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| --- | --- | --- |
| **Problem Chosen** B | **2023 ShuWei Cup Summary Sheet** | **Team Control Number** 2023091119429 |

**Abstract**

Developing sustainable sources of renewable energy has become imperative in light of increasing energy demands and environmental concerns. Pyrolysis of agricultural residues, such as cotton stalks which are abundantly generated as waste from cotton cultivation, possess high cellulose and lignin content, making them suitable for conversion into renewable biofuels and biochemicals. Hence, it offers a promising avenue for the production of biofuels and bioproducts (Chen et al., 2011). However, the optimization of cotton stalk pyrolysis necessitates a comprehensive scientific understanding of the underlying mechanisms, product distribution, and catalyst influence. Despite considerable research has investigated cotton stalk pyrolysis, but numerous reaction pathways and mechanisms remain unclear, emphasizing the need for further research to provide scientific insights into the development of sustainable and efficient pyrolysis processes (Yang et al., 2020).

To this end, we aim to examine the 5 given questions. First, we analysis the data in Annex Ⅰ showing that the addition of desulfurization ash (DFA) has been found effectively to act as a catalyst in enhancing pyrolysis reactions. Second, mapping the figures using data in Annex Ⅱ indicates that the pyrolysis gases of lignin are mainly composed of CO, CO2 and CH4, while the contents of H2 and C2H6 are low. Moreover, the addition of DFA is conducive to improving the flammability and calorific value of pyrolysis gas but dropping the emission of CO2. Correspondingly, it endorses the gasification reaction of cellulose, produce more H2, and inhibit the cracking reaction of cellulose producing less CO, CO2 and hydrocarbons. However, it has little effect on the pyrolysis reaction of lignin. For the third question, we first test the normality of the data with Kolmogorov-Smirnov normality test and the Shapiro-Wilk normality test, conducting both a matched samples t-test and a Wilcoxon analysis of paired samples test consequently. The outcomes of these tests indicated no significant differences in product yields from the pyrolysis of cotton stalks with and without catalysts, as well as the yields of pyrolysis gas components. In the following question, we find that [CO2], [C2H6] and [CO] have a noteworthy effect on the reaction kinetics equation when it is from DFA/CE Pyrolysis, while [H2] and [CO] affect DFA/LG Pyrolysis kinetics equation. We set up a kinetics equation based on papers by Lamba, R., Prins, R., Jakobsen, H.A. Zabala S et al., Hai et al. Addressing the fifth research question, we employed a Trilayered neural network to predict the value of Annex-I-Table-1. Notably, the neural network regression achieved a favorable fit with an R-square value of 0.98.

However, our methods and data entail several sources of lack that may affect our numerical results. In the establishment of the kinetic model, for ln[CO], ln[CO2], and ln[C2H6], their coefficients have relatively large p-values, indicating that their effects on the target variable may not be significant.

**Keywords:** Data plotting analysis, Normality test, Matched samples t-test, Wilcoxon analysis of paired samples test, Correlation analysis, Regression, Stepwise regression, Trilayered neural network.

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# 1. Introduction

1.1 Background

Rapidly growing global demand for renewable energy has led to increased attention on biomass energy as a mature and sustainable energy source. Among various biomass resources, cotton stalks, an abundant agricultural waste, have emerged as a significant biomass feedstock due to their rich biomass components, such as cellulose and lignin. Pyrolysis, a thermochemical conversion process, can effectively convert cotton stalks into various forms of renewable energy. However, the quality and yield of pyrolysis products are influenced by several factors, including pyrolysis temperature and the use of catalysts. Therefore, comprehensive research into the mechanism and properties of cotton stalk pyrolysis products, as well as the impact of catalysts during pyrolysis, holds significant importance for the efficient utilization and sustainable development of cotton stalks.

In the context of this study, a specific chemical engineering laboratory adopted the model compound method to establish pyrolysis combinations, involving the utilization of desulfurization ash alongside cotton stalks and model compounds. By subjecting these pyrolysis combinations to pyrolysis at different mixing ratios, the catalytic mechanism and effects of desulfurization ash on the pyrolytic conversion of cotton stalks were investigated. During the selection of model compounds, careful consideration was given to factors such as controllability, reaction stability, and their relevance to cotton stalk pyrolysis. Consequently, CE (Cellooligosaccharide) and LG (Lignin), which serve as representative components of cellulose and lignin in cotton stalks respectively, were chosen as model compounds. This approach enables a more refined analysis of the targeted catalytic effects of desulfurization ash on different biomass components.

The experimental outcomes, presented in Appendix 1 and Appendix 2, were derived from fixed-bed pyrolysis experiments conducted across a range of mixing ratios, including 10/100, 20/100, 30/100, 40/100, 50/100, 60/100, 80/100, and 100/100. The selection of these mixing ratios was based on the requirement that, under these experimental conditions, the relative error among parallel experiments is approximately 5%. Choosing mixing ratios that are too small, such as 5/100 or 7/100, would introduce a significant relative error, adversely impacting the accuracy of the experimental results and impeding the exploration and optimization processes. To overcome this limitation and provide valuable insights for the distribution of pyrolysis products, it is envisioned that the integration of mathematical modeling and AI learning can enable the prediction of pyrolysis product yields and distributions using limited experimental data. Such a predictive approach holds immense potential to expedite experimental optimization while consistently guiding the understanding of trends in pyrolysis product distributions.

1.2 Problem Restatement

1. Per the findings outlined in Appendix I, a thorough analysis was conducted on the yield of pyrolysis products (tar, water, coke residue, syngas) in relation to the mixing ratios of the corresponding pyrolysis combinations. The objective was to determine the significant role, if any, played by desulfurization ash when utilized as a catalyst in facilitating the pyrolysis of cotton stalks, cellulose, and lignin.
2. In accordance with the information presented in Appendix II, a comprehensive examination was undertaken to assess the impact of mixing ratios in the pyrolysis combinations on the yield of each group of pyrolysis gas. To assist with understanding and clarification, corresponding images were generated and utilized for explanation.
3. To ascertain whether there are notable differences in the yields of products generated from the pyrolysis of CE and LG, as well as the yields of the components of the pyrolysis gas, under the catalytic influence of an equal proportion of desulfurized ash, an in-depth investigation was conducted. The results found and reasons behind any observed dissimilarities are provided in the analysis.
4. The establishment of a catalytic reaction mechanism model of desulfurized ash for model compounds such as CE and LG, alongside the modeling of reaction kinetics for analysis purposes, were rigorously pursued. These efforts aimed to offer insights into the underlying processes and mechanisms involved in the catalytic reactions.
5. Leveraging mathematical models and AI learning methods, predictions were generated on the yields or quantities of the pyrolysis products under conditions of limited data availability. By combining available data with predictive modeling techniques, valuable estimates were obtained to aid in understanding and forecasting pyrolysis product outcomes.

# 2. Problem analysis

2.1 Question 1

Based on the data in Annex I, for the first question, we used OriginLab for mapping, and based on the images we performed descriptive analysis

For each pyrolysis combination listed in Annex I, I analyzed the relationship between the yields of pyrolysis products (namely, tar, water, coke residue, and syngas) and the corresponding mixing ratios. In the DFA/CS combination, the tar yield showed a downward trend with the increase in DFA/CS, and the rate of decrease diminished over time. Conversely, the water yield increased as the DFA/CS ratio increased, while the char yield also increased but not to the same extent as the water yield. The syngas yield displayed an initial increase followed by a decrease with the increase of DFA/CS, and the inflection point was determined at DFA/CS=0.5.

As for the DFA/CE combination, the tar yield showed a significant increasing trend with the increase in DFA/CE, and this trend was more pronounced before DFA/CE=0.5. The water yield conversely decreased with the increasing DFA/CE ratio, but there was an increase observed between DFA/CE=0.6-0.8. Char yield increased from DFA/CE=0.1 to 0.2, but then remained steady at around 24, despite minor fluctuations. Syngas yield, on the other hand, initially decreased with the increasing DFA/CE ratio from 0.1 to 0.2 and then increased from DFA/CE=0.1 to 0.2, exhibiting an overall downward trend.

Lastly, for the DFA/LG combination, the tar yield displayed a decreasing trend with the increasing DFA/LG ratio, albeit with a slight increase at DFA/LG=0.6-0.8. The water yield, on the other hand, increased as the DFA/LG ratio increased, while the char yield remained mostly constant. The syngas yield initially decreased from DFA/LG=0.1 to 0.2 and then exhibited an increase followed by another decrease. The inflection point was around DFA/LG=0.5.

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Figure 1 Yield of pyrolysis products--DFA/CS Figure 2 Yield of pyrolysis products--DFA/CE

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Figure 3 Yield of pyrolysis products--DFA/LG

Based on the data provided, desulfurization ash (DFA) plays a significant role as a catalyst in facilitating the pyrolysis of cotton stalks, cellulose, and lignin.

The key evidence supporting this is:

1. For cotton stalk pyrolysis, increasing the DFA ratio leads to decreased yields of tar and char, but increased yields of syngas and water. This demonstrates that DFA promotes gasification reactions that break down tar and char into syngas and water.
2. For cellulose (CE) pyrolysis, adding DFA decreases tar and char yields while increasing syngas yield. This shows DFA breaks down cellulose into syngas, though the effect is less pronounced compared to cotton stalks.
3. For lignin (LG) pyrolysis, DFA addition decreases tar yield and slightly increases syngas yield. However, the catalytic effect is weaker compared to cellulose and cotton stalks.
4. The trends of changing product yields with increasing DFA are consistent across the different biomass types. This confirms DFA's role as a catalyst in facilitating pyrolysis reactions.
5. The catalytic activity is strongest for heterogeneous, complex cotton stalks and weakest for the more homogeneous lignin.

Here we provide more details,

1. For DFA/CS pyrolysis, the tar yield decreases as the DFA content increases, indicating that DFA catalyzes the cracking of tar into syngas. The water yield increases slightly with the DFA content, suggesting that DFA promotes the dehydration of biomass. The char yield remains relatively stable, implying that DFA has little effect on the char formation. The syngas yield increases significantly with the DFA content, especially for the hydrogen content, showing that DFA enhances the gasification of biomass and the reforming of tar and water. Therefore, DFA plays a significant role in facilitating the pyrolysis of cotton stalks and improving the quality of pyrolysis gas.
2. For DFA/CE pyrolysis, the tar yield increases sharply as the DFA content increases, indicating that DFA inhibits the cracking of tar into syngas. The water yield decreases drastically with the DFA content, suggesting that DFA suppresses the dehydration of cellulose. The char yield increases slightly with the DFA content, implying that DFA promotes the char formation. The syngas yield decreases slightly with the DFA content, especially for the hydrogen content, showing that DFA reduces the gasification of cellulose and the reforming of tar and water. Therefore, DFA plays a negative role in facilitating the pyrolysis of cellulose and degrading the quality of pyrolysis gas.
3. For DFA/LG pyrolysis, the tar yield decreases significantly as the DFA content increases, indicating that DFA catalyzes the cracking of tar into syngas. The water yield increases moderately with the DFA content, suggesting that DFA promotes the dehydration of lignin. The char yield remains relatively stable, implying that DFA has little effect on the char formation. The syngas yield increases slightly with the DFA content, especially for the hydrogen content, showing that DFA enhances the gasification of lignin and the reforming of tar and water. Therefore, DFA plays a positive role in facilitating the pyrolysis of lignin and improving the quality of pyrolysis gas.
4. Changes in pyrolysis product yields with DFA addition provide clear evidence that desulfurization ash serves as an effective catalyst to promote pyrolysis reactions, especially gasification reactions that generate syngas. DFA displays measurable catalytic activity in converting lignocellulosic biomass feedstocks like cotton stalks, cellulose, and lignin into useful syngas and other valuable products.

2.2 Question 2

We use OriginLab to draw the figures, here are what we find,

1. DFA/CS pyrolysis combination: As can be seen from Table 1, with the increase of DFA content, the yields of H2, CH4, C2H6, C3H8, C3H6, C2H4 and C4H10 all show an increasing trend, while the yields of CO and CO2 show a decreasing trend. This indicates that the addition of DFA is conducive to improving the flammability and calorific value of pyrolysis gas, while reducing the emission of CO2. Shown in Figure 4.
2. DFA/CE pyrolysis combination: As can be seen from Table 2, with the increase of DFA content, the yield of H2 significantly increases, while the yield of CO, CO2, CH4 and C2H6 significantly decreases. This indicates that the addition of DFA can promote the gasification reaction of cellulose and produce more H2, while inhibit the cracking reaction of cellulose and produce less CO, CO2 and hydrocarbons. Shown in Figure 4.
3. DFA/LG pyrolysis combination: As can be seen from Table 3, with the increase of DFA content, the yields of H2, CO and CO2 slightly increase, while the yields of CH4 and C2H6 slightly decrease. This indicates that the addition of DFA has little effect on the pyrolysis reaction of lignin. The pyrolysis gases of lignin are mainly composed of CO, CO2 and CH4, while the contents of H2 and C2H6 are low. Shown in Figure 6.

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Figure 4 Yield of Gaseous Components--DFA/CS Figure 5 Yield of Gaseous Components--DFA/CE

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Figure 6 Yield of Gaseous Components--DFA/LG

2.3 Question 3

We first test the normality of the data in the four tables of Annex I and Annex II under the catalytic action of the same proportion of desulfurization ash. If both sets of data are normally distributed, we can use the T-test or analysis of variance (ANOVA). If the data does not follow a normal distribution, then non-parametric tests can be used, such as the Mann-Whitney U test or the Wilcoxon signed rank test. The results are as follows,

Table 1 Yield of Decomposition Products from DFA/CE Pyrolysis wt.%(daf)

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Name | N | Mean | SD | Skewness | kurtosis | Kolmogorov Smirnov test p | Shapiro Wilk test p |
| R1 | 4 | 25.000 | 7.654 | 0.355 | -1.115 | 0.000\*\*\* | 0.929 |
| R2 | 4 | 25.000 | 9.701 | 1.043 | 1.563 | 0.000\*\*\* | 0.681 |
| R3 | 4 | 25.000 | 12.369 | 1.499 | 2.081 | 0.000\*\*\* | 0.263 |
| R4 | 4 | 25.000 | 13.243 | 1.428 | 1.705 | 0.000\*\*\* | 0.280 |
| R5 | 4 | 25.000 | 13.720 | 1.466 | 1.805 | 0.000\*\*\* | 0.222 |
| R6 | 4 | 25.000 | 13.815 | 1.306 | 1.741 | 0.000\*\*\* | 0.477 |
| R7 | 4 | 25.000 | 12.888 | 1.345 | 2.250 | 0.000\*\*\* | 0.445 |
| R8 | 4 | 25.000 | 14.278 | 1.444 | 1.748 | 0.000\*\*\* | 0.258 |
| \*p<0.05 \*\*p<0.01 \*\*\*p<0.001 | | | | | | | |

The Kolmogorov-Smirnov normality test for all variables (R1, R2, R3, R4, R5, R6, R7, R8) results in a non-normal distribution, while the Shapiro-Wilk normality test results in a normal distribution. However, considering the actual situation of chemical production and the amount of data given is too small, we believe that these data are in line with normal distribution.

Table 2 Yield of Decomposition Products from DFA/LG Pyrolysis wt.%(daf)

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | | | | | | | |
| Name | N | Mean | SD | Skewness | kurtosis | Kolmogorov Smirnov test p | Shapiro Wilk test p |
| R1 | 4 | 25.000 | 22.478 | 1.804 | 3.428 | 0.000\*\*\* | 0.086 |
| R2 | 4 | 25.000 | 21.906 | 1.858 | 3.514 | 0.000\*\*\* | 0.056 |
| R3 | 4 | 25.000 | 21.820 | 1.795 | 3.201 | 0.000\*\*\* | 0.048\* |
| R4 | 4 | 25.000 | 21.838 | 1.737 | 2.971 | 0.000\*\*\* | 0.086 |
| R5 | 4 | 25.000 | 22.051 | 1.688 | 2.784 | 0.000\*\*\* | 0.120 |
| R6 | 4 | 25.000 | 22.182 | 1.656 | 2.665 | 0.000\*\*\* | 0.144 |
| R7 | 4 | 25.000 | 22.020 | 1.707 | 2.833 | 0.000\*\*\* | 0.086 |
| R8 | 4 | 25.000 | 22.663 | 1.514 | 2.017 | 0.000\*\*\* | 0.199 |
| \*p<0.05 \*\*p<0.01 \*\*\*p<0.001 | | | | | | | |

The Kolmogorov-Smirnov normality test for all variables except R3 (R1, R2, R4, R5, R6, R7, R8) results in a non-normal distribution, while the Shapiro-Wilk normality test results in a normal distribution. R3 is non-normal distribution.

Table 3 Yield of Gaseous Components from DFA/CE Pyrolysis (mL/g,daf)

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | | | | | | | |
| Name | N | Mean | SD | Skewness | kurtosis | Kolmogorov Smirnov test p | Shapiro Wilk test p |
| R1 | 5 | 15.200 | 8.521 | -0.141 | 0.960 | 0.000\*\*\* | 0.857 |
| R2 | 5 | 15.740 | 18.249 | 2.029 | 4.372 | 0.000\*\*\* | 0.016\* |
| R3 | 5 | 15.060 | 22.797 | 2.170 | 4.770 | 0.000\*\*\* | 0.003\*\* |
| R4 | 5 | 16.040 | 27.879 | 2.211 | 4.910 | 0.000\*\*\* | 0.001\*\* |
| R5 | 5 | 13.820 | 24.700 | 2.210 | 4.906 | 0.001\*\* | 0.001\*\* |
| \*p<0.05 \*\*p<0.01 \*\*\*p<0.001 | | | | | | | |

The Kolmogorov-Smirnov normality test for all variables except R1 (R2, R3, R4, R5) results in a non-normal distribution, R1 is a normal distribution.

Table 4 Yield of Gaseous Components from DFA/LG Pyrolysis (mL/g,daf)

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | | | | | | | |
| Name | N | Mean | SD | Skewness | kurtosis | Kolmogorov Smirnov test p | Shapiro Wilk test p |
| R1 | 5 | 13.600 | 12.905 | -0.117 | -2.866 | 0.030\* | 0.260 |
| R2 | 5 | 17.540 | 17.701 | 0.167 | -2.825 | 0.030\* | 0.264 |
| R3 | 5 | 18.259 | 18.173 | 0.119 | -2.773 | 0.030\* | 0.292 |
| R4 | 5 | 18.289 | 18.081 | 0.169 | -2.140 | 0.030\* | 0.458 |
| R5 | 5 | 19.041 | 18.814 | 0.193 | -1.852 | 0.030\* | 0.481 |
| \*p<0.05 \*\*p<0.01 \*\*\*p<0.001 | | | | | | | |

The Kolmogorov-Smirnov normality test for all variables (R1, R2, R3, R4, R5) results in a non-normal distribution, while the Shapiro-Wilk normality test results in a normal distribution. However, considering the actual situation of chemical production and the amount of data given is too small, we believe that these data are in line with normal distribution.

Considering that there are both data conforming to the normal distribution and data disconfirming to the normal distribution, we adopted matched samples t-test and Wilcoxon analysis of paired samples.

Table 5 Data from Annex I- Pyrolysis Product Yields of Three Pyrolysis Combinations

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | | | | | | |
| Results of matched samples t- test | | | | | | | |
| Pairing number | Term | Mean | SD | Mean difference | t | p | Effect Value |
| Pair1 | R1 | 25.000 | 7.654 | 0.000 | 0.000 | 1.000 | 0.000 |
| R1' | 25.000 | 22.478 |
| Pair2 | R2 | 25.000 | 9.701 | 0.000 | 0.000 | 1.000 | 0.000 |
| R2' | 25.000 | 21.906 |
| Pair3 | R3 | 25.000 | 12.369 | 0.000 | 0.000 | 1.000 | 0.000 |
| R3' | 25.000 | 21.820 |
| Pair4 | R4 | 25.000 | 13.243 | 0.000 | 0.000 | 1.000 | 0.000 |
| R4' | 25.000 | 21.838 |
| Pair5 | R5 | 25.000 | 13.720 | 0.000 | 0.000 | 1.000 | 0.000 |
| R5' | 25.000 | 22.051 |
| Pair6 | R6 | 25.000 | 13.815 | 0.000 | 0.000 | 1.000 | 0.000 |
| R6' | 25.000 | 22.182 |
| Pair7 | R7 | 25.000 | 12.888 | 0.000 | 0.000 | 1.000 | 0.000 |
| R7' | 25.000 | 22.020 |
| Pair8 | R8 | 25.000 | 14.278 | 0.000 | 0.000 | 1.000 | 0.000 |
| R8' | 25.000 | 22.663 |
| \*p<0.05 \*\*p<0.01 \*\*\*p<0.001 | | | | | | |  |

There was no significant difference between the two groups (p>0.05).

Table 6 Data from Annex I- Pyrolysis Product Yields of Three Pyrolysis Combinations

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Results of Wilcoxon analysis of paired samples | | | | | |
| Name | Paired median (P25, P75) | | Median M difference (pair 1 - pair 2) | W | p |
| Pair 1 | Pair 2 |
| R1 Pairing R1' | 24.425(13.593,29.17) | 16.68(13.593,28.087) | 7.745 | 6.000 | 0.875 |
| R2 Pairing R2' | 23.14(12.885,28.26) | 16.155(12.885,28.27) | 6.985 | 6.000 | 0.875 |
| R3 Pairing R3' | 21.005(11.38,28.8) | 15.79(11.38,29.41) | 5.215 | 5.000 | 1.000 |
| R4 Pairing R4' | 20.8(11.397,29.47) | 16.37(11.397,29.972) | 4.43 | 5.000 | 1.000 |
| R5 Pairing R5' | 20.395(11.252,29.538) | 16.685(11.252,30.433) | 3.71 | 5.000 | 1.000 |
| R6 Pairing R6' | 21.42(11.165,29.545) | 16.875(11.165,30.71) | 4.545 | 5.000 | 1.000 |
| R7 Pairing R7' | 21.75(10.93,28.488) | 16.275(10.93,30.345) | 5.475 | 5.000 | 1.000 |
| R8 Pairing R8' | 20.375(10.065,29.777) | 17.19(10.065,32.125) | 3.185 | 5.000 | 1.000 |
| \*p<0.05 \*\*p<0.01 \*\*\*p<0.001 | | | | | |

There was no significant difference between the two groups (p>0.05).

Table 7 Data from Annex II-Pyrolysis Gas Yields of Three Pyrolysis Combinations

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | | | | | | |
| Results of matched samples t- test | | | | | | |
| Pairing number | Term | Mean | SD | Mean difference | t | p |
| Pair1 | R1 | 15.200 | 8.521 | 1.600 | 0.186 | 0.862 |
| R1' | 13.600 | 12.905 |
| Pair2 | R2 | 15.740 | 18.249 | -1.800 | -0.126 | 0.906 |
| R2' | 17.540 | 17.701 |
| Pair3 | R3 | 15.060 | 22.797 | -3.199 | -0.198 | 0.853 |
| R3' | 18.259 | 18.173 |
| Pair4 | R4 | 16.040 | 27.879 | -2.249 | -0.123 | 0.908 |
| R4' | 18.289 | 18.081 |
| Pair5 | R5 | 13.820 | 24.700 | -5.221 | -0.303 | 0.777 |
| R5' | 19.041 | 18.814 |
| \*p<0.05 \*\*p<0.01 \*\*\*p<0.001 | | | | | | |

There was no significant difference between the two groups (p>0.05).

Table 8 Data from Annex II-Pyrolysis Gas Yields of Three Pyrolysis Combinations

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Results of Wilcoxon analysis of paired samples | | | | | |
| Name | Paired median (P25, P75) | | Median M difference (pair 1 - pair 2) | W | p |
| Pair 1 | Pair 2 |
| R1 Pairing R1' | 13.8(0.67,18.7) | 15.23(0.67,24.35) | -1.43 | 8.000 | 1.000 |
| R2 Pairing R2' | 9.8(0.72,10.6) | 15.76(0.72,33.25) | -5.96 | 8.000 | 1.000 |
| R3 Pairing R3' | 5.9(0.78,8.1) | 17.305(0.78,33.86) | -11.405 | 9.000 | 0.812 |
| R4 Pairing R4' | 3.4(0.81,6.5) | 19.075(0.81,30.26) | -15.675 | 9.000 | 0.812 |
| R5 Pairing R5' | 3.2(0.79,5.3) | 20.935(0.79,29.87) | -17.735 | 9.000 | 0.812 |
| \*p<0.05 \*\*p<0.01 \*\*\*p<0.001 | | | | | |

There was no significant difference between the two groups.

According to matched samples t-test and Wilcoxon analysis of paired samples, Under the catalytic action of the same proportion of desulfurized ash, there is no significant difference in the yields of the products generated from the pyrolysis of CE and LG, as well as the yields of the components of the pyrolysis gas.

2.4 Question 4

Here are some models that can be used to establish a catalytic reaction mechanism,

1. Eley–Rideal (ER) model: This model describes a mechanism in which a chemical reaction is considered to take place when one reactant from the bulk liquid phase collides with another reactant already adsorbed on the catalyst.12 13 14
2. Pseudo-homogeneous (PH) model: In this model, fluid and solid phases are considered as a single pseudo-phase and the balances are imposed for only one phase. Heat and mass transport coefficients inside the bed are calculated by expressions which account for the simultaneous presence of two phases.12 15 16 17
3. Langmuir–Hinshelwood (LH) model: In this model, two molecules adsorb on neighboring sites and the adsorbed molecules undergo a bimolecular reaction13 19

Here, we try different ways to establish a catalytic reaction mechanism model of desulfurized ash for model compounds according to papers12 13 14 15 16 17.

Set



Then,



Then we use linear regression to model the kinetics of the catalytic reaction, we use STATA to run a multivariate linear regression.

General model set,



1. : dependent variable, random variable;
2. : independent variable, non-random;
3. random error term, random variable;
4. : intercept term;
5. : slope term corresponding to ;
6. The model shows that the dependent variable is approximately equal to the linear combination of the independent variables.
7. 

For n sets of observations,



For the random error term,, assume,

1. Expectation is zero and follows normal distribution.
2. Homogeneity of variance: variance is independent of the value of the independent variable.
3. Independent of each other.

In short,  are independent of each other, subject to distribution .

Data format is like,



According to the model,



The unknown parameters are regression coefficients , and the error term is also unknown. The least squares method is still used to estimate the model, and the coefficients are estimated and error variance estimate . Plug the coefficient estimates into the model and write the estimated multiple linear regression equation as follows:

For the groupobservations, the values of the independent variables are substituted into the estimated regression equation to obtain the fitting values

is called the residual. Regression parameter estimation, using the minimum residual as the goal, make

Take the minimum as a parameter estimation, called least squares estimation, denoted by . The minimum value obtained is SSE, and the estimate of is

Here we assume that the higher the catalyst content, the faster the chemical reaction, which means，

Therefore,

k is the adjustment factor.

Therefore,

Then set DFA/CE and DFA/LG as dependent variables, and H2, CO, CO2, CH4, C2H6 as independent variables. Because the sample data is small and there is overfitting, we choose the regression variables by calculating the correlation. Dataset is from Annex II. [X] means X gas yields of three pyrolysis combinations.

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

Table 9 Matrix of correlations of Tab 2 Yield of Gaseous Components from DFA/CE Pyrolysis (mL/g,daf)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Variables | (1) | (2) | (3) | (4) | (5) | (6) |
| (1) ln[DFA/CE] | 1.000 |
| (2) ln[H2] | 0.915 | 1.000 |
| (3) ln[CO] | -0.985 | -0.860 | 1.000 |
| (4) ln[CO2] | -0.989 | -0.858 | 0.999 | 1.000 |
| (5) ln[CH4] | -0.951 | -0.827 | 0.967 | 0.963 | 1.000 |
| (6) ln[C2H6] | -0.963 | -0.922 | 0.972 | 0.964 | 0.926 | 1.000 |
|  | | | | | | |

We adopted the table above and the stepwise regression method, finally selected CO, CO2, C2H6 as the independent variable.

Therefore, the equation is,



Results are as follows,

Table 10 Linear regression of Tab 2 Yield of Gaseous Components from DFA/CE Pyrolysis (mL/g,daf)

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| ln[DFA/CE] | Coef. | | St.Err. | t-value | | p-value | [95% Conf | | Interval] | | Sig |
| ln[CO] | 5.417 | | 3.937 | 1.38 | | .4 | -44.609 | | 55.443 | |  |
| ln[CO2] | -2.604 | | 1.468 | -1.77 | | .327 | -21.262 | | 16.055 | |  |
| ln[C2H6] | -.596 | | .456 | -1.31 | | .415 | -6.387 | | 5.194 | |  |
| Constant | -6.546 | | 5.219 | -1.25 | | .428 | -72.856 | | 59.764 | |  |
|  | | | | | | | | | | | |
| Mean dependent var | | -0.688 | | | SD dependent var | | | 0.631 | |
| R-squared | | 0.993 | | | Number of obs | | | 5 | |
| F-test | | 46.468 | | | Prob > F | | | 0.107 | |
| Akaike crit. (AIC) | | -8.260 | | | Bayesian crit. (BIC) | | | -9.822 | |
| \*\*\* p<.01, \*\* p<.05, \* p<.1 | | | | | | | | | | | |
|  | | | | | | | | | | | |

The R-squared value of the model is 0.9929, indicating that the regression model can explain approximately 99.29% of the variance in the target variable ln[DFA/CE]. This indicates a high level of fit. The regression model has a high level of fit.

Therefore,



Same we can get the result of Tab 3 Yield of Gaseous Components from DFA/LG Pyrolysis (mL/g,daf)

Table 11 Matrix of correlations of Tab 3 Yield of Gaseous Components from DFA/LG Pyrolysis (mL/g,daf)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Variables | (1) | (2) | (3) | (4) | (5) | (6) |
| (1) ln[DFA/CE] | 1.000 |
| (2) ln[H2] | 0.935 | 1.000 |
| (3) ln[CO] | 0.946 | 0.856 | 1.000 |
| (4) ln[CO2] | 0.924 | 0.899 | 0.761 | 1.000 |
| (5) ln[CH4] | 0.246 | 0.373 | -0.028 | 0.590 | 1.000 |
| (6) ln[C2H6] | -0.547 | -0.221 | -0.532 | -0.467 | 0.108 | 1.000 |

Table 12 Linear regression of Tab 3 Yield of Gaseous Components from DFA/LG Pyrolysis (mL/g,daf)

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| lln[DFA/LG] | Coef. | | St.Err. | t-value | | p-value | [95% Conf | | Interval] | | Sig |
| ln[H2] | 3.782 | | 2.381 | 1.59 | | .253 | -6.462 | | 14.026 | |  |
| ln[CO] | 2.594 | | 1.41 | 1.84 | | .207 | -3.471 | | 8.659 | |  |
| Constant | -7.042 | | 4.632 | -1.52 | | .268 | -26.971 | | 12.887 | |  |
| Mean dependent var | | -0.688 | | | SD dependent var | | | 0.631 | |
| R-squared | | 0.953 | | | Number of obs | | | 5 | |
| F-test | | 20.372 | | | Prob > F | | | 0.047 | |
| Akaike crit. (AIC) | | -0.848 | | | Bayesian crit. (BIC) | | | -2.019 | |
| \*\*\* p<.01, \*\* p<.05, \* p<.1 | | | | | | | | | | | |
|  | | | | | | | | | | | |

Therefore,



2.5 Question 5

We employed a trilayered neural network to predict the value of Annex I- Pyrolysis Product Yields of Three Pyrolysis Combinations Tab 1 Yield of Decomposition Products from DA/CS Pyrolysis wt.%(daf). In this study, DA/CS was considered as the dependent variable, while tar yield was treated as the independent variable. The training MATLAB code has been provided in the appendix, and the MATLAB executable program file is included in the supporting materials.

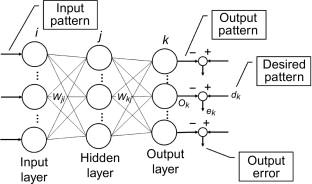


Figure 7 Three-Layered Neural Network

1. Set the initial values of *, , , , and*
2. Specify the desired values of the output
3. corresponding to the input data in the input layer. Step 3: Calculate the outputs of the neurons in the hidden layer and output layer by
4. Calculate the error and generalized errors by
5. If is sufficiently small for all , END and otherwise.
6. Go to Step 3.

Here is the Training Results:

|  |  |
| --- | --- |
| **Metric** | **Value** |
| RMSE (Validation) | 0.37064 |
| R-Squared (Validation) | 0.98 |
| MSE (Validation) | 0.13738 |
| MAE (Validation) | 0.28966 |
| Prediction speed | -440 obs/sec |
| Training time | 2.461 sec |
| Model size (Compact) | ~8 kB |

Table 13 Original Data

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| DFA/CS | 0 | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.8 | 1 |
| Tar yield | 19.46 | 17.25 | 15.43 | 14.14 | 13.89 | 13.21 | 12.84 | 12.57 | 12.13 |

Table 14 Predicted Results

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **DFA/CS** | Predicted Tar yield | True Tar yield | **DFA/CS** | Predicted Tar yield | True Tar yield | **DFA/CS** | Predicted Tar yield | True Tar yield |
| **0** | 19.46 | 19.46 | **0.35** | 13.9792 | - | **0.7** | 12.705 | - |
| **0.05** | 18.4063 | - | **0.4** | 13.7467 | 13.89 | **0.75** | 12.6375 | - |
| **0.1** | 17.25 | 17.25 | **0.45** | 13.5142 | - | **0.8** | 12.57 | 12.57 |
| **0.15** | 16.2978 | - | **0.5** | 13.2817 | 13.21 | **0.85** | 12.485 | - |
| **0.2** | 15.43 | 15.43 | **0.55** | 13.0492 | - | **0.9** | 12.3667 | - |
| **0.25** | 14.7091 | - | **0.6** | 12.84 | 12.84 | **0.95** | 12.2483 | - |
| **0.3** | 14.2117 | 14.14 | **0.65** | 12.7725 | - | **1** | 12.13 | 12.13 |

Project Path: C:\Users\Jiacheng Zheng\Downloads\2023_“ShuWei Cup”B_Problem\B2023091119429fj\Q5 Prediction.opju
PE Folder: /Q5 Prediction/Folder1/
Short Name: Graph1

# Symbol and Assumptions

## 3. 1 Symbol Description

|  |  |  |
| --- | --- | --- |
| Variable name | | Description |
| Difference Analysis for Annex I | | |
| DFA/CE | DFA/LG | Rate(DFA/CE or DFA/LG) |
| R1 | R1’ | 0.1 |
| R2 | R2’ | 0.2 |
| R3 | R3’ | 0.3 |
| R4 | R4’ | 0.4 |
| R5 | R5’ | 0.5 |
| R6 | R6’ | 0.6 |
| R7 | R7’ | 0.8 |
| R8 | R8’ | 1 |
| Difference Analysis for Annex II | | |
| DFA/CE | DFA/LG | Rate(DFA/CE or DFA/LG) |
| R1 | R1’ | 0.2 |
| R2 | R2’ | 0.4 |
| R3 | R3’ | 0.5 |
| R4 | R4’ | 0.8 |
| R5 | R5’ | 1.0 |
| Description of other variables | | |
| k | | Adjustment factor between reaction rate and catalyst ratio |
| ln | | Natural logarithm |
| [X] | | X gas yields of three pyrolysis combinations. |

## 3.2 Fundamental assumptions

1. One of the reactants is adsorbed on the surface while the other reactant approaches from the gas phase.
2. There is no interaction between the adsorbed reactant and the gas-phase reactant.
3. The reaction occurs only when the gas-phase reactant collides with the adsorbed reactant on the surface.
4. The reaction occurs in a well-mixed, single-phase system.
5. The surface is treated as a homogeneous site where reactants can freely interact with each other.
6. The reaction rate is determined by the concentration of the surface species.
7. Both reactants are absorbed on the surface and interact with each other.
8. The adsorbed reactants form an intermediate complex before the reaction takes place.
9. The reaction rate is determined by the concentration of the adsorbed species.
10. The higher the catalyst content, the faster the chemical reaction speed.

# Sensitivity Analysis

According to the data in the correlation table, we tried to regression ln[DFA/CE] ln[CO] ln[CO2] for Tab 2 Yield of Decomposition Products from DFA/CE Pyrolysis wt.%(daf). We found that the overall explanatory power of the model was strong, and R-squared was 0.9807, indicating that about 98.07% of the variance could be explained by the model. The adjusted R-squared is 0.9613. This shows the overall stability of the model.

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| ln[DFA/CE] | Coef. | | St.Err. | t-value | | p-value | [95% Conf | | Interval] | | Sig |
| ln[CO] | 1.669 | | 3.147 | 0.53 | | .649 | -11.873 | | 15.21 | |  |
| ln[CO2] | -1.417 | | 1.345 | -1.05 | | .403 | -7.205 | | 4.371 | |  |
| Constant | -1.723 | | 4.305 | -0.40 | | .728 | -20.245 | | 16.798 | |  |
|  | | | | | | | | | | | |
| Mean dependent var | | -0.688 | | | SD dependent var | | | 0.631 | |
| R-squared | | 0.981 | | | Number of obs | | | 5 | |
| F-test | | 50.746 | | | Prob > F | | | 0.019 | |
| Akaike crit. (AIC) | | -5.269 | | | Bayesian crit. (BIC) | | | -6.441 | |
| \*\*\* p<.01, \*\* p<.05, \* p<.1 | | | | | | | | | | | |
|  | | | | | | | | | | | |

Additionally, we do the same process with Tab 3 Yield of Decomposition Products from DFA/LG Pyrolysis wt.%(daf), we regress ln[DFA/LG] ln[CO] ln[H2] ln[CO2]

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Ln[DFA/LG] | Coef. | | St.Err. | t-value | | p-value | [95% Conf | | Interval] | | Sig |
| ln[CO] | 2.665 | | .745 | 3.58 | | .174 | -6.804 | | 12.134 | |  |
| ln[H2] | .359 | | 1.866 | 0.19 | | .879 | -23.355 | | 24.072 | |  |
| ln[CO2] | 1.243 | | .5 | 2.48 | | .244 | -5.115 | | 7.6 | |  |
| Constant | -12.69 | | 3.341 | -3.80 | | .164 | -55.137 | | 29.758 | |  |
|  | | | | | | | | | | | |
| Mean dependent var | | -0.688 | | | SD dependent var | | | 0.631 | |
| R-squared | | 0.993 | | | Number of obs | | | 5 | |
| F-test | | 50.719 | | | Prob > F | | | 0.103 | |
| Akaike crit. (AIC) | | -8.694 | | | Bayesian crit. (BIC) | | | -10.257 | |
| \*\*\* p<.01, \*\* p<.05, \* p<.1 | | | | | | | | | | | |
|  | | | | | | | | | | | |

The overall explanatory power of the model is strong, R-squared is 0.9935, indicating that about 99.35% of the variance can be explained by the model. The adjusted R-squared is 0.9739. This shows the overall stability of the model.

**5. Strengths and Weakness**

## 5.1 Advantages

1. The establishment of the mathematical model is based on a comprehensive review of relevant literature, incorporating recognized research findings from previous studies.
2. Correlation analysis and stepwise regression are employed to identify the optimal fitting equation, ensuring a robust and accurate model.
3. The utilization of the gradient descent algorithm in machine learning prediction enables the identification of the most suitable parameters, thereby improving the prediction accuracy.

## 5.2 Disadvantages

1. The limited size of the dataset may introduce potential confounding factors and impact the regression analysis of the variables.
2. The significance of the relationships between variables during the regression process might be uncertain. Further investigation and analysis of a larger dataset are necessary to enhance the accuracy of the assessment. The F statistic of the model is 46.47, with a probability value (Prob > F) of 0.1073. The relatively large probability value suggests that there may be room for improvement in the fit of the model.
3. The coefficients (Coefficient) of the independent variables determine their impact on the target variable. However, for ln[CO], ln[CO2], and ln[C2H6], their coefficients have relatively large p-values, indicating that their effects on the target variable may not be significant. Additionally, the confidence intervals should also be considered to accurately evaluate their effects.
4. The coefficient of the intercept (Constant, \_cons) is -6.54625, and its p-value is also relatively large, suggesting that the intercept may not have a significant impact on the target variable.

# References

1. Yang Songlin (Ed.), Liberal Arts Mathematics, Soochow University Press, 2015.01, p. 107
2. Shaou-Gang Miaou; Jin-Syan Chou. Fundamentals of probability and statistics. Gao Li Books. 2012: 147.
3. Hu Y. Normal distribution [J]. Business Weekly, 2009 (24): 94-94.
4. Anderson T W, Anderson T W, Anderson T W, et al. An introduction to multivariate statistical analysis[M]. New York: Wiley, 1958.
5. Zhao Zhengsong, Pan Dengdeng. Analysis of taxi industry operation law based on two independent samples and paired samples T-test [J]. Transportation Construction and Management, 2013 (08): 86-87.
6. Dual-population (σ\_1~2,σ\_2~2 unknown,n≤30) paired sample T-test and independent sample T-test based on SPSS. Reading and Writing (Journal of Education and Teaching), 2016
7. Qi Yongzhong. The impact of two RRR cuts on interest rate risk premium in China in 2014: An empirical analysis based on two paired sample T-test [J]. China Collective Economy, 2016 (10): 57-59.
8. Han Shuguang, Wu Jing, Chen Qiong. Case evaluation of fresh e-commerce logistics service based on paired sample T-test [J]. Journal of Zhejiang University of Science and Technology (Social Science Edition), 2016, 36(03): 246-251.
9. Wu Xizhi and Zhao Bojuan. Nonparametric Statistics: China Statistics Press, 2011
10. Qin Shan, Wang Xiaoyin. Application of rank sum test in feed science research [J]. Feed Wide Angle, 2003(21):30-32. (in Chinese)
11. Committee of the Dictionary of Mathematics. Mathematics Ci Hai (1-6). Volume 6 [M]. Shanxi Education Press, 2002.
12. Lamba, R. Reaction kinetic models for heterogeneous solid catalyzed esterification of decanoic acid with ethanol. Biomass Conv. Bioref. 13, 12157–12166 (2023). [https://doi.org/10.1007/s13399-022-02413-4](https://doi.org/10.1007/s13399-022-02413-4)
13. Wikipedia contributors. "Reactions on surfaces." Wikipedia, The Free Encyclopedia. Wikipedia, The Free Encyclopedia, 1 Dec. 2022. Web. 16 Nov. 2023.
14. Prins, R. Eley–Rideal, the Other Mechanism. Top Catal 61, 714–721 (2018). [https://doi.org/10.1007/s11244-018-0948-8](https://doi.org/10.1007/s11244-018-0948-8)
15. [https://core.ac.uk/download/pdf/213394653.pdf](https://core.ac.uk/download/pdf/213394653.pdf)
16. Jakobsen, H.A. (2014). Packed Bed Reactors. In: Chemical Reactor Modeling. Springer, Cham. [https://doi.org/10.1007/978-3-319-05092-8\_11](https://doi.org/10.1007/978-3-319-05092-8\_11)
17. Zabala S, Reyero I, Campo I, Arzamendi G, Gandía LM. Pseudo-Homogeneous and Heterogeneous Kinetic Models of the NaOH-Catalyzed Methanolysis Reaction for Biodiesel Production. Energies. 2021; 14(14):4192. [https://doi.org/10.3390/en14144192](https://doi.org/10.3390/en14144192)
18. De Falco, M. (2011). Membrane Reactors Modeling. In: De De Falco, M., Marrelli, L., Iaquaniello, G. (eds) Membrane Reactors for Hydrogen Production Processes. Springer, London. [https://doi.org/10.1007/978-0-85729-151-6\_4](https://doi.org/10.1007/978-0-85729-151-6\_4)
19. Hai, Tran & Nguyen, Dinh & Do, Phuong & Tran, Uyen. (2023). Kinetics of photocatalytic degradation of organic compounds: a mini-review and new approach. RSC Advances. 13. 16915-16925. [https://doi.org/10.1039/D3RA01970E](https://doi.org/10.1039/D3RA01970E)
20. Jolliffe, I. T. (2002). Principal component analysis. Wiley Online Library1
21. Abdi, H., & Williams, L. J. (2010). Principal component analysis. Wiley Interdisciplinary Reviews: Computational Statistics, 2(4), 433-4592
22. StataCorp. (2017). Stata Statistical Software: Release 15. StataCorp LLC

# 

# Appendix

function [trainedModel, validationRMSE] = trainRegressionModel(trainingData, responseData)

inputTable = array2table(trainingData', 'VariableNames', {'row\_1'});

predictorNames = {'row\_1'};

predictors = inputTable(:, predictorNames);

response = responseData;

isCategoricalPredictor = [false];

regressionNeuralNetwork = fitrnet(...

predictors, ...

response, ...

'LayerSizes', [10 10 10], ...

'Activations', 'relu', ...

'Lambda', 0, ...

'IterationLimit', 1000, ...

'Standardize', true);

predictorExtractionFcn = @(x) array2table(x', 'VariableNames', predictorNames);

neuralNetworkPredictFcn = @(x) predict(regressionNeuralNetwork, x);

trainedModel.predictFcn = @(x) neuralNetworkPredictFcn(predictorExtractionFcn(x));

trainedModel.RegressionNeuralNetwork = regressionNeuralNetwork;

trainedModel.About = 'This struct is a trained model exported from Regression Learner R2023b.';

trainedModel.HowToPredict = sprintf('To make predictions on a new predictor row matrix, X, use: \n yfit = c.predictFcn(X) \nreplacing ''c'' with the name of the variable that is this struct, e.g. ''trainedModel''. \n \nX must contain exactly 1 rows because this model was trained using 1 predictors. \nX must contain only predictor rows in exactly the same order and format as your training \ndata. Do not include the response row or any rows you did not import into the app. \n \nFor more information, see <a href="matlab:helpview(fullfile(docroot, ''stats'', ''stats.map''), ''appregression\_exportmodeltoworkspace'')">How to predict using an exported model</a>.');

inputTable = array2table(trainingData', 'VariableNames', {'row\_1'});

predictorNames = {'row\_1'};

predictors = inputTable(:, predictorNames);

response = responseData;

isCategoricalPredictor = [false];

partitionedModel = crossval(trainedModel.RegressionNeuralNetwork, 'KFold', 5);

validationPredictions = kfoldPredict(partitionedModel);

validationRMSE = sqrt(kfoldLoss(partitionedModel, 'LossFun', 'mse'));