2023_“ShuWei Cup”

Problem B：The catalytic reaction of cotton stalk pyrolysis

With the increasing global demand for renewable energy, biomass energy has gained widespread attention as a mature renewable energy source. Cotton stalks, as a kind of agricultural waste, are regarded as an important biomass resource because of their rich biomass components, such as cellulose and lignin. Although the pyrolysis of cotton stalk can generate various forms of renewable energy, the quality and yield of its pyrolysis products are influenced by various factors, such as pyrolysis temperature and catalysts. Therefore, studying the mechanism and properties of cotton stalk pyrolysis products (Noun definitions can be found in the appendix), as well as investigating the mechanism and effects of catalysts during the pyrolysis process, is of great significance for the efficient utilization and sustainable development of cotton stalk.

A certain chemical engineering laboratory employed the model compound method to establish pyrolysis combinations: desulfurization ash with cotton stalk and desulfurization ash with model compounds. The pyrolysis combinations were subjected to pyrolysis at different mixing ratios to investigate the catalytic mechanism and effects of desulfurization ash on the generation of pyrolysis products from the cotton stalk. Simultaneously, in selecting model compounds, it was necessary to consider their controllability and stability in reaction performance during the experiment, as well as their contribution to cotton stalk pyrolysis. CE (Cellooligosaccharide) and LG (Lignin) are representative components of cellulose and lignin in the cotton stalk, which can represent the biomass characteristics of the cotton stalk itself. By selecting these two components as model compounds, the experimental conditions could be more finely controlled to study the targeted catalytic effect of desulfurization ash on different biomass components. Therefore, the selection of CE and LG as model compounds was based on a rational judgment of the biomass composition and chemical structure characteristics of the cotton stalk itself. The experimental results are shown in Appendix 1 and Appendix 2.

The desulfurization ash/biomass pyrolysis experiment was conducted with fixed-bed pyrolysis at mixing ratios of 10/100, 20/100, 30/100, 40/100, 50/100, 60/100, 80/100, and 100/100. This choice of mixing ratios was based on the fact that under these experimental conditions, the relative error of parallel experiments is approximately 5%. If the mixing ratios were chosen to be too small, such as 5/100 or 7/100, the relative error would have a significant impact on the experimental results and seriously affect the exploration and optimization process of the experiment. If it is possible to use a mathematical model and AI learning to predict the pyrolysis product yield or production under conditions with limited data, it would not only greatly reduce the time required for experimental optimization but also provide accurate guidance on the trend of changes in the distribution of pyrolysis products.

Please complete the following questions through mathematical modeling:

(1) For each pyrolysis combination in Annex I, analyze the yield of pyrolysis products (tar, water, coke residue, syngas) in relation to the mixing ratios of the corresponding pyrolysis combinations, and explain whether desulfurization ash, as far as it is used as a catalyst, plays a significant role in facilitating the pyrolysis of cotton stalks, cellulose, and lignin?

(2) According to Annex II, for each of the three pyrolysis combinations, the effect of the mixing ratio of the pyrolysis combinations on the yield of each group of pyrolysis gas is discussed and explained by making corresponding images.

(3) Under the catalytic action of the same proportion of desulfurized ash, is there a 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? Please provide reasons.

(4) How do we establish a catalytic reaction mechanism model of desulfurized ash for model compounds such as CE and LG and model the reaction kinetics for analysis?

(5) Please use mathematical models or AI learning methods to make

predictions on the yields or quantities of the pyrolysis products under limited data conditions.

Annexes

Annex I: Pyrolysis Product Yields of Three Pyrolysis Combinations.xlsx

Annex II: Pyrolysis Gas Yields of Three Pyrolysis Combinations.xlsx

Appendix

Pyrolysis Combinations: Desulfurized Ash-Cotton Stalk; Desulfurized Ash-CE; Desulfurized Ash-LG.

Pyrolysis Products: Tar, Water, Char, Syngas.

Pyrolysis Gas Components for Desulfurized Ash and Cotton Stalk: H_2, CO, CO_2, CH_4, C_2H_6, C_3H_8, C_3H_6, C_2H_4, C_4H_{10}.

Pyrolysis Gas Components for Desulfurized Ash and CE: H_2, CO, CO_2, CH_4, C_2H_6.

Pyrolysis Gas Components for Desulfurized Ash and LG: H_2, CO, CO_2, CH_4, C_2H_6.

All experiments in this study were conducted at the same temperature.