tansig','purelin'},'traingdx'); %Establish a model and train it using gradient descent method.

net.trainParam.show=1000;                    %Display results once every 1000 cycles
net.trainParam.Lr=0.05;                      %The learning speed is 0.05
net.trainParam.epochs=50000;                 %The maximum training cycle is 50000 times
net.trainParam.goal=0.65*10^(-3);            %mean squared error
net=train(net,pn,tn);                        %Start training, where pn and tn are input and output samples respectively
%Simulating BP Networks Using Raw Data
an=sim(net,pn);                              %Simulate with trained models
a=postmnmx(an,mint,maxt); % Restore the simulated data to the original order of magnitude;
pnew=[p

    ]  %%Enter the parameters of the independent variable, with each row representing one independent variable and the number of columns representing the number of predictions

pnewn=tramnmx(pnew,minp,maxp); %Normalize the new data using the normalization parameters of the original input data;
anewn=sim(net,pnewn);                        %Simulate using normalized data;
anew=postmnmx(anewn,mint,maxt);    %Restore the simulated data to the original order of magnitude;

disp('Using BP neural network to predict')
disp(anew)
wucha=abs(t-anew)./t;      %relative error
disp('The error predicted using the BP neural network is')
disp(wucha)
```