

Article

Preparation Method of Simulated Deep Sandstone Materials Based on Dual Equivalence of Principal Components and Mechanical Properties, and Quantitative Evaluation of Simulation Effectiveness

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Abstract

Intact deep sandstone cores are scarce, heterogeneous with poorly repeatable, limiting systematic laboratory studies of deep-rock mechanical behavior. This study selected dense sandstone recovered from 1050 m in the Pingdingshan mining area as the prototype system for the development of a targeted-sandstone-constrained screening strategy for simulated deep sandstone. The strategy integrates mineral-composition matching, orthogonal mixture design, mechanical testing, PCA-based comprehensive similarity evaluation, GMM classification, stress–strain curve comparison and fracture-morphology verification. Candidate materials were prepared using a cement–silica-fume matrix with quartz sand, K-feldspar, Na-feldspar, nanoclay and superplasticizer. Results show that the water–binder ratio dominated uniaxial compressive strength, tensile strength and elastic modulus, whereas superplasticizer and nanoclay had secondary effects. The PCA-based index assigned weights of 52.9%, 29.2% and 17.9% to uniaxial compressive strength, elastic modulus and brittleness index, respectively. Among the 25 mixtures sampled, S5 showed the highest mechanical similarity, with a simulation index of 71.65% and a stress–strain curve similarity of 0.958. GMM clustering identified S5 and S10 as the closest high-strength, high-stiffness and high-brittleness group, while S10 better reproduced natural crack geometry. These results indicate that the optimal simulated sandstone depends on the target response and provide a task-oriented route for reproducible simulated deep sandstone.

Keywords: simulated rock material; principal component analysis; Gaussian mixture clustering; principal component equivalence; comprehensive simulated index

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1. Introduction

As mineral resource exploitation has progressively shifted from shallow to deep levels, the existing theoretical framework of deep rock mechanics has been confronted with unprecedented challenges [1–3]. To advance this body of theory, researchers have attempted to obtain rock specimens directly from great depths for controlled laboratory investigations [4,5]. However, due to the limitations of current coring technologies, rock masses are prone to cutting-induced fragmentation during deep drilling, making it difficult to recover intact and representative specimens [6–10]. In addition, deep drilling operations are typically associated with considerable time, labor, and financial costs, which further constrain the efficiency of sample acquisition [11,12]. More critically, the in situ geological environment at depth is often highly heterogeneous; many targets are located within faulted, fractured, or otherwise strongly disturbed zones, rendering the recovery of structurally sound, laboratory-scale rock samples even more challenging [13–16].

Against this background, the development of simulated rock-like materials with physical and mechanical properties equivalent to deep in situ rocks has gradually become a research frontier in recent years [17]. Concrete, whose formation process and macroscopic mechanical behavior are highly comparable to those of natural rock, has played a pivotal role in this line of research on rock-like materials [18]. In recent years, concrete technology has evolved from conventional low-strength mixes toward high-strength and high-brittleness systems, providing a solid material basis for replicating the response of deep rocks. At the same time, rock-like materials are attractive because their raw ingredients are readily available, their preparation procedures are relatively simple, and their physical and mechanical properties can be designed and tuned within a wide range, which makes them highly promising substitutes for deep rock specimens in laboratory testing [19,20]. Therefore, developing high-performance concrete-based rock-like materials that closely match the physical and mechanical characteristics of deep rocks is expected not only to alleviate the difficulty of obtaining deep in situ cores, but also to provide an essential technical pathway for advancing the theoretical framework of deep rock mechanics.

Scholars have made numerous attempts to develop simulated rocks that are equivalent to the physical and mechanical properties of real rocks. TIAN et al. [21] utilized 3D printing technology to create simulated rock samples, whose stress–strain characteristics were similar to those of real rocks, suggesting that this technology could make the mechanical properties of the samples closer to those of real rocks than previous methods. SU et al. [22] developed a program for optimizing the mixture ratio of rock-like materials based on a genetic algorithm, and using this, they identified the optimal mixture ratio for gneiss-like granite materials. FEDRIZZI et al. [23] created a carbonate rock from raw materials such as sand and calcite, discovering that this artificial rock exhibited a high similarity in physical characteristics, such as porosity and permeability, to natural mudstones. Zhuang et al. [24] proposed a method for quantitatively adjusting rock mechanical properties using 3D printing technology, successfully simulating the stress–strain characteristics of real rocks by adjusting material ratios and curing temperatures.

In addition to these studies, MA et al. [25] developed rockburst-similar materials for white sandstone and showed that the optimized material reproduced the general strength–brittleness characteristics of the prototype, although its compressive strength, tensile strength and elastic modulus remained lower than those of the original sandstone. PERRAS and VOGLER [26] compared natural sandstones with several 3D-printed sand-based materials and found that Sand-Furan specimens were close to weak natural

sandstone in terms of strength, but clear differences still existed in stiffness and damage thresholds. GE et al. [27] prepared transparent hard rock-like materials and found that their stress–strain response and brittle failure pattern were similar to sandstone, whereas their elastic modulus was much lower than that of the prototype sandstone. GOU et al. [28] developed a gypsum-mixed sandstone-like material whose mechanical properties followed a proportional relationship with those of the target sandstone, but the absolute values of UCS and elastic modulus were still substantially lower. WANG et al. [29] prepared damaged sandstone-like materials using polystyrene foam particles and achieved small errors relative to similarity-scaled target parameters, but the model material parameters were still governed by the adopted similarity ratio.

In summary, and as shown in Table 1, the gap between simulated rocks developed by scholars and real rocks has not been resolved, especially for deep rocks, where the differences in simulation effects are even more pronounced. The development of simulated rocks that are completely equivalent to the physical and mechanical properties of real rocks remains an urgent task.

Table 1. Comparison of mechanical parameters between real rocks and simulated rocks.

No.	Producer	Real Rock Parameters			Simulated Rock Parameters		
		σ_c /MPa	σ_t /MPa	E/GPa	σ_c /MPa	σ_t /MPa	E/GPa
1	TIAN [21]	9.7	--	--	8.97	--	1.696
2	SU [22]	80	5.33	26	20.66	1.41	6.48
3	ZHUANG [24]	44.57	--	6.87	8.15	--	0.73
4	MA [25]	29.76	6.14	7.41	11.50	2.37	2.86
5	PERRAS and VOGLER [26]	3.74	1.02	0.13	3.47	1.38	1.31
6	GE [27]	--	--	12.74	3.29	0.259	0.384
7	GOU [28]	69.20	--	3.68	6.96	--	0.53
8	WANG [29]	62.91	11.25	5.24	3.36	0.53	0.29

Scholars have selected various mechanical parameters of rocks as equivalent bridges between simulated rocks and real rocks. DEERE et al. [30] compiled the range of ratios between the tangent elastic modulus (E) at 50% of the compressive peak strength and uniaxial compressive strength for different types of sedimentary rocks, and proposed a classification standard for sedimentary rocks based on this. SIMPSON [31] used this indicator to compile the relevant values for various granular and nongranular materials used as rock-like materials, determining that materials falling within this deformation indicator range could be used as rock substitutes. TATONE [32] introduced the tensile-to-compressive strength ratio as a brittleness index, which was used to assess the suitability of rock-like materials. He emphasized that the deformation and brittleness indices of rock-like materials must fall within the statistical ranges of the corresponding natural rock indicators in order to replace rocks in mechanical testing. LIU et al. [33] adopted Tatone's approach [32] and created mortar-like rock materials using deformation and brittleness indices, verifying that these materials fell within the range of natural rock parameters. However, the mechanical behavior of real rocks, especially deep rocks, is complex, and judging the effectiveness of simulation based solely on a single macro parameter (such as uniaxial compressive strength) is overly simplistic. There is an urgent need to evaluate the effectiveness of simulated rock materials in simulating real rocks from multiple perspectives and indicators. This would enable the study of deep in situ rock mechanics behavior in the laboratory using only simulated rock materials.

This study took dense sandstone at a depth of 1050 m in the Pingdingshan mining area as the prototype and prepared a simulated rock material characterized by high strength, high elastic modulus and pronounced brittleness. The mix design was adjusted so that the major constituents of the simulated material were equivalent to those of the target sandstone. Laboratory-scale tests showed that the macroscopic mechanical response of the deep sandstone was successfully reproduced. Furthermore, Principal Component Analysis (PCA) and Gaussian Mixture Model (GMM) clustering were introduced to construct a data-driven framework for quantitatively evaluating the restoration performance of the simulated deep rock. The results demonstrated that the simulated material achieved a high degree of consistency with the deep sandstone in terms of key mechanical parameters, providing both a reliable material basis and a methodological tool for in-depth investigations of rock-mass mechanical behavior under deep in situ conditions.

2. Sample Preparation and Experimental Scheme

2.1. Physical and Mechanical Parameters of Pingdingshan Sandstone

The real rock selected for this experiment was sandstone from the Pingdingshan Coal Mine area, located at a depth of 1050 m in Pingdingshan City, Henan Province. As shown in Figure 1, petrographic analysis of thin sections revealed that the main clastic minerals in the sandstone were quartz and feldspar, with contents of approximately 50% and 45%, respectively. The grain size ranged from 0.1 to 0.4 mm. The mechanical parameters were as follows: uniaxial compressive strength of 160.4 MPa, elastic modulus of 44.61 GPa, tensile strength of 22.91 MPa, brittleness index of 7, and Poisson's ratio of 0.17.

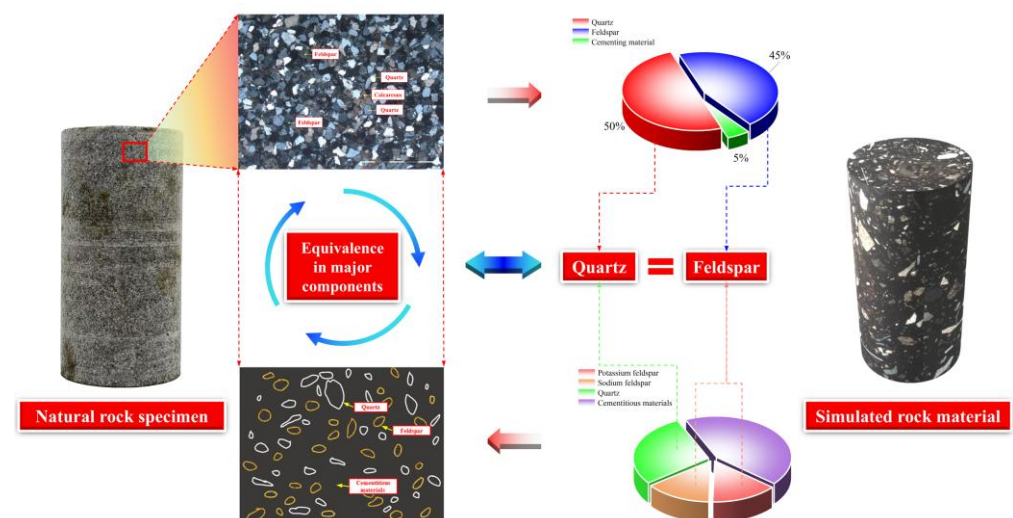


Figure 1. Petrographic thin section of Pingdingshan sandstone.

2.2. Selection of Raw Materials

The raw materials used in this experiment included cement, potassium feldspar, sodium feldspar, quartz sand, nanoclay, water, a polycarboxylate high-performance superplasticizer, and a defoamer. The binding materials consisted of cement and silica fume. Ordinary Portland cement (P.O. 52.5) was selected as the cementitious material, while silica fume played two important roles in the simulated rock material due to its pozzolanic activity and ultrafine particle size. The reaction between SiO_2 and the Ca(OH)_2 generated during cement hydration formed calcium silicate hydrate gel, which significantly enhanced the strength of the material. Although Ca(OH)_2 itself tended to reduce the strength of the simulated rock material, the formation of calcium silicate hydrate improved the overall mechanical performance. In addition, silica fume, with a fineness about 100 times

greater than that of cement, could fill the pores within the material and further improve its compactness.

The filling aggregates selected for this experiment included quartz sand and feldspar. The grain size ranges of quartz sand were 10–20 mesh (1.5–0.75 mm), 20–40 mesh (0.75–0.38 mm), 40–80 mesh (0.38–0.19 mm), and 80–120 mesh (0.19–0.13 mm). The multiscale particle-size distribution of quartz sand was designed to improve particle packing efficiency and reconstruct the granular skeleton characteristics of the prototype sandstone. Both potassium feldspar (KAlSi_3O_8) and sodium feldspar ($\text{NaAlSi}_3\text{O}_8$) powders had a purity of 95%. As shown in Figure 2a, the particle size of potassium feldspar ranged from 0.02 to 0.12 mm, and the composition ratio of potassium feldspar to quartz was 95.7:4.3. As shown in Figure 2b, the particle size of sodium feldspar ranged from 0.02 to 0.26 mm, and the composition ratio of sodium feldspar, muscovite, calcite, and quartz was 96.2:2:0.9:0.9. The particle-size distribution curves in Figure 2 demonstrate the fine-grained characteristics of feldspar powders, which enables them to act as filling components between coarse quartz particles and contributes to the adjustment of packing structure and pore characteristics. Therefore, the particle-size characteristics of quartz sand and feldspar were considered as an important factor in reproducing the mineralogical framework and mechanical response of the prototype sandstone.

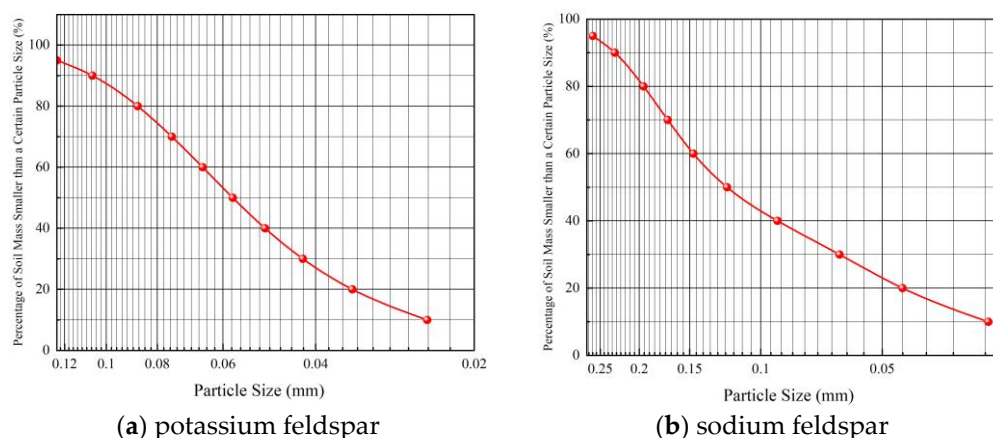


Figure 2. Feldspar particle-size distribution curve.

Erolite nanoclay ($\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4$) has a tubular morphology, similar to montmorillonite, and is composed of two layers of aluminosilicate in halloysite. When halloysite nanotubes are incorporated into polymer composites, they can significantly improve the material's thermal and mechanical properties.

The polycarboxylate high-performance superplasticizer used is the HLX standard type, which exhibits strong water-reducing and dispersing properties for cement. Its primary function is to reduce the water content in cement, enhance strength, improve workability and durability, and reduce shrinkage. As the water content decreases, the cement strength typically increases further. As shown in Figure 3, the raw materials used for simulated deep sandstone can be divided into four categories: granular aggregates (quartz sand and feldspar), binding materials (cement and silica fume), microstructural modification materials (nanoclay), and chemical additives (superplasticizer and defoamer). This material system combines mineral composition control with cement-based structural modification, providing the basis for achieving both mineralogical similarity and mechanical similarity with the prototype sandstone.



Figure 3. Raw materials for simulated deep sandstone.

2.3. Experimental Scheme

Based on the selected raw materials and the physical and mechanical parameters of Pingdingshan sandstone, the main components of Pingdingshan sandstone are quartz and feldspar, with their mass ratio being approximately 1:1. Therefore, quartz sand and potassium/sodium feldspar were selected as the main granular components to reproduce the mineralogical framework of the prototype sandstone. In addition to the mineral proportion, the particle-size characteristics of the granular components were considered during material design because particle-size distribution influences particle packing, pore structure, interparticle contacts, and stress-transfer behavior, which are closely related to the mechanical response of rock-like materials. However, due to the differences between natural rock formation processes and laboratory preparation methods, an exact reproduction of the particle-size distribution of natural sandstone is difficult to achieve. In this study, the particle-size ranges of the selected aggregates were therefore designed to approximate the dominant grain-size characteristics of the prototype sandstone. The prototype Pingdingshan sandstone has a particle-size range of 0.1–0.4 mm, while the quartz sand used in this study ranges from 0.13 to 1.5 mm, covering the main grain-size range of the prototype sandstone, and the potassium/sodium feldspar powders range from 0.02 to 0.26 mm to provide fine particle filling and regulate the packing structure.

Based on the above mineral composition and particle-size considerations, an orthogonal experimental design [34,35] was adopted to further optimize the mechanical properties of the simulated sandstone. The mass ratios of silica fume, quartz sand, potassium and sodium feldspar, and defoamer were set as fixed values. The specific mass ratios are as follows: the mass ratio of quartz sand to feldspar is 1:1, the mass ratio of silica fume to cement is 0.3, the mass ratio of quartz sand to cement is 1.3, the mass ratio of potassium feldspar to cement is 0.65, the mass ratio of sodium feldspar to cement is 0.65, and the mass ratio of defoamer to cement is 0.001. The mass ratios of water to binder materials, superplasticizer to binder materials, and nanoclay to binder materials were set as the three factors for the orthogonal experiment, with each factor having five levels. The specific configurations are shown in Tables 2 and 3.

Table 2. Orthogonal experimental factor levels for simulated rock materials.

Level	Water	Superplasticizer	Nanoclay
1	0.34	0.007	0.02
2	0.35	0.009	0.04

3	0.36	0.011	0.06
4	0.37	0.013	0.08
5	0.38	0.015	0.10

Table 3. Orthogonal design combinations for simulated rock materials.

No.	Water	Superplasticizer	Nanoclay
S1	0.34	0.007	0.02
S2	0.34	0.009	0.06
S3	0.34	0.011	0.10
S4	0.34	0.013	0.04
S5	0.34	0.015	0.08
S6	0.35	0.007	0.10
S7	0.35	0.009	0.04
S8	0.35	0.011	0.08
S9	0.35	0.013	0.02
S10	0.35	0.015	0.06
S11	0.36	0.007	0.08
S12	0.36	0.009	0.02
S13	0.36	0.011	0.06
S14	0.36	0.013	0.10
S15	0.36	0.015	0.04
S16	0.37	0.007	0.06
S17	0.37	0.009	0.10
S18	0.37	0.011	0.04
S19	0.37	0.013	0.08
S20	0.37	0.015	0.02
S21	0.38	0.007	0.04
S22	0.38	0.009	0.08
S23	0.38	0.011	0.02
S24	0.38	0.013	0.06
S25	0.38	0.015	0.10

2.4. Sample Preparation

The specimen preparation process is illustrated in Figure 4. The raw materials were sequentially added into a mortar mixer and mixed for 3 min. After mixing, the mixture was poured into a 15 cm cubic mold and vibrated on a vibration table for 3 min, until no more bubbles emerged from the specimen. The surface of the mold was then wrapped with plastic film, and the specimen was allowed to sit for one day. After the specimen had set, it was demolded and placed in a curing chamber for 28 days. During the curing period, the temperature was maintained at 20 ± 1 °C, and the relative humidity was kept above 99%. After curing, core samples were taken from the cubic specimens and prepared as standard specimens for uniaxial compression tests ($\varphi 50 \times 100$ mm) and Brazilian splitting tests ($\varphi 50 \times 25$ mm). The tensile splitting response of heterogeneous brittle materials may be affected by specimen size [36]. To control the influence of the size effect on the comparative analysis, all specimens used in the Brazilian splitting tests were prepared with identical dimensions and tested under the same loading configuration and boundary conditions. Therefore, although the intrinsic size effect could not be completely eliminated, its influence remained consistent among the different material groups. Accordingly, the measured splitting tensile strength was used only for comparative evaluation and similarity analysis at the specified specimen scale, rather than for extrapolation to specimens of other sizes or to the engineering scale. This sample preparation method effectively

prevents the formation of bubbles at the contact points between the standard mold and the specimen, ensuring the homogeneity of the sample. It also mirrors the sample preparation process of real rock specimens, thereby restoring the preparation process of real rock as much as possible and ensuring the accuracy of the test results.

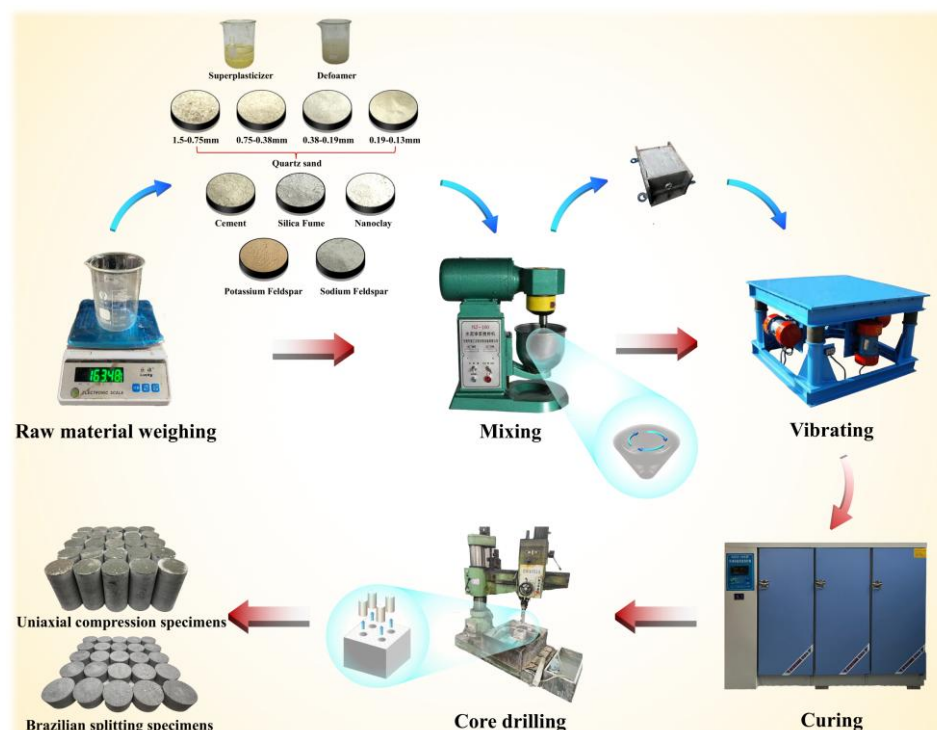


Figure 4. Schematic diagram of the specimen preparation process for simulated deep sandstone.

2.5. Testing Method

The basic physical and mechanical property tests were conducted using the GCTS rock mechanics testing system from the State Key Laboratory of Intelligent Construction and Healthy Operation and Maintenance of Deep Underground Engineering at Sichuan University, as shown in Figure 5. This GCTS comprehensive rock testing system employs closed-loop servo control and is capable of testing rock compressive strength, tensile strength, elastic modulus, and P-wave and S-wave velocities under high-temperature and high-pressure conditions. The system has a maximum axial compressive load of 1000 kN and a maximum confining pressure of 70 MPa, with high control accuracy, allowing for complex rock mechanics testing. In the uniaxial compression test, the sample was pre-loaded with 1 kN before testing, and the displacement control method was used with a loading rate of 0.04 mm/min.

During the uniaxial compression tests, the axial and circumferential deformations were simultaneously measured using the on-specimen deformation measurement system equipped with linear variable differential transformers (LVDTs) in the GCTS system. The elastic modulus and Poisson's ratio were determined based on the stress–strain response within the elastic deformation stage. Specifically, the stress range of 30–60 MPa was selected, and linear regression was performed on the corresponding stress–strain data. The elastic modulus was calculated from the slope of the axial stress–axial strain relationship:

$$E = \frac{\Delta\sigma}{\Delta\varepsilon_a} \quad (1)$$

where E is the elastic modulus, $\Delta\sigma$ represents the stress increment, and $\Delta\epsilon_a$ represents the corresponding axial strain increment. Poisson's ratio was calculated from the slope relationship between circumferential strain and axial strain:

$$\nu = -\frac{\Delta\epsilon_r}{\Delta\epsilon_a} \quad (2)$$

where ϵ_r and ϵ_a represent circumferential strain and axial strain, respectively. The least-squares linear fitting method was adopted to minimize the influence of measurement fluctuations and improve the reliability of the calculated mechanical parameters.

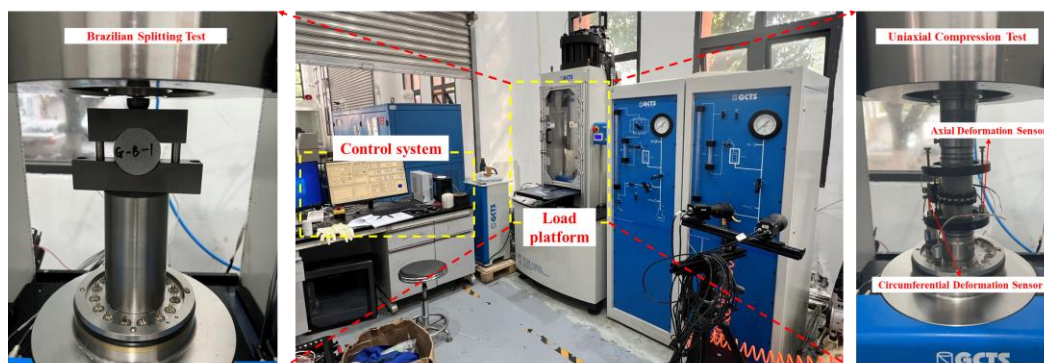


Figure 5. GCTS rock mechanics testing system.

3. Experimental Results

3.1. Sensitivity Analysis of Factors in Simulated Deep Sandstone

The physical and mechanical test results of the simulated deep rock material are shown in Table 4, where the calculation formula for the brittleness index B is as follows:

$$B = \frac{\sigma_c}{\sigma_t} \quad (3)$$

Table 4. Physical and mechanical parameters of each sample group under orthogonal experimental design.

No.	σ_c/MPa	σ_t/MPa	E/GPa	μ	B
S1	101.28	11.62	30.26	0.13	8.72
S2	95.22	11.13	36.53	0.05	8.56
S3	111.71	12.04	33.19	0.17	9.28
S4	111.67	11.19	33.7	0.19	9.98
S5	118.85	11.21	36.31	0.17	10.60
S6	107.28	10.54	31.42	0.19	10.18
S7	102.7	11.86	30.4	0.17	8.66
S8	105.36	12.06	31.96	0.18	8.74
S9	98.93	10.58	31.79	0.18	9.35
S10	111.69	9.5	35.89	0.13	11.76
S11	85	9.87	52.3	0.2	8.61
S12	79.24	8.66	42.24	0.2	9.15
S13	84.47	7.95	46.91	0.13	10.63
S14	85.04	8.14	49.18	0.25	10.45
S15	77.48	8.33	44.31	0.2	9.30
S16	77.25	8.43	29.77	0.28	9.16
S17	88.52	9.27	39.77	0.21	9.55

S18	88.08	8.16	30.54	0.19	10.79
S19	78.09	8.94	42.89	0.27	8.73
S20	87.73	9.05	37.13	0.2	9.69
S21	83.5	9.46	34.16	0.17	8.83
S22	69.78	7.13	27.65	0.25	9.79
S23	84.59	7.84	36.73	0.24	10.79
S24	80.26	8.41	32.49	0.15	9.54
S25	82.71	9.87	34.44	0.22	8.38

A range analysis was performed on the data obtained from the orthogonal experiment, aiming to determine the sensitivity of each factor to uniaxial compressive strength, tensile strength, and elastic modulus. In the range analysis, only the influence of individual factors was considered, with interference from other factors excluded. The range value represents the difference between the maximum and minimum response values under different levels of a particular factor. Its magnitude can be used to initially assess the sensitivity of the response values to changes in the factor levels.

Based on Figure 6 and Table 5, the relative importance of the influencing factors on uniaxial compressive strength (UCS) can be ranked as follows: water-to-binder ratio > superplasticizer > nanoclay. As shown in Table 5, the range values of the water-to-binder ratio, superplasticizer, and nanoclay for UCS were 27.28, 8.60, and 5.27, respectively, corresponding to fluctuation amplitudes of 34.4%, 9.87%, and 5.87%. These results indicate that the water-to-binder ratio exerted a much stronger effect on UCS than either superplasticizer or nanoclay, confirming it as the primary control variable. With increasing water-to-binder ratio, the UCS of the simulated rock material decreased monotonically. The UCS at water-to-binder ratios of 0.34–0.35 was 24.35 MPa, or 29.66%, higher than that at 0.36–0.38, indicating that strength enhancement was particularly pronounced when the water-to-binder ratio was below 0.35. With increasing superplasticizer dosage, the UCS showed only a modest fluctuation. With increasing nanoclay content, the UCS increased slowly and reached its maximum when the nanoclay content was 10%.

Table 5. Influence of factor levels on each response value in orthogonal experimental design.

Response Values	Water-to-Binder Ratio	Superplasticizer	Nanoclay
σ_c /MPa	27.28 (34.4%)	8.60 (9.87%)	5.27 (5.87%)
Rank	1	2	3
E /GPa	14.70 (45.52%)	2.69 (7.62%)	3.60 (10.4%)
Rank	1	3	2
σ_t /MPa	2.90 (33.96%)	0.53 (5.61%)	0.89 (9.80%)
Rank	1	3	2
μ	0.09 (61.97%)	0.03 (18.18%)	0.07 (44.59%)
Rank	1	3	2
B	0.31 (3.29%)	0.95 (10.33%)	0.63 (6.89%)
Rank	3	1	2

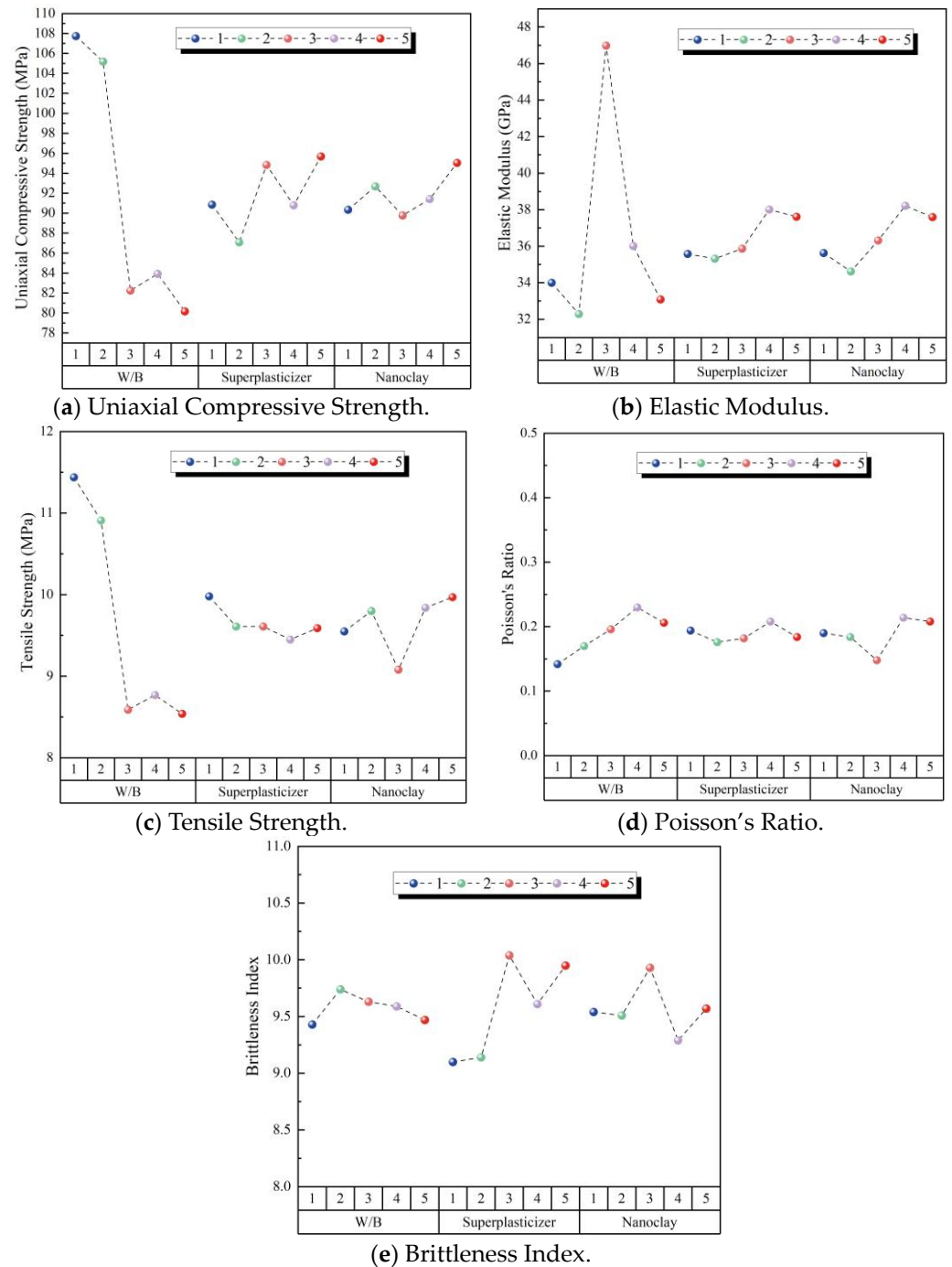


Figure 6. Variation of each response value with different levels of water–cement ratio, superplasticizer, and nanoclay.

For the elastic modulus (E), the ranking of influencing factors was water-to-binder ratio > nanoclay > superplasticizer. As listed in Table 5, the range values of the water-to-binder ratio, nanoclay, and superplasticizer for E were 14.70, 3.60, and 2.69, respectively, corresponding to fluctuation amplitudes of 45.52%, 10.4%, and 7.62%. This indicates that the water-to-binder ratio was the dominant factor controlling the deformation resistance of the simulated rock material. As the water-to-binder ratio increased, E first increased and then decreased, attaining its maximum at a water-to-binder ratio of 0.36. With increasing superplasticizer content, E fluctuated within 35.32–38.01 GPa, showing an overall upward trend and peaking at a superplasticizer dosage of 1.3%, beyond which it gradually decreased. As the nanoclay content increased, E varied between 34.62 and 38.22 GPa,

following a trend of first increasing and then decreasing, with a maximum at a nanoclay content of 8%.

For tensile strength, the influencing factors were ranked as water-to-binder ratio > nanoclay > superplasticizer. According to Table 5, the range values of the water-to-binder ratio, nanoclay, and superplasticizer for tensile strength were 2.90, 0.89, and 0.53, respectively, corresponding to fluctuation amplitudes of 33.96%, 9.80%, and 5.61%. This shows that tensile strength was mainly governed by the water-to-binder ratio, whereas nanoclay and superplasticizer produced relatively minor effects within the studied ranges. Tensile strength gradually decreased with increasing water-to-binder ratio. At water-to-binder ratios of 0.34–0.35, the tensile strength was 2.54 MPa, or 29.44%, higher than that at 0.36–0.38, indicating that a water-to-binder ratio below 0.35 was more favorable for improving the tensile performance of the simulated rock material. With increasing superplasticizer and nanoclay contents, tensile strength showed only small fluctuations.

For Poisson's ratio, the ranking of influencing factors was water-to-binder ratio > nanoclay > superplasticizer. As shown in Table 5, the range values of the water-to-binder ratio, nanoclay, and superplasticizer for Poisson's ratio were 0.09, 0.07, and 0.03, respectively, corresponding to fluctuation amplitudes of 61.97%, 44.59%, and 18.18%. These results suggest that the water-to-binder ratio had the greatest influence on the lateral deformation behavior of the simulated rock material, while nanoclay also had a relatively notable effect. As the water-to-binder ratio increased, Poisson's ratio first increased and then decreased, peaking at a ratio of 0.37. With increasing superplasticizer content, Poisson's ratio followed an S-shaped evolution, decreasing initially, then increasing, and subsequently decreasing again. In contrast, with increasing nanoclay content, Poisson's ratio exhibited a V-shaped trend, first decreasing and then increasing, reaching its minimum at 6% nanoclay. At this dosage, the lateral deformation capacity was the lowest, and the material was least prone to transverse expansion.

For the brittleness index, the ranking of influencing factors was superplasticizer > nanoclay > water-to-binder ratio, which differed from the rankings obtained for the other four mechanical parameters. As shown in Table 5, the range values of superplasticizer, nanoclay, and water-to-binder ratio for the brittleness index were 0.95, 0.63, and 0.31, respectively, corresponding to fluctuation amplitudes of 10.33%, 6.89%, and 3.29%. Overall, the effects of all three variables on brittleness were relatively small compared with their effects on the other mechanical parameters. As shown in Figure 6, the brittleness index changed only slightly with variations in water-to-binder ratio. With increasing superplasticizer dosage, the brittleness index increased, then decreased, and then increased again, reaching its maximum at a superplasticizer content of 1.1%, at which the simulated rock material exhibited the highest brittleness. With increasing nanoclay content, the brittleness index remained essentially stable, indicating only a marginal influence on the brittleness characteristics.

The range analysis results indicate that the water–binder ratio is the dominant factor affecting the mechanical properties of simulated sandstone, whereas superplasticizer and nanoclay exhibit relatively weaker effects. This difference can be attributed to their distinct roles in controlling the material structure. The water–binder ratio directly determines the amount of free water involved in hydration and the development of the pore structure after hardening. A lower water–binder ratio reduces capillary porosity, improves matrix compactness, and enhances stress transfer within the cementitious skeleton, thereby exerting a fundamental influence on strength and deformation characteristics.

In comparison, superplasticizer mainly improves the dispersion of cement particles by reducing particle agglomeration, which enhances packing efficiency and hydration uniformity. However, its effect is highly dependent on the initial water–binder condition, and it cannot fundamentally compensate for the adverse effects of excessive water content

on pore structure. Therefore, although superplasticizer contributes to improving the internal structure, its influence on macroscopic mechanical properties is secondary to that of the water–binder ratio.

Nanoclay improves material performance mainly through filler effects, nucleation effects, and microstructural refinement. The incorporation of nanoclay can promote the formation of hydration products and refine local pore structures, particularly within the cement matrix and interfacial regions. However, because the nanoclay content used in this study was relatively low, its influence was mainly limited to local microstructural optimization rather than the overall pore structure evolution. Consequently, its contribution to the macroscopic mechanical response was weaker than that of the water–binder ratio.

3.2. Variance Analysis of Influencing Factors for Simulated Deep Sandstone

The above analysis, based on a relatively small computational load, preliminarily assessed the influence of water-to-binder ratio, superplasticizer, and nanoclay on five response variables: uniaxial compressive strength, tensile strength, elastic modulus, Poisson's ratio, and brittleness index. However, range analysis cannot assess errors and does not accurately determine the significance of each factor's impact on the response variables. Therefore, based on the results of the range analysis, an analysis of variance (ANOVA) from orthogonal design experiments was applied to correct the results, providing statistical validation for the effects of each factor on the response variables.

Analysis of variance (ANOVA) is used to determine whether the effects of factors are significant by comparing the sum of squares for each factor with the sum of squares for error [37]. Based on the orthogonal experimental design in this study, the arrangement was made using an orthogonal table, with each column having the same number of trials, $t = 5$. It is assumed that the experimental results $y_1, y_2, \dots, y_n$ are independent and follow a normal distribution with variance σ^2 , i.e., $y_i \sim N(\mu, \sigma^2), i = 1, 2, \dots, n$.

Total sum of squares of the experimental results:

$$S_T = \sum_{i=1}^n (y_i - \bar{y})^2 = \sum_{i=1}^n y_i^2 - \frac{T^2}{n} \quad (4)$$

$$S_j = t \sum_{i=1}^r (\bar{K}_{ij} - \bar{y})^2 = \frac{1}{t} \sum_{i=1}^r K_{ij}^2 - \frac{T^2}{n} \quad (5)$$

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i; \quad T = \sum_{i=1}^n y_i; \quad K_{ij} = \sum_{k=1}^t y_{ij,k}; \quad \bar{K}_{ij} = \frac{K_{ij}}{t}.$$

In the formula:

S_j represents the sum of squares for the deviation of the j -th factor. If factor A is arranged in the j -th column of the orthogonal table, it is denoted as $S_A = S_j$; K_{ij} represents the statistical parameter for the j -th factor at the i -th level, and $y_{ij,k}$ represents the k -th experimental result value for the j -th factor at the i -th level.

The experimental design is based on orthogonal table design, which leads to the following:

$$S_T = \sum_{j=1}^m S_j \quad (6)$$

The degrees of freedom for S_T and S_j are as follows:

$$\begin{aligned} f_T &= n - 1 \\ f_j &= r - 1 \end{aligned} \quad (7)$$

If $\alpha > 0.05$, no significant statistical difference was found, and no symbol was assigned. When $0.01 < \alpha \leq 0.05$, a “(*)” was used to indicate a significant statistical difference. For $0.001 < \alpha \leq 0.01$, a “**” was assigned to represent a highly significant statistical difference. When $\alpha \leq 0.001$, “***” was used to denote an extremely significant difference.

According to the variance analysis results in Table 6 and the influence of each factor on different response values shown in Figure 7, the following conclusions were drawn.

Table 6. Analysis of variance results.

Response Value	Significance Analysis	Water-to-Binder Ratio	Superplasticizer	Nanoclay	Residuals
Uniaxial Compressive Strength	F	24.44	1.64	0.60	
	P	<0.0001	0.23	0.67	
	Significance	**	--	--	
	η^2	82.35%	5.52%	2.02%	10.11%
Tensile Strength	F	11.76	0.23	0.73	
	P	<0.001	0.914	0.586	
	Significance	**	--	--	
	η^2	74.8%	1.5%	4.7%	19%
Elastic Modulus	F	10.35	0.44	0.6	
	P	<0.001	0.779	0.668	
	Significance	**	--	--	
	η^2	71.9%	3.0%	4.2%	20.9%
Poisson’s Ratio	F	3.42	0.47	2.01	
	P	0.044	0.758	0.157	
	Significance	(*)	--	--	
	η^2	38.5%	5.3%	22.6%	33.6%
Brittleness Index	F	0.07	0.862	0.232	
	P	0.99	0.514	0.915	
	Significance	--	--	--	
	η^2	1.7%	20.7%	5.6%	72%

(1) The content of superplasticizer and nanoclay had no significant effect on the five macroscopic parameters: uniaxial compressive strength, tensile strength, elastic modulus, brittleness index, and Poisson’s ratio.

(2) The water-to-binder ratio had an extremely significant effect on uniaxial compressive strength, tensile strength, and elastic modulus, a significant effect on Poisson’s ratio, but no significant effect on the brittleness index.

(3) For factors with no significant effect, their influence on the response values could be further assessed through η^2 . The larger the η^2 , the greater the influence of the factor on the macroscopic mechanical parameters.

$$\eta^2 = \frac{S_j}{S_T} \quad (8)$$

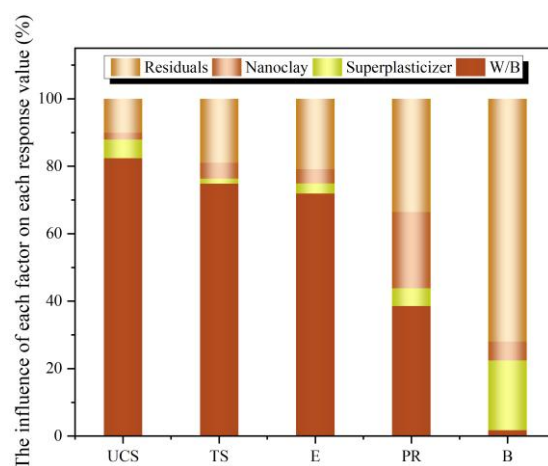


Figure 7. The influence of each factor on each response value.

Based on the results of range analysis and variance analysis, the ranking of the influencing factors for each response value was as follows.

- (1) Uniaxial compressive strength: Water-to-binder ratio > Superplasticizer > Nanoclay.
- (2) Tensile strength: Water-to-binder ratio > Nanoclay > Superplasticizer.
- (3) Elastic modulus: Water-to-binder ratio > Nanoclay > Superplasticizer.
- (4) Poisson's ratio: Water-to-binder ratio > Nanoclay > Superplasticizer.
- (5) Brittleness index: Superplasticizer > Nanoclay > Water-to-binder ratio.

4. Discussion

4.1. The Effect Evaluation of Simulated Deep Sandstone Based on Principal Component Analysis

Principal Component Analysis (PCA) was a widely used dimensionality reduction method in the field of artificial intelligence. In the study of practical problems, multiple indicators were often considered to comprehensively reveal the underlying laws of a system. However, an excessive number of indicators not only reduced computational efficiency but also led to data overlap due to correlations between variables, thereby increasing the complexity of the analysis [38–41]. Therefore, researchers sought to replace the original multiple variables with fewer variables, while retaining as much of the original information as possible. This approach allowed for the generation of a composite index to explain most of the original data. The basic idea of Principal Component Analysis (PCA) was dimensionality reduction, where, under the premise of minimizing data loss, a small number of uncorrelated new variables replaced the correlated original variables. These new variables, called “principal components,” were able to explain most of the original data, thus achieving dimensionality reduction.

This study aimed to establish a comprehensive index for evaluating the simulation effectiveness of simulated rock materials. Considering that the mechanical similarity of deep sandstone should reflect not only the load-bearing capacity but also the deformation response and failure tendency under high in situ stress conditions, three representative mechanical parameters, namely uniaxial compressive strength, elastic modulus, and brittleness index, were selected as the input variables for Principal Component Analysis (PCA). Specifically, uniaxial compressive strength characterizes the bearing capacity of deep sandstone, elastic modulus reflects its stiffness and deformation compatibility, and brittleness index represents the tendency toward brittle failure. These three parameters collectively describe the strength, deformation, and failure characteristics of deep sandstone and therefore provide a comprehensive mechanical basis for similarity evaluation. The PCA method was then employed to reduce the dimensionality of these multi-

parameter mechanical characteristics and construct a comprehensive similarity index, enabling the quantitative evaluation of the simulation effectiveness of simulated rock materials.

As illustrated in Figure 8, the specific steps of Principal Component Analysis (PCA) are described as follows [42,43]:

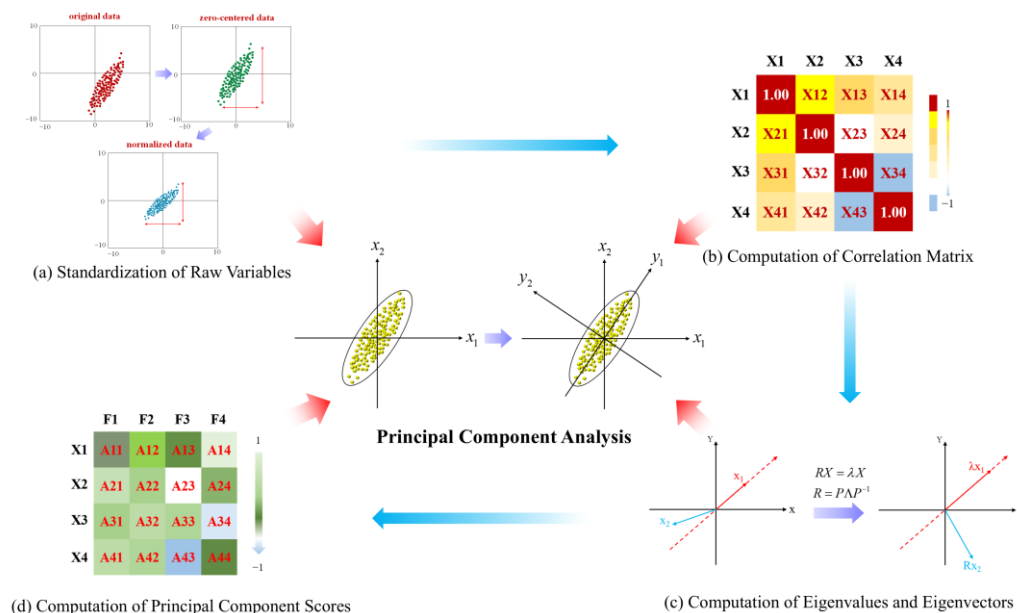


Figure 8. Schematic of the specific steps in Principal Component Analysis.

(1) To eliminate the analytical bias caused by differences in the dimensions of the indicators, the original data matrix X was standardized.

$$x_{ij}^* = \frac{x_{ij} - \bar{X}_j}{S_j} \quad (9)$$

$$\bar{X}_j = \frac{1}{n} \sum_{k=1}^n x_{kj}; \quad S_j = \sqrt{\frac{1}{n-1} \sum_{k=1}^n (x_{kj} - \bar{X}_j)^2}$$

In the formula:

(2) Calculate the correlation matrix. Since the original data matrix has been standardized (denoted as X^*), its covariance matrix is equal to the correlation coefficient matrix, i.e.,

$$R = \frac{1}{n-1} X^* X^{*T} \quad (10)$$

(3) Solve for the eigenvalues of R . By solving the characteristic equation of R , p non-negative eigenvalues were obtained, which were arranged in order of magnitude, i.e., $\lambda_1 \geq \lambda_2 \geq \lambda_3 \dots \geq \lambda_p \geq 0$. The variance contribution of the j -th principal component

was denoted as λ_j , and the variance contribution rate of the j -th principal component was denoted as $\lambda_j / \sum_{i=1}^p \lambda_i \times 100\%$.

(4) Calculate the principal component scores.

$$\begin{cases} F_1 = a_{11}X_1 + a_{12}X_2 + \dots + a_{1p}X_p \\ F_2 = a_{21}X_1 + a_{22}X_2 + \dots + a_{2p}X_p \\ \dots \\ F_p = a_{p1}X_1 + a_{p2}X_2 + \dots + a_{pp}X_p \end{cases} \quad (11)$$

where F_1 represents the first principal component, F_2 represents the second principal component, and so on.

The uniaxial compressive strength (X_1), elastic modulus (X_2), and brittleness index (X_3) of the simulated deep sandstone were selected for dimensionality reduction. By using the dimensionality reduction algorithm of Principal Component Analysis (PCA), the intrinsic relationships among these three indicators were revealed, allowing for the identification of a composite index to describe the simulation effect of the simulated deep sandstone.

Using Python version 3.10.16 for computation, these three indicators were reduced to two principal components to explain all the data. The two principal components were orthogonal and independent of each other. The relationships between the first and second principal components and the three original variables were as follows:

$$\begin{aligned} F_1 &= 0.7275X_1 - 0.5405X_2 + 0.4226X_3 \\ F_2 &= 0.0233X_1 + 0.6351X_2 + 0.7721X_3 \end{aligned} \quad (12)$$

As shown in Figure 9, the cumulative contribution rate of the first two principal components was 79.62%, meaning that these two principal components were able to reasonably explain 79.62% of the information in the original data. At the same time, the principal components provided a good representation of each original variable, and the extracted principal components performed excellently.

The relationship between each principal component and a given original variable is referred to as the factor loading:

$$\rho(y_k, x_i) = \frac{\sqrt{\lambda_k} \alpha_{ik}}{\sqrt{\sigma_{ii}}} \quad (13)$$

In the formula, $\rho(y_k, x_i)$ represents the factor loading, whose magnitude indicates the correlation between the principal component and the variable; λ_k is the eigenvalue of the k -th principal component; α_{ik} is the coefficient corresponding to the k -th principal component for the i -th original variable; σ_{ii} is the variance of the i -th variable. The sum of the squares of all coefficients for a principal component with respect to a given original variable equals 1, i.e., $\sum_{k=1}^m \rho^2(y_k, x_i) = 1$.

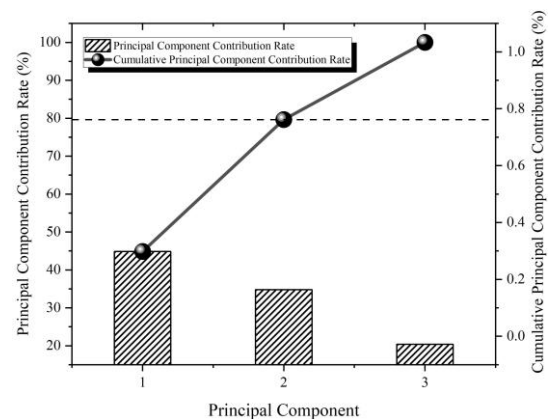


Figure 9. Contribution rates and cumulative contribution rates of each principal component.

As shown in Figure 10, the first principal component (PC1) exhibits its largest positive loading on uniaxial compressive strength (UCS), while the loading on elastic modulus is negative and that on the brittleness index is positive; the absolute values of all three loadings exceed 0.5. This pattern indicates that PC1 is strongly correlated with UCS, elastic modulus and brittleness index. By contrast, the second principal component (PC2) has relatively large loadings on elastic modulus and brittleness index, with the brittleness index clearly dominating PC2, implying a close association between PC2 and these two indicators. As shown in Figure 11, PC1 makes the largest contribution to UCS, with a pronounced leading advantage, reaching 73.96%. The contributions of PC1 and PC2 to elastic modulus are comparable, at 40.96% and 43.56%, respectively. PC2 contributes most strongly to the brittleness index, with a contribution of 64%. Combining the factor loadings with the contribution rates of each principal component to UCS, elastic modulus and brittleness index, PC1 can be interpreted as a strength–brittleness component, primarily reflecting the rock’s uniaxial compressive strength and brittleness characteristics. PC2 can be interpreted as an elasticity–brittleness component, primarily reflecting the rock’s deformation-related brittleness characteristics.

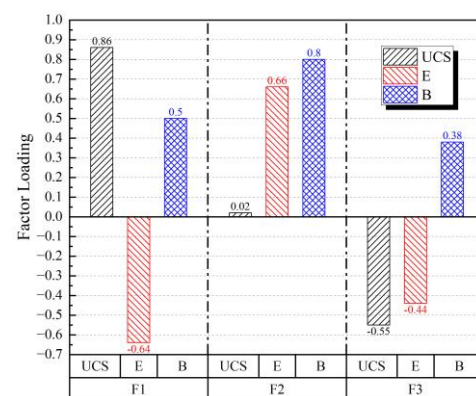


Figure 10. Factor loadings of each principal component on uniaxial compressive strength (UCS), elastic modulus (E), and brittleness index (B).

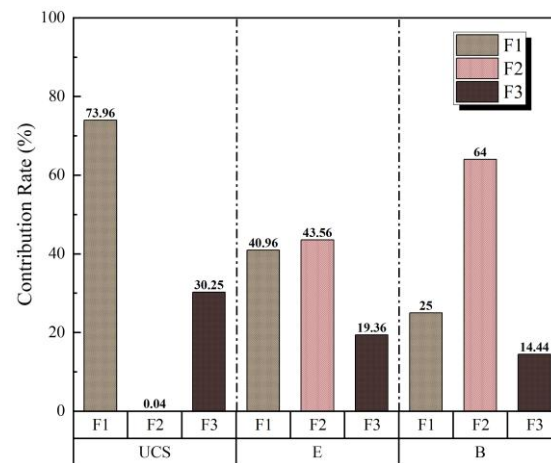


Figure 11. Contribution rates of uniaxial compressive strength (UCS), elastic modulus (E), and brittleness index (B) to each principal component.

In summary, the first principal component explained most of the data from the original variables, and the factor loadings also demonstrated that the first principal component had a strong correlation with uniaxial compressive strength, elastic modulus, and brittleness index. Therefore, based on the dimensionality reduction concept of Principal Component Analysis (PCA) and the definition of the first principal component, a Comprehensive Simulation Index (CSI) based on PCA was proposed to quantitatively evaluate the simulation effect of multi-parameter simulated deep sandstone:

$$CSI = \max \left(0, 1 - \left| \frac{\sigma - \sigma_r}{\sigma_r} \right| \right) \times \alpha_{11}^2 + \max \left(0, 1 - \left| \frac{E - E_r}{E_r} \right| \right) \times \alpha_{12}^2 + \max \left(0, 1 - \left| \frac{\frac{\sigma_c}{\sigma_t} - \left(\frac{\sigma_c}{\sigma_t} \right)_r}{\left(\frac{\sigma_c}{\sigma_t} \right)_r} \right| \right) \times \alpha_{13}^2 \quad (14)$$

$$\alpha_{11}^2 = 0.529, \alpha_{12}^2 = 0.292, \alpha_{13}^2 = 0.179$$

$$\alpha_{11}^2 + \alpha_{12}^2 + \alpha_{13}^2 = 1$$

As shown in Equation 14, the weights of uniaxial compressive strength, elastic modulus, and brittleness index were 52.9%, 29.2%, and 17.9%, respectively. In Equation 14, σ , E , and σ_c / σ_t denote the uniaxial compressive strength, elastic modulus, and brittleness index of the simulated sandstone, respectively, whereas σ_r , E_r , and $(\sigma_c / \sigma_t)_r$ represent the corresponding values of the prototype sandstone. The three PCA-derived weights sum to 1. To prevent the similarity from being overestimated when a mechanical parameter of the simulated sandstone exceeds the corresponding prototype value, the similarity of each parameter was calculated using its absolute relative deviation from the prototype. Accordingly, positive and negative deviations of the same magnitude receive equal penalties, while the maximum function constrains each individual similarity score to a non-negative value. An exact match with the prototype therefore yields an individual similarity score of 1, whereas an increasing deviation in either direction progressively reduces the score. The resulting CSI ranges from 0 to 1 and is multiplied by 100% when expressed as a percentage. In the evaluation of the simulation effect of simulated deep sandstone, uniaxial compressive strength played a dominant role, followed by elastic modulus, and lastly brittleness index. This ranking of importance was consistent with the importance of rock mechanics parameters proposed in this study. As shown in Figure 12, the Comprehensive Simulation Index of the simulated deep sandstone ranged from 52% to 72%, with S5 having the best simulation effect at 72%, while S22 had the poorest simulation effect at only 52%.

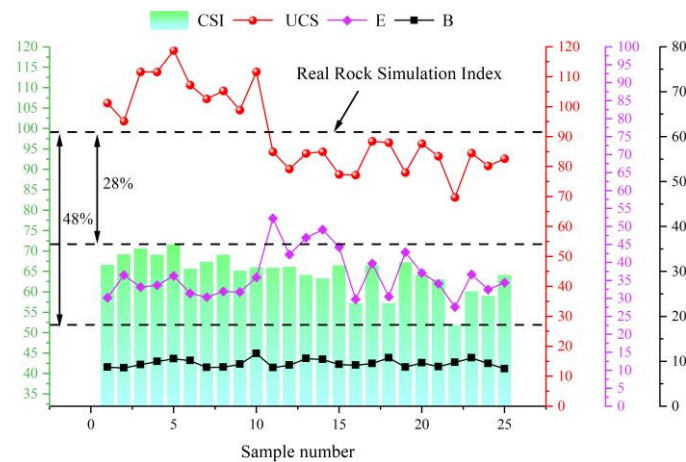


Figure 12. Relationship between the simulation index of simulated deep sandstone and each parameter.

4.2. Classification Analysis Based on Gaussian Mixture Model (GMM)

The Gaussian Mixture Model (GMM) clustering algorithm used multiple individual Gaussian probability density distributions to quantify sample data, ensuring that the likelihood probability of the sample data points under this distribution was maximized. It combined the advantages of both parametric and non-parametric estimation, and was not limited by the form of a specific probability density function [44]. The complexity of the model was only related to the nature of the research problem and the size of the sample set. Theoretically, the more models there were, the higher the precision, which could be made arbitrarily close to any continuous distribution [45,46]. However, increasing the number of models also led to an increase in model complexity. Therefore, when applying the Gaussian Mixture Model, it was necessary to seek a balance between model accuracy and model complexity. Although the Gaussian Mixture Model had been widely applied in various fields, its application in rock mechanics remained relatively limited.

The Gaussian Mixture Model (GMM) was composed of multiple individual Gaussian distributions, each with a different weight. However, the weighted average of all the Gaussian distribution weights summed to 1. The probability density function of the Gaussian Mixture Model was defined as follows [47]:

$$p(x|\lambda) = \sum_{i=1}^M \omega_i g(x|\mu_i, \Sigma_i) \quad (15)$$

In the equation, x was the feature vector of the input data; μ_i and Σ_i were the mean and covariance matrix of the i -th Gaussian density function; M was the number of Gaussian components in the model; and ω_i was the weight coefficient for each Gaussian component, with the condition that $\sum_{i=1}^M \omega_i = 1$; λ is a parameter combination consist of ω_i , μ_i and Σ_i . The definition of each Gaussian density function is as follows [48]:

$$g(x|\mu_i, \Sigma_i) = \frac{1}{(2\pi)^{D/2} |\Sigma_i|^{1/2}} \exp \left\{ -\frac{1}{2} (x - \mu_i)^T \Sigma_i^{-1} (x - \mu_i) \right\} \quad (16)$$

Since directly solving the maximum likelihood function of the Gaussian Mixture Model was very challenging, the Expectation-Maximization (EM) algorithm was used to estimate the parameters of the Gaussian Mixture Model in order to maximize the following likelihood function [49]:

$$p(x|\lambda) = \prod_{i=1}^N p(x_i|\lambda) \quad (17)$$

Using the first and second principal components obtained through Principal Component Analysis in the previous section, Gaussian Mixture Clustering was performed on the original data, dividing the 25 data points into three categories. The clustering results are shown in Figure 13.

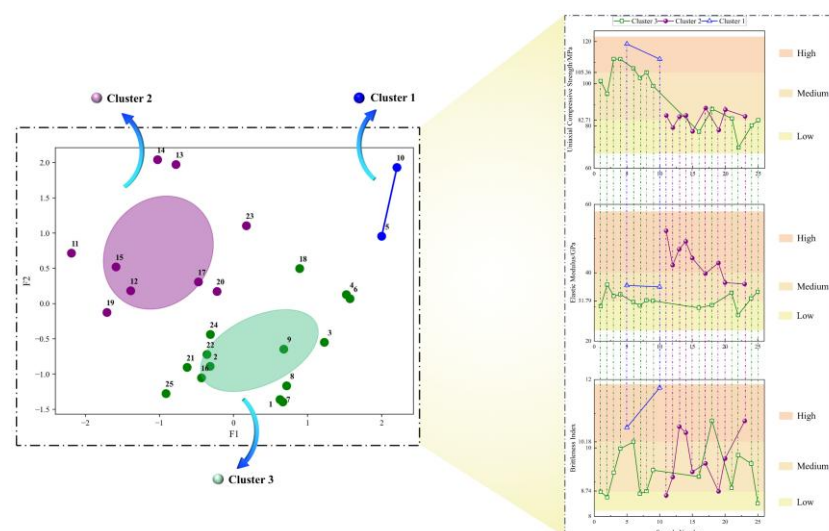


Figure 13. Gaussian Mixture Clustering results.

From Figure 13, it can be seen that Category I comprises samples S5 and S10, which are located in the region where both F1 and F2 attain high values. These mixes exhibit distinctly elevated uniaxial compressive strengths of 118.85 MPa and 111.69 MPa, respectively, together with high elastic moduli of 36.31 GPa and 35.89 GPa. Their brittleness indices are also higher than those of the other two categories, particularly S10, which reaches 11.76. In addition, the simulation indices of S5 and S10 are 71.65% and 66.06%, indicating the best overall agreement with the mechanical response of the Pingdingshan sandstone. Overall, Category I simulated deep sandstones are characterized by high strength and high stiffness under elevated stress levels, but also pronounced brittleness; once the peak stress is reached, they are prone to sudden brittle failure with minimal plastic deformation.

Category II (S11–S15, S17, S19, S20, S23) occupies the region with relatively low F1 and relatively high F2, indicating that these mixes generally possess high stiffness but only moderate strength. The average elastic modulus of this group is 43.5 GPa, with S11 reaching as high as 52.3 GPa, implying limited deformability under load. In contrast, their uniaxial compressive strength lies in a lower range of 77.48–88.52 MPa, reflecting a weaker load-bearing capacity compared with Category I. The brittleness index is of intermediate level (8.61–10.79). In summary, Category II simulated deep sandstones are relatively rigid materials with only average bearing capacity.

Category III (S1–S4, S6–S9, S16, S18, S21, S22, S24, S25) is distributed in the region of moderate F1 and relatively low F2. These samples are concentrated in the low-to-moderate range of elastic modulus; for example, S22 has an elastic modulus of only 27.65 GPa, indicating low stiffness and a high tendency to deform under stress. Their uniaxial compressive strength displays a clear two-level differentiation: some samples retain relatively high strengths (111.71 MPa and 111.67 MPa for S3 and S4), whereas others are markedly weaker (e.g., 69.78 MPa for S22). The brittleness indices of this group are generally low, suggesting that these rocks are more likely to undergo substantial plastic deformation

prior to failure. Overall, Category III simulated deep sandstones are characterized by low elastic modulus, poor resistance to deformation, a pronounced two-tier pattern in bearing capacity, and low brittleness.

Overall, the first category of simulated deep sandstone is characterized by the “three-high” combination of high strength, high stiffness and high brittleness, which is fully consistent with the design objectives of this study and delivers the best reproduction of the mechanical response of the Pingdingshan sandstone. The second category exhibits generally high stiffness but only moderate compressive strength and brittleness. The third category is distinguished by a low elastic modulus and low brittleness, enhanced deformability, and a pronounced two-tier pattern in load-bearing capacity.

4.3. Comparative Analysis of Stress–Strain Curves Between Simulated Deep Sandstone and Real Rock

By comparing the stress–strain curves of the selected S5 and S10 simulated deep sandstone with that of the real rock, it was observed that the real rock and the simulated rock exhibited similar evolution patterns. During the initial loading stage, the initial compaction phase of the simulated deep rock material was relatively short, indicating that there were few inherent fractures and pores within the material and that it possessed good compactness. As the stress increased, the material entered the elastic deformation stage, during which the propagation of inherent fractures and the formation of internal microcracks were both minimal. After the material entered the elastoplastic deformation stage, it experienced only very small plastic deformation before rapidly losing stability and failing, and the stress–strain curve displayed an abrupt drop, marking the end of the test. These observations indicated that the mechanical response of the simulated deep sandstone was highly similar to that of the Pingdingshan sandstone.

In addition, the one-dimensional Wasserstein distance (also known as the Earth Mover’s Distance, EMD) was used to quantify the similarity between the value distributions of two stress–strain curves. The procedure was as follows: the curves were first resampled over a common strain interval to obtain stress samples and construct one-dimensional empirical distributions. The Wasserstein distance is defined as the area between the cumulative distribution functions of the two distributions and represents the minimum amount of “work” required to transport one distribution into the other, thereby providing greater robustness to local misalignment and small-amplitude noise. To enable comparison between different datasets, the interquartile range (IQR) of the reference curve was used for scale normalization, yielding a dimensionless similarity index: $S = 1 / (1 + d / IQR) \in [0, 1]$, where values closer to 1 indicate higher similarity between the two curves. The calculated similarity indices for the stress–strain curves of samples S5 and S10 relative to the real rock were 0.958 and 0.941, respectively, indicating (as shown in Figure 14) that both simulated curves were highly consistent with the real curve in terms of value distribution, with S5 performing slightly better than S10. According to the commonly adopted criterion (similarity greater than 0.9 can be regarded as highly similar), both samples met the similarity requirement. Therefore, S5 can be preferentially selected as the representative curve, with S10 serving as an alternative.

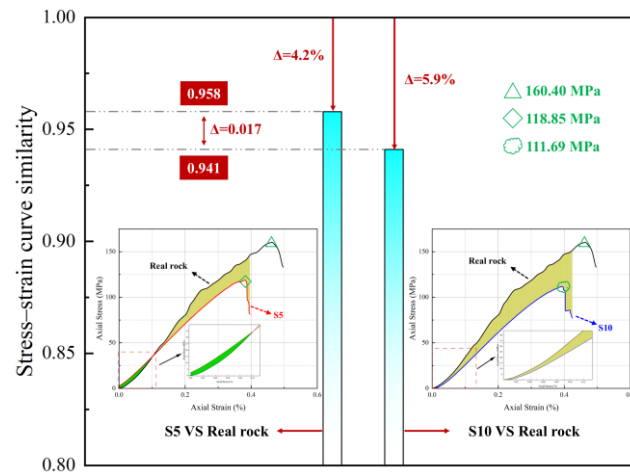


Figure 14. Similarity of the stress–strain curves of samples S5 and S10 relative to the real rock.

4.4. Comparative Analysis of Macroscopic Mechanical Properties Between Simulated Deep Sandstone and Real Rock

By comparing the failure crack patterns of simulated rocks S5 and S10 with that of the real rock (Figure 15), it was found that the principal orientation angle of the S10 crack differed from that of the real rock by only about 1°, and its crack height was essentially identical to that of the real rock. In contrast, the inclination of S5 deviated by about 5°, and its height was only about 75% of that of the real rock. In terms of tortuosity, the principal cracks in S5 and the real rock were both close to 1.2, indicating relatively straight compressive–tensile cracks, whereas the tortuosity of S10 was about 1.7, reflecting more pronounced bending and branching. Taking into account the crack orientation, scale, and network morphology, S10 was considered to more closely reproduce the overall geometric characteristics of the real rock fractures, while S5 more closely represented a simplified form of the main fracture in the real rock.

The divergence between mechanical similarity and fracture morphology similarity observed between S5 and S10 can be attributed to the differences in their mixture parameters. Specifically, S5 had a lower water–binder ratio (0.34) and a higher nanoclay content (0.08), whereas S10 had a slightly higher water–binder ratio (0.35) and lower nanoclay content (0.06). The lower water–binder ratio of S5 reduced the amount of free water and capillary porosity during hydration, resulting in a denser cementitious matrix and improved stress-transfer efficiency. Meanwhile, the higher nanoclay content enhanced microstructural refinement through filler and nucleation effects, further improving the compactness of the matrix. These effects contributed to the better agreement of S5 with the prototype sandstone in terms of strength, elastic modulus, and brittleness characteristics, leading to the highest mechanical similarity index.

However, fracture morphology is controlled not only by macroscopic mechanical parameters but also by local heterogeneity, particle contacts, pore distribution, and crack propagation paths. Compared with S5, the slightly higher water–binder ratio and lower nanoclay content of S10 may result in relatively different matrix heterogeneity and interfacial characteristics, which can provide crack propagation conditions closer to those of natural sandstone. Therefore, although S10 exhibits slightly lower mechanical similarity, it achieves a closer reproduction of fracture geometric characteristics.

This difference indicates that there is no universally optimal simulated sandstone for all research purposes. S5 is more suitable for investigations focusing on mechanical responses, such as strength, stiffness, and stress–strain behavior, whereas S10 may be more appropriate for studies emphasizing crack evolution and fracture morphology. Therefore,

the selection of simulated sandstone should be determined according to the specific experimental objective.

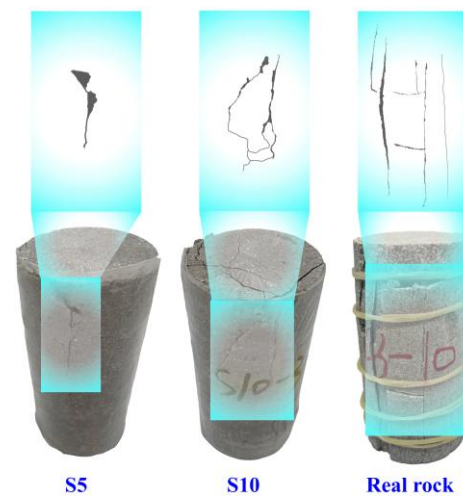


Figure 15. Comparison of failure crack patterns of simulated rocks S5 and S10 and the real rock.

4.5. Engineering Implications of Simulated Deep Sandstone for Deep Rock Mechanics Testing

In the current practice of deep rock engineering, intact deep cores remain the most direct specimens for evaluating the strength, deformation and failure behavior of deep surrounding rocks. Nevertheless, deep coring and laboratory testing still face critical limitations, including drilling-induced disturbance, stress release, core damage, strong lithological heterogeneity and poor repeatability of destructive tests [1,50,51]. For deep mining, tunneling and geo-energy engineering, these limitations are particularly restrictive because the surrounding rock is commonly subjected to high in situ stress, stress redistribution, impact disturbance, creep deformation and water–rock interaction [52–54]. Therefore, a controllable simulated deep sandstone is not intended to fully replace natural deep rock, but to provide a reproducible experimental carrier for preliminary mechanism verification and parameter comparison when intact deep cores are limited or highly scattered.

Based on the findings of this study, a possible engineering application route of “prototype-constrained material preparation–task-oriented specimen selection–deep-condition experimental verification” can be proposed. First, the mineral composition and key mechanical responses of the target sandstone are extracted as prototype constraints. Then, a batch of simulated deep sandstone specimens is prepared under controllable mixture conditions. Subsequently, different simulated materials can be selected according to different engineering testing purposes: S5 is more suitable for tests focusing on strength, stiffness and complete stress–strain behavior, whereas S10 is more suitable for tests focusing on macroscopic fracture geometry and crack-network morphology. In this way, the simulated materials can be used as standardized specimens for laboratory studies on excavation unloading, dynamic disturbance, support–rock interaction, rockburst tendency, active rock weakening and multi-field coupling processes [19,55]. Compared with directly relying on a small number of natural deep cores, this route can reduce the uncertainty caused by sample discreteness and improve the comparability of repeated experiments.

It should be noted that the proposed simulated deep sandstone is currently developed as a laboratory-scale material design and evaluation method, and its applicability under true deep geological conditions requires further validation. The objective of this methodology is not to completely reproduce all geological characteristics of natural deep sandstone, but to provide a controllable and repeatable experimental material by achieving equivalence in key mineralogical and mechanical characteristics. In this study,

mineralogical equivalence mainly refers to the matching of major mineral constituents of the prototype sandstone, such as quartz and feldspar, while mechanical equivalence is evaluated through macroscopic mechanical parameters. Therefore, the established equivalence does not necessarily indicate complete similarity in pore structure, cementing matrix, intergranular contacts, and other microscale structural characteristics. These differences may influence deformation behavior, crack initiation, and failure evolution under complex loading conditions.

Furthermore, the current validation of fracture behavior is mainly based on macroscopic crack comparison and geometric characterization, which provides preliminary evidence of fracture similarity but cannot fully describe the statistical and three-dimensional characteristics of fracture networks. Therefore, quantitative analyses involving crack density, orientation distribution, connectivity, and three-dimensional fracture evolution are required to further validate the fracture similarity between simulated and prototype sandstones. In addition, the present study mainly focuses on material screening and mechanical similarity evaluation under laboratory conditions. The effects of deep in situ environmental factors, including confining pressure, temperature, seepage, cyclic loading, dynamic disturbance, unloading paths, and long-term durability, have not yet been systematically considered. These coupled factors may further affect material degradation, deformation characteristics, damage accumulation, and long-term mechanical stability. Future studies should therefore investigate optimized materials such as S5 and S10 under more representative deep-rock conditions through triaxial testing, hydro-mechanical-thermal coupling experiments, acoustic emission, digital image correlation, CT scanning, and field-calibrated similarity criteria. Once these validations are completed, the simulated deep sandstone system developed in this study may provide a practical and reproducible material platform for repeated laboratory testing, mechanism-oriented physical modeling, and preliminary engineering evaluation of deep sandstone stability.

5. Conclusions

This study focused on the dense sandstone at a depth of 1050 m in the Pingdingshan mining area. A simulated rock material with high strength, high elastic modulus, and high brittleness was developed, ensuring that its primary material composition was equivalent to that of Pingdingshan sandstone. Through laboratory-scale simulation, the mechanical properties of deep sandstone were successfully replicated. By combining Principal Component Analysis (PCA) and Gaussian Mixture Clustering (GMM) methods from artificial intelligence, a novel method was proposed to assess the simulation effectiveness of deep rock restoration. The main conclusions are as follows:

(1) The water-binder ratio was the dominant factor controlling the macroscopic mechanical properties of the simulated deep sandstone. It had a highly significant effect on uniaxial compressive strength, tensile strength and elastic modulus, and a significant effect on Poisson's ratio. In contrast, the effects of superplasticizer and nanoclay were not statistically significant within the investigated ranges, indicating that they mainly played secondary roles in adjusting workability and local mechanical response.

(2) A PCA-based comprehensive simulation index was constructed using uniaxial compressive strength, elastic modulus and brittleness index as the principal mechanical indicators. The corresponding weights were 52.9%, 29.2% and 17.9%, respectively, showing that strength was the primary contributor to the mechanical similarity assessment, followed by stiffness and brittleness. Among all candidate mixtures, S5 showed the highest comprehensive similarity to the prototype sandstone, with a simulation index of 71.65%.

(3) GMM clustering divided the 25 simulated sandstone mixtures into three mechanically distinct groups. The first group, represented by S5 and S10, exhibited the closest

combination of high strength, high stiffness and high brittleness to the target Pingdingshan sandstone. The other two groups showed either relatively high stiffness but insufficient strength, or lower stiffness and brittleness with greater deformability.

(4) The stress–strain curve and fracture morphology comparisons further showed that the optimal simulated material depends on the target response to be reproduced. S5 achieved the best agreement with the prototype sandstone in terms of the complete stress–strain curve, with a similarity index of 0.958, whereas S10 more closely reproduced the principal crack orientation, crack height and overall fracture geometry of the real rock. Therefore, S5 is more suitable for studies focusing on strength, stiffness and deformation response, while S10 can serve as a better candidate for fracture morphology and crack-network analysis.

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