

Research Article

Study on the Parameter Optimization and Strength Mechanism of Coal Gangue Emulsified Asphalt Mixture

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Emulsified asphalt mixture has the characteristics of convenient construction and durable performance, but its poor early strength and demulsification seriously restrict the popularization and application of this material. At present, the coal gangue produced by coal-fired power plants is generally discarded, resulting in serious environmental pollution. The combination of coal gangue and emulsified asphalt can explore an efficient utilization way for more and more coal gangue and also solve the curing problem of asphalt. In order to give full play to the advantages of existing materials and make rational use of resources, this paper studies the factors affecting the performance of coal gangue emulsified asphalt mixture based on orthogonal experimental design and optimizes its material composition parameters by considering the coupling effect of two factors. The water stability of coal gangue emulsified asphalt mixture is evaluated by the immersion Marshall test. Finally, the strength formation mechanism of coal gangue emulsified asphalt mixture is analyzed from the microscopic point of view. The results determined 7.5% as the optimum amount of emulsified asphalt in coal gangue emulsified asphalt mixture and recommended the best parameter combination of 7.5% emulsified asphalt, 6% coal gangue, and 5% water consumption. With the increase of coal gangue content, the water loss resistance of emulsified asphalt mixture increases gradually, and the water stability of emulsified asphalt mixture can be improved by adding coal gangue. According to the microscopic analysis, the strength of the mixture is formed by the joint action of emulsified asphalt and coal gangue, in which the hydration products of coal gangue and asphalt play the role of cementation and strength together. The ordinary emulsified asphalt mortar mainly contains CaCO_3 , which mainly plays the role of physical filling.

1. Introduction

The construction temperature of the modified asphalt mixture is generally between 155°C and 165°C. Such a high temperature will cause a large consumption of heat energy, which will adversely affect the environment and construction personnel [1]. On the other hand, for areas with lower temperatures, the time for road construction will also be limited. Today, with the increasing shortage of energy and materials, it is very urgent to find materials that can replace hot mix asphalt mixture. Emulsified asphalt mixture refers to the asphalt mixture mixed and paved at room temperature, which does not need to be heated during mixing and construction, which not only reduces the construction cost but also reduces environmental pollution and energy

consumption. Emulsified asphalt mixture has the characteristics of “simple and flexible construction, ultrathin and durable performance, and open and fast traffic” [2]. However, this environmentally friendly material also has some disadvantages, such as poor early strength and demulsification, which have seriously restricted the popularization and use of this material [3]. At the same time, the coal industry in China emits about 280 million tons of coal gangue every year. At present, this kind of industrial waste is generally discarded, so the resource utilization of waste coal gangue has become an urgent problem to be solved [4, 5]. If the combination of coal gangue and emulsified asphalt is studied, on the one hand, we can explore an efficient utilization way for more and more coal gangue; on the other hand, it can also solve the curing problem of asphalt, so as to

meet the normal-temperature construction of asphalt. Thus, it can be seen that the efficient use of coal gangue and the research and development of room temperature asphalt pavement materials can reduce emissions, save resources, and have important economic and social value. Amir and Morteza [6] investigated the effects of using coal waste and its ignited product on roller compacted concrete pavement (RCCP). They also studied the combination of limestone powder (LS) and coal waste ash (CWA). Yang et al. [7] adopted cone penetration test, dynamic shear rheological (DSR) test, and bending beam rheological (BBR) test to investigate the high- and low-temperature rheological properties of the activated coal gangue-modified asphalt mortar under the condition of different filler-bitumen ratios. Shafabakhsh and Ahmadi [8] evaluated the effects of coal waste ash and rice husk ash and compared the mechanical properties of pervious concrete pavement with concrete having ash. Rui et al. [9] evaluated the durability properties of nonair entrained roller compacted concrete pavement containing coal waste ash as partial replacement of cement in the presence of deicing salts. Rad and Modarres [10] used dynamic shear rheological (DSR) test, bending beam rheometer (BBR), and brook-field viscometer (BV) test to study the high- and low-temperature performance of asphalt mortar which was made of limestone slag and three types of activated coal gangue. Mohsen and Amir [11] presented the physical-mechanical performances of coal gangue aggregate and the result indicates that coal gangue aggregate can meet the specifications except the content of the flat and elongated particles. Wu et al. [12], according to the erosion of asphalt pavement by precipitation, fog, and chloride molecules in the atmosphere in coastal areas of China, selected polyester fibers with six different mass percentages and fillers of coal gangue powder with five different replacement rates for asphalt mixture SCB test. Xinjun et al. [13] used coal waste powder (CWP), coal waste ash (CWA), and limestone (LS) powder to prepare asphalt mortar with 5 kinds of filler asphalt ratio, and the technical performance tests and the microcosmic action mechanisms analyses were conducted to compare the road performance of different asphalt mortar. Shamsaei et al. [14] investigated the use of ceramic and coal waste powders as partial replacement of cement in roller compacted concrete pavement mixture, and the mixtures were produced with the ceramic waste powder contents at 5% and 10% of total cementitious material (by weight). In view of the disadvantage that coal waste powder (CWP) can reduce the crack resistance of asphalt mortar at low temperature, Fenga et al. [15] used silane coupling agent KH-550 to modify coal waste powder. Thus, it can be seen that scholars' research on the strength improvement of emulsified asphalt mixture is mainly focused on mixture optimization design, fiber reinforcement, performance prediction, and so on and rarely complements the performance of coal gangue and emulsified asphalt, and the strength formation mechanism of coal gangue emulsified asphalt mixture is rarely analyzed. In this paper, the factors affecting the performance of coal gangue emulsified asphalt mixture are studied based on orthogonal experimental design, the material composition parameters are optimized by

considering the coupling effect of two factors, and its water stability is evaluated by immersion Marshall test. Finally, the strength formation mechanism of coal gangue emulsified asphalt mixture is analyzed from the microscopic point of view.

2. Technical Performance of Raw Materials

2.1. Emulsified Asphalt. According to the field investigation, cationic emulsified asphalt is widely used in China's road industry, and it has an excellent performance in domestic application effect. Therefore, this paper adopts the finished cationic emulsified asphalt of slow crack and fast setting type and tests it according to the relevant regulations of "Test Code of Asphalt and Asphalt mixture for Highway Engineering" JTGE20-2011. Its technical index is shown in Table 1 [16].

2.2. Aggregate. The coarse and fine aggregates used in the test are all limestone, and their mechanical properties are tested according to the "Test Methods of Aggregate for Highway Engineering (JTGE42-2015)" as shown in Table 2 [17].

2.3. Coal Gangue. The coal gangue used in the test comes from the waste coal gangue produced by a coal-fired plant, and its physical appearance is shown in Figure 1.

This paper mainly uses coal gangue of 1~3 mm specification. The chemical composition of coal gangue was studied by X-ray fluorescence (XRF) analysis, as shown in Table 3.

It can be seen from Table 3 that this type of coal gangue is a low-calcium mineral with high contents of SiO_2 and Al_2O_3 and potential high activity. Based on the experiment specification of activity index test of coal gangue (GB/T17671-1999), the coal gangue was prepared into coal gangue cement mortar, and the cement mortar was used as the reference group to test the compressive strength of 28 days. The activity index was determined by the ratio of their compressive strength. The higher the compressive strength ratio ($\geq 70\%$), the higher the activity. The test results are shown in Table 4.

From the above results, the compressive strength ratio is 89.5%. According to the ratio of compressive strength, it can be concluded that this type of coal gangue has higher activity.

2.4. Mixture Gradation. At present, there is no unified standard and requirement for the selection of gradation form of emulsified asphalt mixture, and many studies have found that the type of dense gradation of emulsified asphalt mixture is better [18]. In this paper, the dense gradation AC-25C is selected as the test gradation, and the mineral gradation is shown in Table 5.

3. Test Method

Considering that coal gangue emulsified asphalt mixture is a new type of emulsified asphalt mixture, the amount of emulsified asphalt, coal gangue content, and water

TABLE 1: Technical index of emulsified asphalt.

Properties	Unit	Test result	Specification [13]
Particle charge	—	Cationic	Cationic
Residue on the 1.18 mm sieve	%	0.076	≤0.1
Wrap ratio with coarse aggregate	—	0.86	≥2/3
Saybolt viscosity (25°C)	S	61	6~100
Penetration (5 s, 100 g, 25°C)	0.1 mm	79	45~150
Ductility (15°C)	Cm	74	≥40
Storage stability (1 days, 25°C)	%	0.7	≤1
Storage stability (5 days, 25°C)	%	4.1	≤5

TABLE 2: Experimental results of mechanical properties for aggregate.

Properties	Unit	Test result	Specification
Apparent density	g/cm ³	2.83	≥2.50
Crushing value	%	15.3	≤20
Wear loss in Los Angeles	%	18.5	≤24
Elongated particle content	%	8.7	—



FIGURE 1: Coal gangue.

TABLE 3: Chemical composition of coal gangue/wt. %.

Chemical component	SiO ₂	Al ₂ O ₃	Fe ₂ O ₃	CaO	MgO	K ₂ O	Others
Value	48.52	34.83	11.25	2.03	1.68	1.22	0.47

TABLE 4: Activity test of coal gangue.

Properties	Unit	Test group		Activity index (%)
		Coal gangue	Cement	
Compressive strength	MPa	46.94	52.43	89.5

consumption are the three key factors that affect the performance of the mixture. Orthogonal design method is scientific and reasonable [19]. According to the value range of various mixing amounts obtained from the previous trial

mixing and combined with the mixing state of the mixture, the orthogonal table L16 (4³) with three factors and four levels is determined, as shown in Table 6.

In this paper, Marshall test is used to study the factors affecting the performance of coal gangue emulsified asphalt mixture. The specimen is formed by Marshall compaction method. In order to make the result closer to the actual construction situation, mineral powder, coal gangue, and aggregate are added first, and then emulsified asphalt is added. According to the test specification (JTGE20-2011) requirements, the Marshall test should conduct 75 times of compaction on double-sided of the specimen. In this paper, the two stages of compaction are used, that is, 50 times of double-sided compaction after mixing and 25 times of compaction after curing at 110°C for one day. Because after curing, there will be no chemical reaction inside the specimen, and the better compaction quality can be obtained by compaction again. In addition, because the emulsified asphalt mixture is often used for pavement maintenance and maintenance, it is in direct contact with the external environment and is greatly harmed by water, so the water stability of emulsified asphalt mixture has a great influence on its performance. In this paper, the water stability of emulsified asphalt mixture was studied by immersion Marshall test.

4. Results and Discussion

4.1. Analysis of Influencing Factors. The Marshall test of asphalt mixture is carried out by using the test combination in Table 6 and combined with the specification, and the results are shown in Table 7 [20].

The range analysis of the test results in the above table is carried out to study the influence weight of each parameter on the test results, as shown in Table 8.

In Table 8, the greater the range R , the greater the influence of factors on the test results. Through the range analysis, it can be found that, in terms of stability, for coal gangue emulsified asphalt mixture, the order of the influence degree of each factor is water consumption > coal gangue content > emulsified asphalt dosage [21]. The preliminary analysis is that because the emulsified asphalt mixture is different from the hot mix asphalt mixture, the water consumption is very important to the compaction process of the asphalt mixture, and the insufficient water consumption can easily lead to the early demulsification of the asphalt mixture and the poor overall performance of the mixture and then affect the stability of the mixture. From the results of the K value analysis of the stability in Table 8, we can see that there is an extreme value of the effect of each factor on the stability of the mixture, from which it can be preliminarily obtained that the corresponding parameter combination of the best stability is 6% of coal gangue, 7.5% of emulsified asphalt, and 5% of water. In terms of flow value, for coal gangue emulsified asphalt mixture, the order of various factors according to the degree of influence is coal gangue content > emulsified asphalt content > water consumption. The parameter combination corresponding to the optimal flow value is 5% of coal gangue, 7.5% of emulsified

TABLE 5: Gradation of AC-25C asphalt mixture.

Mixture type	Sieve size passing (%)											
AC-25C	26.5 mm	19 mm	16 mm	13.2 mm	9.5 mm	4.75 mm	2.36 mm	1.18 mm	0.6 mm	0.3 mm	0.15 mm	0.075 mm
	100	86.2	73.1	66.3	56.2	36.8	27.5	20.8	16.2	10.8	6.8	3.6

TABLE 6: Orthogonal test designs table.

Level	Parameters		
	Parameter A Coal gangue	Parameter B Content of emulsified asphalt	Parameter C Water consumption
1	3%	6.5%	4%
2	4%	7%	4.5%
3	5%	7.5%	5%
4	6%	8%	5.5%

asphalt, and 5% of water. In terms of voidage, for coal gangue emulsified asphalt mixture, the order of various factors according to the degree of influence is water consumption > emulsified asphalt dosage > coal gangue content. Preliminary results show that the corresponding parameter combination of the best flow value is 6% of coal gangue, 7.5% of emulsified asphalt, and 4% of water. From the comprehensive analysis of the orthogonal test, it can be concluded that the asphalt dosage of 7.5% is the best, while the water consumption and the content of coal gangue need to be further analyzed.

4.2. Optimization of Material Composition. Considering that the amount of coal gangue is different, it may affect the optimal amount of water used for asphalt mixture, so based on the two-factor coupling analysis method, this paper further studies the influence of different coal gangue content and water consumption on the Marshall stability, flow value, and voidage of emulsified asphalt mixture when the amount of emulsified asphalt is 7.5%. Thus, the material composition is optimized [22].

4.2.1. Effect of Coal Gangue Content and Water Consumption on Marshall Stability of Mixture. Under the condition of the optimum asphalt dosage of 7.5%, the coal gangue content is 3%, 4%, 5%, and 6%, respectively, and the water consumption is 4%, 4.5%, 5%, and 5.5%, respectively. The Marshall stability of the mixture is obtained by the Marshall test as shown in Figure 2.

It can be seen from Figure 2(a) that the stability of coal gangue emulsified asphalt mixture increases gradually with the increase of coal gangue content. When the coal gangue content is 6% and the water consumption is 5%, the stability of the mixture reaches the maximum value 13.42 kN. The test results show that the addition of coal gangue can improve the stability of emulsified asphalt mixture. The preliminary analysis is that coal gangue has certain activity, and its own active components can produce certain hydration products under the action of water. The hydration products

can be cemented with asphalt mortar, and the more the coal gangue is added, the more obvious this effect is. At the same time, the unhydrated coal gangue can be used as a kind of fine aggregate, which plays the effect of microaggregate [11]. As can be seen from Figure 2(b), when the amount of coal gangue is constant, the stability of the mixture increases at first and then decreases with the increase of water consumption (the water consumption reaches the peak when the water consumption is 5%), which shows that too large or too small water consumption is not conducive to the stability of the mixture. The water consumption has a certain influence on the mixing forming of the mixture. When the water consumption is less, the mixture is uneven, the emulsified asphalt is easy to demulsify earlier, and the fine aggregate is easy to agglomerate, which has a great influence on the strength of the mixture. When the water consumption is too large, the fluidity of the mixture is too large, and even overflow phenomenon occurs, resulting in the fact that the mixture in the compaction process is easy to compact out of the asphalt mortar, affecting the strength of the mixture [23]. On the other hand, compared with mineral powder, coal gangue has hydration activity and larger specific surface area, so it needs more water to improve the workability of the mixture. Therefore, based on the above analysis results, it is preliminarily determined that the optimal water consumption is 5%.

4.2.2. Influence of Coal Gangue Content and Water Consumption on Mixture Flow Value. Under the condition of 7.5% of the optimum amount of asphalt, the content of coal gangue is 3%, 4%, 5%, and 6%, respectively, and the water consumption is 4%, 4.5%, 5%, and 5.5%, respectively. The flow value of the mixture is obtained by Marshall test as shown in Figure 3.

It can be seen from Figure 3(a) that when the water consumption is constant, the flow value decreases with the increase of coal gangue content. When the water consumption is relatively small, the effect of the amount of coal gangue on the mixture flow value is not obvious. The test results show that the addition of coal gangue can reduce the flow value of emulsified asphalt mixture. The preliminary analysis is that the hydration product of coal gangue hydration is a kind of rigid material and asphalt mixture is a kind of flexible material. This kind of coal gangue emulsified asphalt mixture can form a kind of semirigid material. With the increase of coal gangue content, the mixture tends to be more rigid, and its flow value is smaller [14]. It can be seen from Figure 3(b) that when the content of coal gangue is constant, the flow value of the mixture decreases at first and then increases with the increase of water consumption. Particularly, when the water consumption is too large, the flow value of emulsified asphalt mixture will increase

TABLE 7: Marshall test results of coal gangue emulsified asphalt mixture.

Test ID	Parameters			Marshall test results		
	Parameter A	Parameter B	Parameter C	Stability (kN)	Flow value (0.1 mm)	Void ratio (%)
1	3%	6.5%	4%	8.77	36.2	8.33
2	3%	7%	4.5%	11.64	35.5	7.11
3	3%	7.5%	5%	11.94	39.4	8.79
4	3%	8%	5.5%	12.12	35.6	6.98
5	4%	6.5%	4.5%	11.25	36.4	7.05
6	4%	7%	4%	7.95	37.6	8.35
7	4%	7.5%	5.5%	10.88	38.3	8.21
8	4%	8%	5%	11.24	36.8	7.56
9	5%	6.5%	5%	9.38	40.4	6.07
10	5%	7%	5.5%	9.08	39.5	7.58
11	5%	7.5%	4%	8.52	38.6	8.17
12	5%	8%	4.5%	9.21	39.1	7.72
13	6%	6.5%	5.5%	10.27	38.4	8.57
14	6%	7%	5%	11.57	36.8	7.92
15	6%	7.5%	4.5%	11.14	39.2	7.68
16	6%	8%	4%	9.53	39.7	8.07

TABLE 8: Range analysis.

Properties	Parameters			
	Parameter A	Parameter B	Parameter C	
Stability (kN)	K_1	11.12	9.92	8.69
	K_2	10.33	10.06	10.81
	K_3	9.05	10.62	11.03
	K_4	10.63	10.53	10.59
	R	2.07	0.7	2.34
Flow value (0.1 mm)	K_1	36.68	37.85	38.03
	K_2	37.28	37.35	37.55
	K_3	39.40	38.88	38.35
	K_4	38.53	37.80	37.95
	R	2.72	1.53	0.80
Void ratio (%)	K_1	7.80	7.51	8.23
	K_2	7.79	7.74	7.39
	K_3	7.39	8.21	7.59
	K_4	8.06	7.58	7.84
	R	0.67	0.70	0.84

Note: K_i ($i = 1, 2, 3, 4$) is the mean value of the corresponding test results at level i of the parameters. R is the range, which is the difference value between the maximum and the minimum of K_i .

accordingly, thus affecting the performance of the mixture. The decrease of the mixture flow value is mainly due to the fact that the hydration products from the hydration of coal gangue can provide a rigid effect, and the appropriate water consumption can make the hydration of coal gangue in the mixture more sufficient.

4.2.3. Effect of Coal Gangue Content and Water Consumption on Voidage of Mixture. Under the condition of 7.5% of the optimum amount of asphalt, the content of coal gangue is 3%, 4%, 5%, and 6%, respectively, and the water consumption is 4%, 4.5%, 5%, and 5.5%, respectively. The voidage of the mixture is obtained by Marshall test as shown in Figure 4.

It can be seen from Figure 4(a) that when the water consumption is relatively small, the voidage of the mixture increases with the increase of the content of coal gangue;

when the water consumption is relatively large, with the increase of the content of coal gangue, the voidage of the mixture decreases. When the content of coal gangue is 6% and the water consumption is 5%, the voidage of the mixture is the smallest, but it meets the requirements of the specification [24]. The test results show that when the water consumption is too small, the addition of coal gangue will increase the voidage of emulsified asphalt mixture. The preliminary analysis is that because the specific surface area of coal gangue is relatively small, it will easily absorb water, resulting in uneven mixture in the mixing process, leaving more voids, although the hydration products of coal gangue hydration can play a certain improvement effect. However, the content of coal gangue is relatively small, the activity is not very high, and it does not have a great impact on it. Under this condition, the problem caused by uneven mixing to the mixture is greater than the benefits brought by the hydration products produced by the hydration of coal gangue. When the water consumption is appropriate, the mixture can be more uniform when mixing; with the increase of the amount of coal gangue, the hydration products will increase accordingly, which can play a certain role in filling the void and reduce the voidage of the mixture. From Figure 4(b), it can be seen that when the content of coal gangue is constant, the voidage of the mixture decreases at first and then increases with the increase of water consumption. The voidage of the mixture with different coal gangue content varies greatly with the change of water consumption, indicating that the increase of water consumption has an obvious effect on the voidage of the mixture. When the water consumption is appropriate, the mixture is better in the molding process, and the addition of coal gangue can reduce the density of the mixture and achieve the best [25]. To sum up, in order to make the asphalt mixture achieve a rigid and flexible effect, the flow value of the mixture should not be too large or too small, and the addition of too much coal gangue should increase the rigidity of the mixture and reduce the failure strain. At

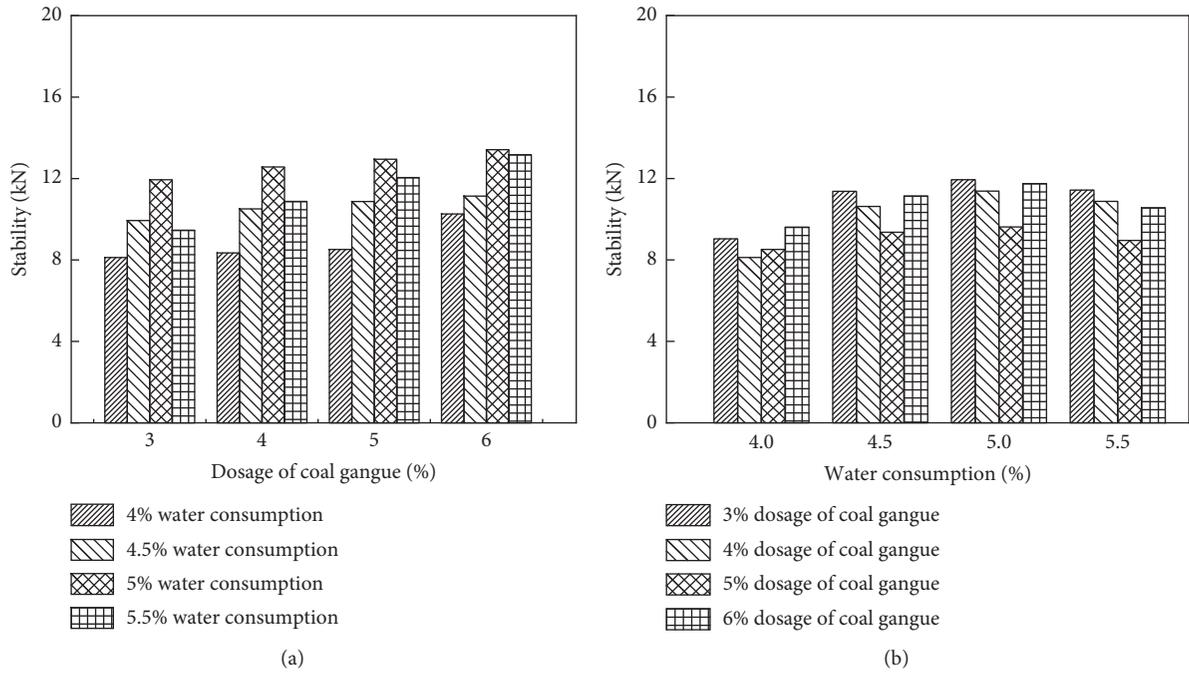


FIGURE 2: Effect of coal gangue and water consumption on the Marshall stability of mixture. (a) Coal gangue. (b) Water consumption.

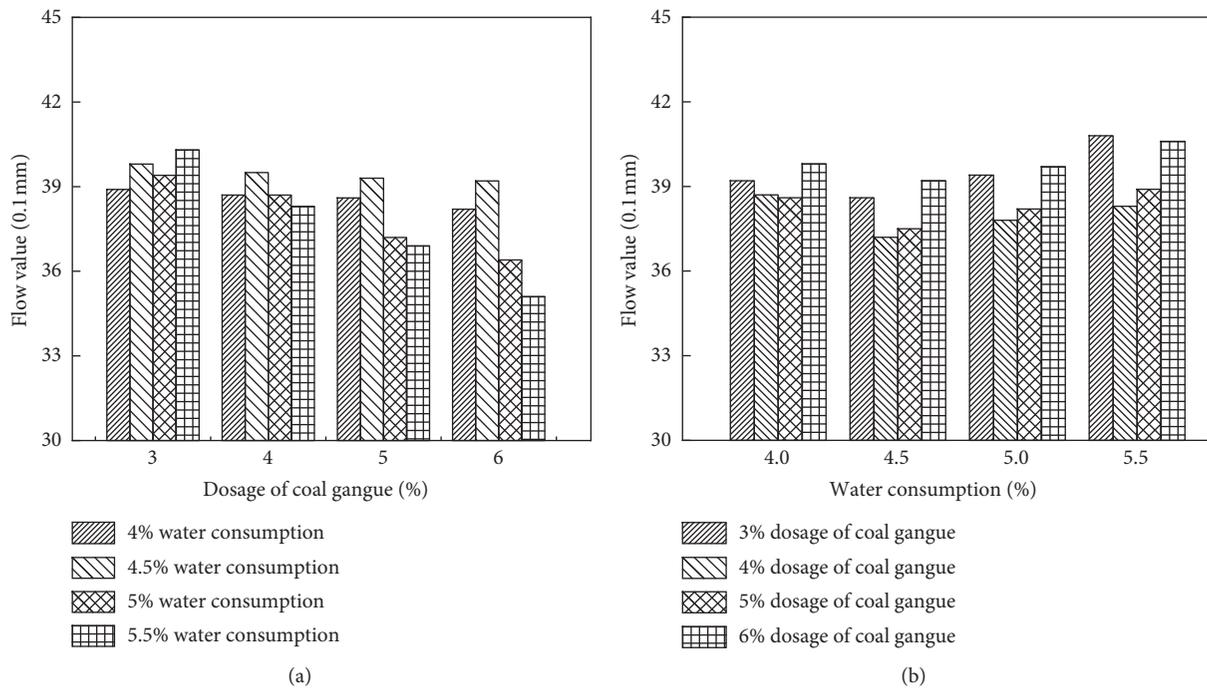


FIGURE 3: Effect of coal gangue and water consumption on the flow value of mixture. (a) Coal gangue. (b) Water consumption.

the same time, the phenomenon of uneven mixing should be avoided in the actual production. Based on the above analysis, the best combination of parameters is recommended as follows: the content of emulsified asphalt is 7.5%, the content of coal gangue is 6%, and the water consumption is 5%.

4.3. *Water Stability of Coal Gangue Emulsified Asphalt Mixture.* Using AC-13 gradation, the content of emulsified asphalt is 7.5%, the water consumption is 5%, and the content of coal gangue is 0%, respectively. The water stability of coal gangue emulsified asphalt mixture is studied by immersion Marshall test. The loading rate of the specimen is

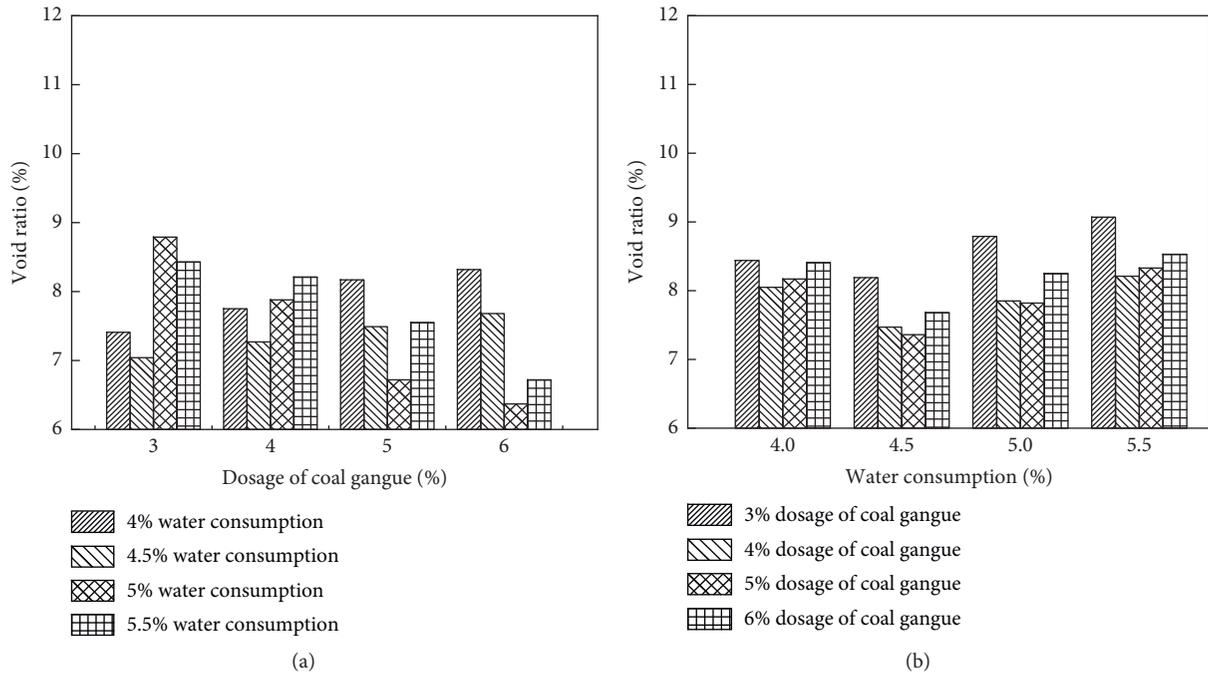


FIGURE 4: Effect of coal gangue and water consumption on the void ratio of mixture. (a) Coal gangue. (b) Water consumption.

50 mm/min \pm 5 mm/min. In order to simulate the situation that the pavement is often eroded by rainwater after rolling in summer and the emulsified asphalt is easy to be secondary emulsified, this paper takes the water bath at 60°C for 48 hours as the most unfavorable condition, and the results are shown in Table 9 and Figure 5.

From the results of the immersion Marshall test in Table 9, it can be seen that the residual stability of each group of tests is more than 85%, which meets the requirements of the specification. It can be seen from Figure 5 that the water loss resistance of emulsified asphalt mixture increases gradually with the increase of coal gangue content, which shows that adding coal gangue can improve the water stability of emulsified asphalt mixture. This is because the hydration products formed by the hydration of coal gangue further bond the components of the mixture together, thus improving the water stability of coal gangue emulsified asphalt mixture [26].

4.4. Analysis of Strength Formation Mechanism. The asphalt material in the mixture contributes to the appropriate “flexibility,” while the aggregate skeleton and the hydration products of coal gangue contribute to a certain strength. The demulsification of emulsified asphalt is a process in which the matrix asphalt is separated from water, and the matrix asphalt will gradually adhere to the surface of the aggregate to form a film, and the hydration of coal gangue will consume the excess water in the mixture, so as to avoid water damage to the mixture [27]. In this paper, the micromorphology of the mixture is explored by scanning electron microscope (SEM) and X-ray diffraction (XRD) analysis, the structural composition characteristics of coal gangue emulsified asphalt mixture are analyzed from the micro

point of view, and the strength formation mechanism is analyzed. Through the observation of the morphology of the mixture, the hydration result, bonding state, and pore distribution of the mixture can be judged efficiently, and the morphological differences between different types of mixture can also be seen directly. First of all, two kinds of samples of ordinary emulsified asphalt mixture (without coal gangue) and coal gangue emulsified asphalt mixture (6%) were analyzed by scanning electron microscope (SEM) at 1000 times, and the results are shown in Figure 6.

Compared with Figures 6(a) and 6(b), it can be found that there are many pores in 1000 times emulsified asphalt mixture, which is due to the fact that a large amount of water in emulsified asphalt mixture is not removed in time and formed after water evaporation. From the micromorphology of coal gangue emulsified asphalt mixture under 1000 times, it can be seen that a large number of flocs are combined with plate or block hydration products to fill the interior of the mixture and play a cementing role to improve the performance of the mixture. The strength of coal gangue emulsified asphalt mixture is formed by the joint action of emulsified asphalt and coal gangue, in which the hydration products of coal gangue and asphalt play the role of cementation and strength. In the process of mixture formation, tiny pores can be filled by hydration products of coal gangue, and the gap between aggregate and cement can be filled by coal gangue, so that the internal structure of the mixture is dense and the strength is increased [28]. At the same time, the hydration of coal gangue needs to consume the excess water in the emulsified asphalt, which further accelerates the strength formation of the mixture. The asphalt mortar without coal gangue and 6% coal gangue is ground into powder for XRD test, and the test results are shown in Figure 7.

TABLE 9: The results data of immersion Marshall test.

Type	Dosage of coal gangue (%)	Stability (kN)	Immersion stability (kN)	Residual stability (%)
Emulsified asphalt mixture	0	11.24	9.68	86.1
	3	11.94	10.42	87.3
Desulphurization fly ash emulsified asphalt mixture	4	12.13	10.76	88.7
	5	12.38	11.12	89.8
	6	12.56	11.52	91.7

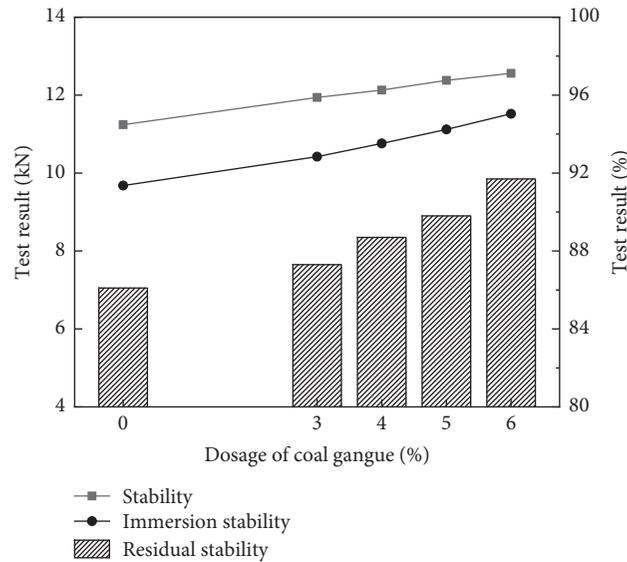


FIGURE 5: The results plot of immersion Marshall test.

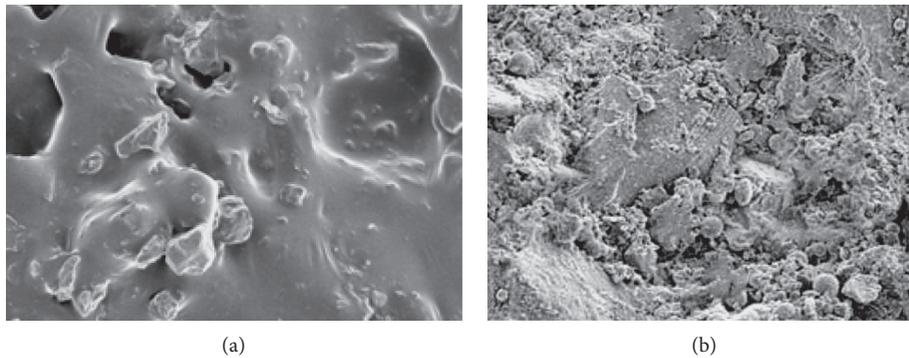


FIGURE 6: Micromorphology of asphalt mixture. (a) Emulsified asphalt mixture. (b) Coal gangue emulsified asphalt mixture.

According to the above XRD diagram, in the ordinary emulsified asphalt mixture, the basic composition of asphalt mortar mainly contains CaCO_3 , and this mineral is the basic composition of mineral powder, which shows that the addition of mineral powder will not have any reaction with it but only plays a role of physical filling. In coal gangue emulsified asphalt mixture, the basic composition of asphalt mortar not only contains CaCO_3 but also contains some hydration products, such as C-S-H gel, SiO_2 , Al_2O_3 , and CaSO_4 .

5. Molecular Dynamics Simulation

In order to clarify the mechanism of the coal gangue on the properties of asphalt, the Molecular Dynamics (MD) simulation is employed in this paper. To create the realistic and applicable asphalt binder molecular model, some researchers have separated asphalt binder into three, four, or six fractions [29, 30] and then created asphalt binder according to the proportion of the fractions. In this paper, the 12-component asphalt binder model, which was first proposed to

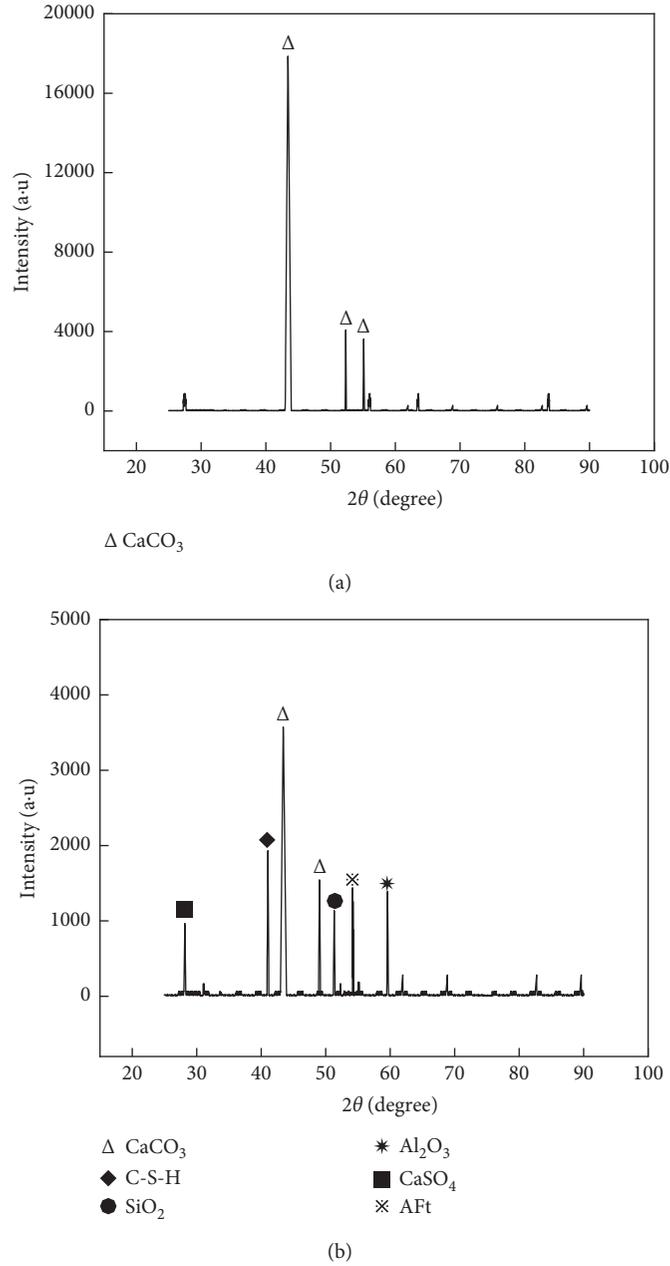


FIGURE 7: XRD analysis of asphalt mixture. (a) XRD analysis of emulsified asphalt. (b) XRD analysis of coal gangue emulsified asphalt.

represent SHRP core asphalt AAA-1, was used to represent the virgin asphalt binder following the literature [31].

The MD simulation was done via a two-step optimization: 100 ps of NVT at a temperature of 60°C, followed by 200 ps of NPT ensemble. After this stage, the simulation was run for 1 ns at NPT to calculate the viscosity and diffusion coefficient. Based on the previous articles [32, 33], the COMPASS force field is employed in the simulation.

The interaction behavior occurs between asphalt binder and the main chemical composition of coal gangue, SiO₂ or Al₂O₃, which is important for the mechanical properties of mixture. To evaluate the interaction behavior, the interaction energy needs to be calculated using (1) first; the

interaction work between asphalt and SiO₂ or Al₂O₃ can be obtained using (2):

$$\Delta E_{\text{interaction}} = E_{\text{total}} - (E_{\text{asphalt}} + E_{\text{chemical composition}}), \quad (1)$$

$$W_{\text{interaction}} = \frac{\Delta E_{\text{interaction}}}{A}, \quad (2)$$

where $\Delta E_{\text{interaction}}$ is the interaction energy between asphalt binder and SiO₂ or Al₂O₃; E_{total} is the total potential energy of asphalt binder and SiO₂ or Al₂O₃ showed in Figure 8; E_{asphalt} and $E_{\text{chemical composition}}$ are the potential energies of asphalt and SiO₂ or Al₂O₃ separated in vacuum at equilibrium, respectively; $W_{\text{interaction}}$ is the interaction work

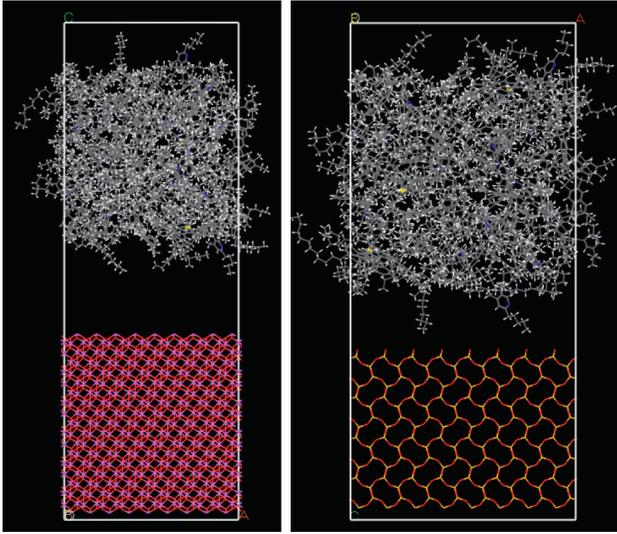


FIGURE 8: Asphalt binders' modes with different Al_2O_3 (left) and SiO_2 (right).

between asphalt and SiO_2 or Al_2O_3 ; and A is the interface contact area between asphalt and SiO_2 or Al_2O_3 .

Based on the abovementioned theory of computation for interaction work, the interaction between asphalt binders and SiO_2 or Al_2O_3 in different contents is shown in Figure 9.

To compare conveniently the interaction energy and the cohesive energy of asphalt, the surface free energy of asphalt is added in Figure 9. In order to simulate the surface free energy, bulk and confined models were created, respectively. The equation for surface free energy is shown in

$$\gamma_a = \frac{(E_{\text{surface}} - E_{\text{bulk}})}{2A}, \quad (3)$$

where γ_a is the surface free energy; E_{surface} and E_{bulk} are the potential energy of the confined asphalt layer and bulk asphalt, respectively; and A is the area where the new surface is created.

Figure 9 shows that the interaction energy of the asphalt and main chemical composition of coal gangue, SiO_2 and Al_2O_3 , is larger than the surface free energy of asphalt, indicating that the coal gangue improves the internal interaction of asphalt. Based on this feature of coal gangue, the mechanical properties of mixture after modification are improved.

6. Conclusions

- (1) Through orthogonal test, the influence weights of coal gangue content, emulsified asphalt dosage, and water consumption on Marshall stability, flow value, and voidage of coal gangue emulsified asphalt mixture are analyzed. It is determined that the optimum amount of emulsified asphalt in coal gangue emulsified asphalt mixture is 7.5%. Combined with the Marshall test, the effects of water consumption and coal gangue content on the performance of the mixture are further studied. Finally, it is

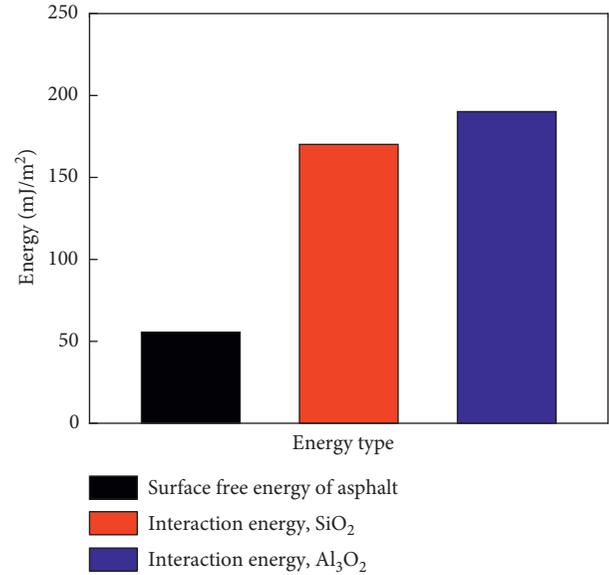


FIGURE 9: Interaction energy between asphalt binder and SiO_2 or Al_2O_3 .

recommended that the best parameter combination of the mixture is 7.5% emulsified asphalt, 6% coal gangue, and 5% water consumption.

- (2) With the increase of coal gangue content, the water loss resistance of emulsified asphalt mixture increases gradually, and the water stability of emulsified asphalt mixture can be improved by adding coal gangue. This is because the coal gangue is alkaline, and the alkalinity increases rapidly in the wet environment, thus increasing the bonding effect between the aggregate and asphalt in the asphalt mixture. In addition, the hydration products formed by the hydration of coal gangue further bond the components of the mixture together, thus improving the water stability of coal gangue emulsified asphalt mixture.
- (3) According to the SEM analysis, the strength of the mixture is formed by the joint action of emulsified asphalt and coal gangue, in which the hydration products of coal gangue and asphalt play the role of cementation and strength together. In the process of mixture formation, the hydration of coal gangue needs to consume the excess water in the emulsified asphalt, so that the strength of the mixture can be further accelerated. The tiny pores in the mixture can be filled by the hydration products of coal gangue, and the gap between aggregate and binder can be filled by unhydrated coal gangue, so that the internal structure of the mixture is dense and the strength is increased.
- (4) According to the results of XRD analysis, ordinary emulsified asphalt mortar mainly contains CaCO_3 , which mainly plays the role of physical filling. After adding coal gangue, the basic composition of asphalt mortar not only contains CaCO_3 but also contains

some hydration products, such as C-S-H gel, SiO₂, Al₂O₃, and CaSO₄.

- (5) The interaction behavior between asphalt binder and the main chemical composition of coal gangue, SiO₂ or Al₂O₃, is calculated by MD simulation; it is found that the interaction energy of the asphalt and SiO₂ or Al₂O₃ is larger than the surface free energy of asphalt. Based on this feature of coal gangue, the mechanical properties of mixture after modification are possibly improved.

Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

Acknowledgments

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