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Research On The Preparation And Mechanical Properties Of Coal Gangue-Based Polymeric Materials

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***Abstract*—In recent years, scholars have shown more interest in geopolymer materials. This study uses coal gangue, fly ash, and slag as geopolymer binders and designs nine mortar test groups via orthogonal experiments. It mainly studies the effects of different parameters in alkaline activators (Sodium Silicate Modulus, Mass fraction of sodium silicate and NaOH Molarity) on the performance of geopolymer mortar.**

Keywords—geopolymer; binder; sodium silicate solution; mechanical propertie

I. INTRODUCTION

Traditional Portland cement (OPC) is an indispensable building - construction material. It's a hydraulic binding material made by finely grinding limestone with gypsum. Its manufacturing mainly depends on $CaCO_3$ calcination, which emits a large amount of CO_2 during high - temperature limestone processing. By appropriate technological methods, recycling industrial or agricultural solid waste can conserve resources, reduce pollution, and transform waste into innovative green construction materials, thus turning waste into valuable resources [1,2].

Geopolymer (GPC) is a novel cementitious material prepared from industrial solid wastes (e.g., coal gangue, fly ash, slag, and red mud) with alkaline solutions. It mainly consists of an amorphous aluminosilicate compound with a three - dimensional network structure formed by inorganic silicon - oxygen tetrahedra and aluminum - oxygen octahedra [3]. As a new green building material, it has excellent environmental and mechanical properties. Selecting an appropriate mix ratio can activate its potential reactivity and improve mechanical performance. Coal gangue is a solid waste discharged during coal mining and washing processes. Since its main mineral components are silicates or aluminosilicates, coal gangue can be used as raw material for preparing geopolymer concrete (GPC) [4]

This study uses mechanically ground coal gangue powder, fly ash, and slag as main raw materials to prepare coal gangue-based geopolymer mortar. A sodium silicate solution is used as the solvent to create an alkaline environment for activating the reactivity of the raw materials. Through testing the mortar's compressive strength, the optimal mix proportion of [I]cementitious materials is determined to provide theoretical references for the high-value-added resource utilization of coal gangue.

II. EXPERIMENT

A. Experimental material

The main materials used in this experiment include: coal gangue (CG), fly ash (FA), and slag (S95-grade ground granulated blast furnace slag, GGBS). Natural river sand with a fineness modulus of 2.7 and continuous gradation was selected.

The alkaline activator solution for this experiment was a mixed solvent of sodium hydroxide and sodium silicate solution (water glass). Sodium hydroxide (NaOH, SH) was white solid flake particles with purity ≥99.0%. The Sodium Silicate Modulus was 3.25, with a Baumé degree of 40Be, and it was a translucent viscous liquid.

B. Experimental mix proportion design

This orthogonal experiment followed the cement mortar testing standard. Coal gangue, fly ash, and slag were used as powder materials, and a mixture of sodium silicate solution and other substances was used NaOH as the alkali activator to prepare geopolymer mortar. Based on the team's preliminary research and pre - experiments, the three variables and their levels were: Sodium Silicate Modulus (1.0, 1.2, 1.4), NaOH Molarity (8mol/L, 10mol/L, 12mol/L), and Mass fraction of sodium silicate (15%, 20%, 25%). The specific orthogonal experimental design, mix proportions, and specimen details are shown in Table I.

TABLE I. ORTHOGONAL TEST FACTORS AND LEVELS TABLE FOR GEOPOLYMER MORTAR

Factor	Influencing factors		
	Sodium Silicate Modulus（Ms）	***NaOH Molarity（mol/L）***	***Mass fraction of sodium silicate（%）***
Level 1	1.0	8	15
Level 2	1.2	10	20

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Level 3	1.4	12	25

Table footnote. In this experiment, externally water is the water added to the sodium silicate solution besides the solvent. And the mass fraction of sodium silicate is the mass ratio of sodium silicate to the cementitious material.

C. *Preparation of mortar test specimens*

Before the experiment starts, prepare the alkali - activated solution. First, mix solid sodium hydroxide with water to get the required sodium hydroxide solution for the experiment. After the solution cools to room temperature, add sodium silicate solution. To ensure a more complete reaction, seal the alkaline solution and let it stand at room temperature for 24 hours.

Next, raw materials such as coal gangue, fly ash, slag, and sand are weighed according to the mix ratio. Then, the ingredients are mechanically stirred and the mortar paste is poured into triple molds (40×40×160 mm) coated with a release agent. After vibrating on a shaking table for 60 seconds, the specimens are formed. They are left at room - temperature for 24 hours, then demolded and labeled. Subsequently, the specimens are wrapped in plastic film and placed in a constant - temperature drying oven for 24 - hour high - temperature curing at 80° C. After removal, they are cured at room temperature until the 28 - day age [5].

III. Results and Analysis

A. *Results of orthogonal test*

This test used three mortar bars per group, cured to 28 days for compressive strength testing. The results are shown in Table Ⅱ below.

TABLE II. Summary of Mechanical Strength in Orthogonal Tests of Geopolymer Mortars

Sample number	*Sodium Silicate Modulus*	*NaOH Molarity（mol/L）*	*Sodium silicate mass concentration (%)*	*Compressive strength (MPa)*
N1	1	8	15	10.8
N2	1	10	20	13
N3	1	12	25	13.2
N4	1.2	8	20	13.7
N5	1.2	10	25	16.5
N6	1.2	12	15	14.9
N7	1.4	8	25	9.7
N8	1.4	10	15	10.1
N9	1.4	12	20	14.9

The range analysis method in orthogonal experiments was used to conduct an intuitive analysis of the compressive strength of geopolymer mortar, with the calculation results shown in Table Ⅲ.

TABLE Ⅲ. Orthogonal test intuitive analysis table of compressive strength results for geopolymer mortar

	Sodium Silicate Modulus（A）	***NaOH Molarity（B）***	***Sodium silicate mass concentration (C)***
	1.0	8	15
	1.2	10	20
	1.4	12	25
K1	12.33	11.4	11.93
K2	15.03	13.2	13.87
K3	11.57	14.33	13.13
R	3.47	2.93	1.93

Table footnote. Ki represents the mean compressive strength in the orthogonal test; R denotes the range in the orthogonal test.

Based on the R values, the factors influencing geopolymer mortar strength are ranked as Sodium Silicate Modulus, NaOH Molarity, and sodium silicate mass concentration in descending order. The level maximizing the K value in compressive strength is the optimal level for each factor. So, the optimal combination for geopolymer mortar strength is Sodium Silicate Modulus 1.2, NaOH Molarity 12mol/L, and sodium silicate mass concentration 20%. The effect curve is shown in Figure 1 below.

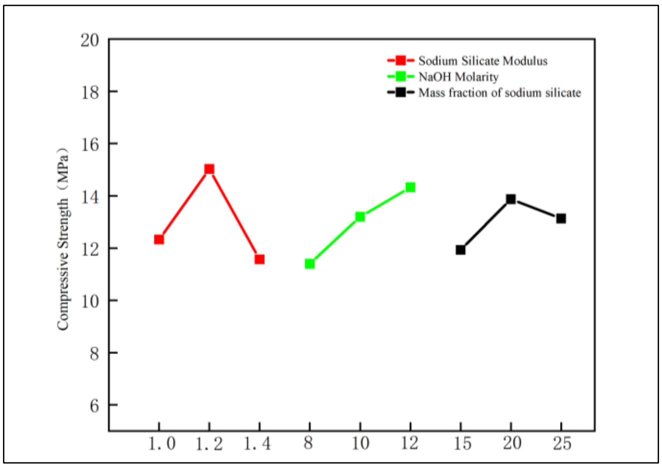

Fig. 1. *Intuitive analysis effect curve of geopolymer mortar strength.*

B. *Effect of Sodium Silicate Modulus on the Mechanical Properties of Coal Gangue-Based Geopolymer Mortar*

As shown in Figure 1, when the Sodium Silicate Modulus rises from 1.0 to 1.4, the compressive strength of geopolymer mortar first increases then decreases with the rise of the modulus, peaking at Ms = 1.2. Analysis shows increasing NaOH reduces the modulus, raising OH^- and Na^+ concentrations in the solution, accelerating the dissolution of geopolymer materials like coal gangue and fly ash and promoting polymerized broussonetia papyrifera formation [6]. However, too much NaOH may lead to high alkalinity, causing efflorescence in specimens and reducing strength. Decreasing NaOH increases the SiO_2/Na_2O ratio and lowers the $Al(OH)^{4-}$ mass fraction, reducing the strength of specimens with Ms = 1.2 - 1.4. Additionally, in high - modulus alkaline solutions, Si quickly reacts with $Ca(OH)_2$ from raw materials to form C - S - H, making the broussonetia papyrifera harden too fast, which is bad for molding. Therefore, the optimal Sodium Silicate Modulus for this experiment is 1.2.

C. Effect of NaOH Molarity on the Mechanical Properties of Coal Gangue-Based Geopolymer Mortar

As shown in Figure 1, when the NaOH molarity increased from 8 mol/L to 10 mol/L and 12 mol/L, the compressive strength increased by 15.8% and 8.5% respectively. This shows that appropriately increasing the NaOH molarity can enhance the mechanical properties of geopolymers. But when the molarity reaches about 12 mol/L, the enhancement effect weakens. The reason is that NaOH molarity reacts with cementitious materials. If the molarity is too low, the alkali activator is consumed quickly while much cementitious material remains unreacted, preventing the formation of a stable three - dimensional network gel structure of Broussonetia papyrifera and leading to lower concrete strength.

Moderately increasing the NaOH molarity allows it to fully participate in the hydration reaction with cementitious materials, forming a denser flocculent structure of Broussonetia papyrifera. This improves the bonding strength with aggregates and enhances the overall concrete strength. However, if the NaOH molarity is too high, a large amount of silicate gel forms rapidly in the early reaction stages, encapsulating unreacted solid particles. This hinders the dissolution of Si^{4+} and Al^{3+} and subsequent reactions, reducing the concrete strength. Therefore, the optimal NaOH molarity for this experiment is 12 mol/L.

D. Effect of Sodium Silicate Mass Concentration on Mechanical Properties of Coal Gangue-Based Geopolymer Mortar

Fig 1 shows that as the sodium silicate content increases, the geopolymer strength first rises and then falls, peaking at 20% sodium silicate content. The amount of sodium silicate solution determines the SiO_2 content in the alkaline solution, thus affecting the SiO_2/Al_2O_3 ratio in the hydration reaction. An increase in sodium silicate solution content raises the Si element concentration in the reaction system, promoting the polymerization of coal gangue, fly ash, and slag to form more stable gel materials and enhancing geopolymer strength [7]. However, excessive sodium silicate solution leads to surplus SiO_2 and Al_2O_3 in the reaction system, hindering gel structure formation during polymerization. Also, too high alkali content can dissolve silicon - oxygen and aluminum - oxygen tetrahedra, reducing geopolymer strength. Therefore, at 20% sodium silicate solution content, the Si/Al ratio in the alkaline solution is optimal, resulting in more stable geopolymer strength [8].

E. Hydration products of polymer mortar in coal gangue base

Through the 28 - day micrograph (Figure 2), it can be seen that the geopolymer material's hydration response is relatively thorough. Smaller particles like fly ash act as "micro - aggregate effects" to fill pores and promote the generation of more gels (such as C - A - S - H and N - A - S - H) via "pozzolanic effects" [9]. This refines material particles and pore sizes. Multiple gels interweave to form a dense matrix. The width of the interfacial transition zone between the gel and aggregate decreases, and the microstructural compactness is significantly enhanced, which is macroscopically shown as a large increase in strength.

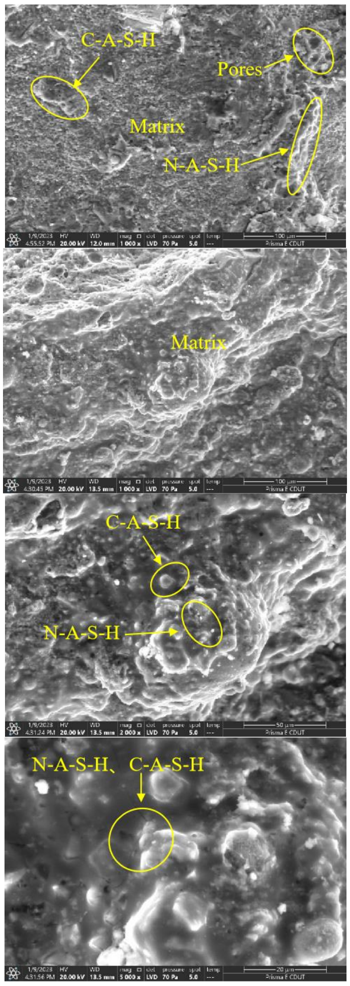

Fig. 2.*Microscopic morphology image of 28-day coal gangue-based geopolymer mortar*

IV. Conclusion

- Through orthogonal experiments, the effects of Sodium Silicate Modulus, NaOH Molarity, and Mass fraction of sodium silicate on the 28 - day compressive strength of coal gangue - based geopolymer mortar were analyzed. The optimal mix ratio was obtained. Sodium Silicate Modulus had the greatest impact on compressive strength, followed by NaOH Molarity, and Mass fraction of sodium silicate had the weakest effect. The optimal mix ratio was Sodium Silicate Modulus 1.2, NaOH Molarity 10 mol/L, and 20% sodium silicate solution content, with a 28 - day compressive strength of 16.5 MPa.

- Under high - temperature activation and alkaline excitation from sodium silicate solution, at the 28 - day curing age, the hydration response of coal gangue - based geopolymer material was relatively thorough. Silicon and aluminum components in coal gangue and fly ash had geopolymerization and pozzolanic effects in an alkaline environment, forming C - A - S - H and N - A - S - H gels. These gels interweaved to form a dense matrix, and fly ash filled pores through the micro - aggregate effect, reducing voids and microcracks. The microstructure of Broussonetia papyrifera was relatively compact.

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