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Pyrolysis Reaction and Kinetic Analysis of Model Compounds

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Abstract

In this paper, Pearson correlation analysis was used to correlate the different mixing ratios of the three pyrolysis combinations with the associated pyrolysis product yields. Then, a paired-sample t-test model was used to explore whether the catalyst DFA plays an important catalytic role in promoting the pyrolysis of CS, CE and LG. In order to address the effect of mixing ratios of pyrolysis combinations on the yields, this paper plotted line graphs with the mixing ratios of pyrolysis combinations as the horizontal axis and the pyrolysis gas yields as the vertical axis, and interpreted the effect of mixing ratios on the yields of each gas according to the trend of each gas.

Keywords: Pearson correlation coefficient, paired sample T test, catalytic reaction

1. Introduction

With the increasing global demand for renewable energy, biomass has received widespread attention as a mature renewable energy source. Cotton straw, as an agricultural waste, is considered as an important biomass resource because it is rich in biomass components such as CE and LG. A chemical laboratory used the model compound method to establish pyrolysis combinations: DFA/CS, DFA/CE and DFA/LG. The pyrolysis combinations were pyrolyzed at different mixing ratios to investigate the catalytic mechanism and the effect of the generation of DFA/CS pyrolysis products. In this experiment, CE and LG were selected as two representative components of CS as model compounds, and the targeted catalytic effects of DFA on different biomass components were investigated.

2. Research Design

2.1 The Relationship Between Pyrolysis Products and Mixture Ratio of Pyrolysis Combinations was Analyzed Based on Pearson Correlation Coefficient

This paper uses Pearson correlation coefficient to conduct correlation analysis. The relationship between the yield of pyrolysis products (Tar yield, Water yield, Char yield, Syngas yield) and the mixing ratio of the three pyrolysis combinations of (DFA/CS, DFA/CE, DFA/LG) was analyzed[1]. In this paper, whether there is a statistically significant relationship between different mixture ratios of pyrolysis products and pyrolysis combinations is tested to determine whether the P-value is significant ($P<0.05$).

The Pearson correlation coefficient between pyrolysis products and pyrolysis combinations is defined as the quotient of covariance and standard deviation between them, the calculated results are shown in the table 1.

Table 1. Correlation coefficient between pyrolysis combination and products

	DFA/CS	DFA/CE	DFA/LG
Tar yield	-0.883(0.002***)	0.759(0.029**)	-0.794(0.019**)
Water yield	0.984(0.000***)	-0.604(0.113)	0.866(0.005***)
Char yield	0.898(0.001***)	0.367(0.371)	-0.394(0.334)
Syngas yield	0.416(0.265)	-0.79(0.020**)	0.428(0.290)

The Pearson's correlation coefficient is calculated as follows:

$$\rho_{X,Y} = \frac{\operatorname{cov}(X,Y)}{\sigma X \sigma Y} = \frac{E\left[\left(X-\mu x\right)\left(Y-\mu y\right)\right]}{\sigma X \sigma Y} \tag{1}$$

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

$$r = \frac{1}{n-1}\sum_{i=1}^{n}(\frac{X_i - \overline{X}}{\sigma X})(\frac{Y_i - \overline{Y}}{\sigma Y}) \tag{3}$$

It can be concluded from the table that DFA/CS is significantly negatively correlated with Tar yield. There was significant positive correlation with Water yield and Char yield, but no correlation with Syngas yield. DFA/CE was negatively correlated with Syngas yield, significantly positively correlated with Tar yield, and had no correlation with Water yield and Char yield. DFA/LG has a significant negative correlation with Tar yield, a significant positive correlation with Water yield, and no linear relationship with Char yield and Syngas yield.

2.2 Whether DFA has an Effect on Promoting the Pyrolysis of CS,CE and LG was Analyzed Based on Paired Sample T Test

In order to study whether DFA as a catalyst plays an important role in promoting the pyrolysis of CS, CE and LG, the paired sample T test was used to calculate whether there are differences in the yields of paired pyrolysis products among the pyrolysis combinations[2].

First of all, Shapiro-Wilk test was conducted on the data, and the test results were as follows. To check its significance, it can be concluded from the table that the absolute value of sample kurtosis is less than 10, and the absolute value of skewness is less than 3, so it can be described as basically conforming to normal distribution, and thus pairing can be performed.

The test formula is as follows.

$$t = \left(\bar{x}d - \mu d\right) / (sd / \sqrt{n}) \tag{4}$$

Table 2. Normality test results of DFA/CE paired pyrolysis products

Variable name	Average value	Standard deviation	Skewness	Kurtosis	S-W inspect
DFA/CE paired tar yields	-41.595	3.539	1.616	1.816	0.767(0.013**)
DFA/CE paired water yield	-18.775	3.95	-1.691	3.063	0.835(0.067*)
DFA/CE paired Char yield	-23.578	1.068	1.543	2.474	0.855(0.106)
DFA/CE Paired Syngas yield	-14.102	1.523	-0.264	-0.665	0.955(0.766)

The matching results are shown in the table 3.

Table 3. Paired sample T test of DFA/CE and pyrolysis products

paired variable	Mean ± standard deviation			t	df	P	Cohn's d
	Pairing 1	Pairing 2	Pairwise difference				
DFA/CE paired tar yields	0.488±0.304	42.082±3.764	-41.595±3.459	-33.25	7	***	11.755
DFA/CE paired water yield	0.488±0.304	19.262±3.759	-18.775±3.454	-13.45	7	***	4.753
DFA/CE paired Char yield	0.488±0.304	24.065±1.141	-23.577±0.837	-62.46	7	***	22.084
DFA/CE paired Syngas yield	0.488±0.304	14.59±1.271	-14.102±0.966	-26.19	7	***	9.261

According to the analysis results, under the DFA/CE combination, the yield of each product is significantly different from that of the pyrolysis combination, and the Cohen's d values of tar, water, coke and syngas are 11.755, 4.753, 22.084 and 9.261, respectively. In other words, desulfurization ash plays an important role in promoting the pyrolysis of cellulose as a catalyst.

Similarly, the normality test between the pyrolysis combination (DFA/CS) and the pyrolysis products shows that the distribution is basically in line with normal distribution.

The matching results are shown in the table 4.

Table 4. Paired sample T test of DFA/CS and pyrolysis products

paired variable	Mean ± standard deviation			t	df	P	Cohen's d
	Pairing 1	Pairing 2	Pairwise difference				
DFA/CS paired tar yields	0.433±0.328	14.547±2.431	-14.113±2.103	-15.54	8	***	5.18
DFA/CS paired water yield	0.433±0.328	28.913±1.415	-28.48±-1.087	-78.07	8	***	26.025
DFA/CS paired Char yield	0.433±0.328	29.379±0.246	-28.946±0.081	-571	8	***	190.34
DFA/CS paired Syngas yield	0.433±0.328	27.161±1.279	-26.728±0.951	-67.93	8	***	22.64

According to the analysis results, under the DFA/CS combination, there was a significant difference between the yield of each product and the pyrolysis combination. The Cohen's d value of tar, water, coke and syngas was 5.18, 26.025, 190.34 and 22.64, respectively, indicating a very large difference. That is, desulfurization ash as a catalyst plays an important role in promoting the pyrolysis of cotton straw.

Similarly, the normality test between the pyrolysis combination (DFA/LG) and the pyrolysis products shows that the distribution is basically in line with normal distribution.

The matching results are shown in the table 5.

Table 5. Paired sample T test of DFA/LG and pyrolysis products

paired variable	Mean ± standard deviation			t	df	P	Cohen's d
	Pairing 1	Pairing 2	Pairwise difference				
DFA/LG paired tar yields	0.488±0.304	11.3±3.207	-10.812±2.902	-8.86	7	***	3.131
DFA/LG paired water yield	0.488±0.304	20.435±2.539	-19.948±2.234	-24.74	7	***	8.748
DFA/LG paired Char yield	0.488±0.304	57.336±0.373	-56.849±0.068	-283.7	7	***	100.301
DFA/LG paired Syngas yield	0.488±0.304	10.929±1.153	-10.441±0.849	-27.88	7	***	9.857

According to the analysis results, under the DFA/LG combination, there is a significant difference between the yield of each product and the pyrolysis combination. The Cohen's d value of tar, water, coke and syngas is 3.131, 8.748, 100.301 and 9.857, respectively, indicating a very large difference range. That is, desulfurization ash as a catalyst plays an important role in promoting the pyrolysis of lignin.

2.3 Effect of Mixing Ratio of Pyrolysis Combinations on Yield And the Effect of Pyrolysis Gas Per Group

In this paper, the yield of each gas component (H2, CO, CO2, CH4, C2H6, C3, H8, C3H6, C2H4, C4H10) in three pyrolysis combinations (DFA/CS, DFA/CE, DFA/LG) was analyzed with the mixing

ratio. The result is visualized by line chart[3].

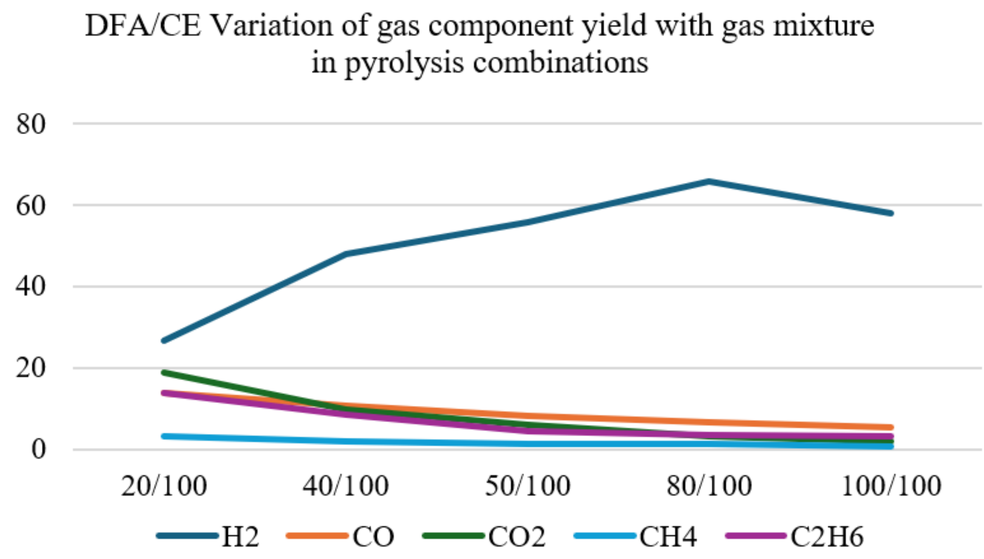

Figure 2. DFA/CE Variation

H2: The H2 yield increases significantly with the increase of the mixture ratio of DFA/CE pyrolysis combination. This is due to the accelerated water vapor displacement of desulfurization ash in the pyrolysis reaction, which significantly promotes the chemical reaction of H2 generation from hydrogen free radicals generated by CE pyrolysis, thus resulting in a rapid increase in H2 yield.

CO and CO2: With the continuous increase of the content of desulfurization ash in the pyrolysis reaction, the oxidation of carbon is promoted, and its catalytic effect inhibits the reaction of CE decomposition to produce CO and CO2, so that the production of CO and CO2 in the pyrolysis gas of desulfurization ash is constantly reduced.

CH4: The component yield of the pyrolysis gas CH4 in DFA/CE is very low, indicating that the thermal decomposition of CE can only produce a very small amount of CH4, and the desulfurization ash has obvious inhibition on the process.

C2H6: The promotion effect of desulfurization ash on CE pyrolysis makes CE produce more and smaller molecular weight free radicals, such as hydroxyl, carbonyl, etc., which inhibits the ring-opening and isomerization of CE structural units to produce 5.C2H6 free radicals, thus reducing the production rate of CH4 and C2H6.

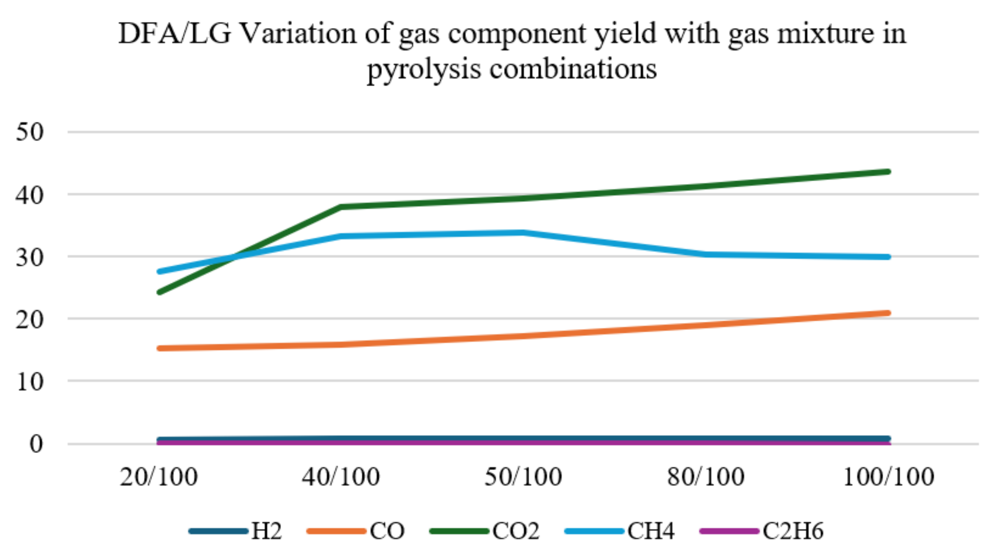

Figure 3. DFA/LG Variation

CH4: component in the CH4 DFA/LG pyrolysis combination is mainly from the break of LG-rich methoxy side chain, and desulfurization ash has a significant inhibition on this process, so the rate of CH4 production slows down in the later process.

C2H6, H2: In this pyrolysis combination reaction, the yields of C2H6 and H2 are very small, indicating that DFA has no obvious catalytic effect on C2H6 and H2 in DFA/LG pyrolysis combination.

CO, CO2: The yield of CO and CO2 increased steadily, indicating that DFA has a certain catalytic effect on CO and CO2.

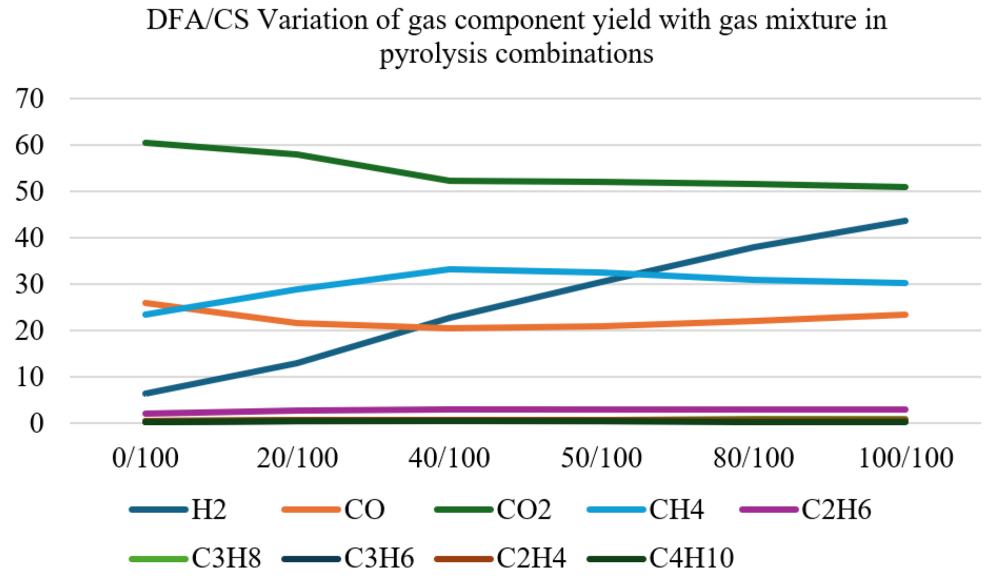

Figure 4. DFA/CS Variation

In this paper, the catalytic mechanism and effects of DFA/CS pyrolysis products (CE, LG) were studied, and it was found that the effects of DFA on the yield of combined gas components in different pyrolysis processes were different. It shows that DFA as catalyst has different catalytic effects in different combinations, so the dosage of DFA can be properly controlled according to the situation of use, so that the gas production rate can achieve an ideal effect, so as to ensure the yield and quality of pyrolysis gas.

3. Conclusion

In this paper, based on each pyrolysis combination, the yields of the relevant pyrolysis products (tar yield, water yield, coke yield, syngas yield) were analyzed at the mixing ratios of the corresponding pyrolysis combinations, and also based on the analyses, it can be concluded that the DFA as a catalyst plays an important role in facilitating pyrolysis at both CS, CE and LG. After producing the corresponding images of the three pyrolysis combinations, the effect of the mixing ratio of the pyrolysis combinations on the pyrolysis gas yield of each group is specifically discussed and explained.

Reference

[1] Li, S., & Jing, D. F. (2006). Distributed activation energy modeling of biomass pyrolysis. Agricultural *Mechanization Research,* (8), 131-133, 140.

[2] Du, Q., Tang, C. Y., An, X. Y., et al. (2023). Study of catalytic biomass pyrolysis gas extraction from desulfurization ash based on model compounds. *Renewable Energy, 41*(6), 711-716. https://doi.org/10.13941/j.cnki.21-1469/tk.2023.06.011

[3] Che, Y. F. (2019). Study on the reaction kinetics and catalysts of carbon dioxide hydrogenation to methanol [Dissertation, East China University of Science and Technology].

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