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RESEARCH

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Uncertainty-Based Performance Prediction and Optimization of High-Fluidization Cement Grouting Material Using Machine Learning and Bayesian Inference

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Abstract

In pavement engineering, cement grouting material is widely used to pour into large void asphalt concrete to prepare semi-flexible composite mixtures. It plays an essential role in the performance of the semi-flexible composite mixture. To meet specific engineering requirements, various additives are mixed into the grouting material to improve the physical and mechanical properties. As a result, the uncertainty of the grouting material is also more significant as the complexity of material composition increases during the material design. It will bring some unknown risks for the engineering application. Hence, it is necessary to quantize the uncertainty during the material design of the grouting material and evaluate the reliability of the material formula. In this study, a novel framework of material design was developed by combing the Multioutput support vector machine (MSVM), Bayesian inference, and laboratory experiments. The MSVM was used to approximate and characterize the complex and nonlinear relationship between the grouting material formula and its properties based on laboratory experiments. The Bayesian inference was adopted to deal with the uncertainty of material design using the Markov Chain Monte Carlo. An optimized formula of the cement grouting material is obtained based on the developed framework. Experimental results show that the optimized formula improves engineering properties and performance stability, especially early strength. The developed framework provides a helpful, valuable, and promising tool for evaluating the reliability of the material design of the grouting material considering the uncertainty.

Keywords: Cement grouting material, Uncertainty, Optimization design, Bayesian inference, Multioutput support vector machine

1 Introduction

In pavement engineering, cement grouting material is widely used to pour into large void asphalt concrete to prepare semi-flexible composite mixtures (Cai et al., 2019; Ren et al., 2022a). The semi-flexible composite mixtures can significantly improve the rutting resistance and bearing capacity of the pavement because of the existence of the cement grouting material (Hong et al., 2019; Zhang et al., 2020). Obviously, the cement grouting material plays an important role in the performance of the semi-flexible composite mixture. Guo et al. considered that the cement grouting material is the main factor influencing the performance of semi-flexible composite mixture (Guo & Hao, 2021). To meet various functional requirements of the semi-flexible composite mixture, the grouting material should provide various properties of high-fluidization, early

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strength, and low-shrinkage (Hu et al., 2008). Hence, many different additives such as the expansion agent, accelerating agent, water-reducing agent, and early strength agent are mixed with cement and water to prepare the cement grouting material (Li & Hao, 2018; Zhang et al., 2017). Although these additives can significantly improve the engineering properties of the grouting material, the nonuniformity of physical spatial distribution and the uncertainty of hydration reaction degree is more significant as the complexity of material composition increases (Su & Miao, 2003). It is inevitable to affect the performance of the grouting material. As a result, a frequent case is that there is performance fluctuation of the grouting material, although the raw materials, formula, experimental conditions, and operating personnel are all the same, which will bring unknown risk in engineering application (Ren et al., 2021a, 2021b, 2022b; Zhao, 2022; Zhao et al., 2021a, 2021b, 2021c). The performance fluctuation results from the uncertainty mentioned above during material design (Ren et al., 2020). It is necessary to quantize the uncertainty during the material design of the grouting material and evaluate the reliability of the material formula to reduce the potential engineering risk.

The uncertainty is an essential attribute of engineering materials and influences the properties and performance of engineering materials (Nahvi et al., 2018; Ni et al., 2022; Zhao et al., 2021a, 2021b). The uncertainty analysis of cement materials has been paid more attention in the past decade. Venkovic et al. (2013) investigated the uncertainty of elastic modulus, Biot–Willis parameter, and skeleton Biot modulus on the vulnerability of concrete structure at early age based on the polynomial chaos expansions. Tsamatsoulis and Nikolakakos (2013) analyzed the strength variability of cement grouting material caused by cement composition and curing time using a variance analysis based on the error propagation technique. Kim et al. (2020) evaluated the effect of the uncertainty of the porosity and pore continuity on the stiffness and thermal conductivity of cement grouting material using the first-order second-moment method. Zhu et al. (2021) studied the uncertainty of cement fraction in the binder and the binder concentration resulting from mixing binder slurry with in situ clays in the cement stabilized soil using Monte Carlo simulations. Jones et al. (2021) investigated the unknowns in the cement paste degradation process and the cost of uncertainty quantification based on a minimally complex model. Miller (2021) addressed the uncertainty analysis of concrete production on environmental pollution using the Monte Carlo method. These studies contribute considerably to improving our understanding of the uncertainty of cement-based materials.

However, the existing studies mainly focused on the uncertainty of the durability and mechanical properties of engineering materials. There is no related discussion on the uncertainty evaluation and quantification for material design, especially for the cement grouting material—a complex material composed of various components. The objective of this study is to establish a framework to realize the uncertainty evaluation and quantification during material design to optimized the formula of the cement grouting material.

With probabilistic methods and machine learning development (Nahvi et al., 2018; Pham et al., 2020), the Bayesian theory and support vector machine has been widely applied in various engineering fields. The Bayesian theory is a useful tool to quantify the uncertainty, because it is able to determine a complete estimation of the posterior probability density function of unknown parameters (Doh & Lee, 2018; Markus et al., 2019). An alternative approach was developed to explore parameter space and compute Bayesian evidence based on Bayesian inference and Nested Sampling (Vigliotti et al., 2018). Bayesian inference was combined with a support vector machine to update the geomechanical parameters and determine their uncertainty based on field monitoring (Zhao et al., 2021b). Thomas et al. (2022) presented a Bayesian methodology to infer the elastic modulus of the constituent polymer and the fiber orientation state in a short-fiber reinforced polymer composite. Based on the experimental design process, a machine learning technique based on Bayesian inference was developed to predict the optimum strength gain in sustainable geomaterials (Jong et al., 2022). A probabilistic method was developed to quantify the uncertainty of the mechanical behavior of rockbolts based on the Bayesian method (Zhang et al., 2022). Support vector machine has been a commonly used surrogated model which is conducive to avoid the costly computation of the engineering system to improve efficiency in uncertainty analysis. However, the traditional support vector machine has only one output, which hinders its application in practical engineering problems. The traditional support vector machine is unsuitable for material design problems that deal with multiple outputs. This limitation increases the computation time required and introduces errors, because the correlation between different outputs is not considered. Fortunately, Multi-output support vector machines (MSVM) can overcome the above shortcomings and consider the relationship between outputs (Tuia et al., 2011). MSVM regression was applied to estimate the biophysical parameter based on the remote sensing data (Tuia et al., 2011). An MSVM-based surrogated model was developed to evaluate the geomaterial mechanical parameters and their uncertainty (Li et al., 2016). MSVM was utilized to replace the numerical model to improve the efficiency of inverse analysis in geotechnical engineering (Zhao & Yin, 2016). Zhou et al. (2019) explored a novel framework by combining the MSVM and the Multi-Task Learning algorithm to improve the effectiveness and the accuracy of regional multi-step-ahead PM2.5 forecasting. Lu et al. (2020) developed a novel framework to predict wind power output from multiple wind farms based on MSVM and grey wolf.

The Bayesian inference is a fundamental way of combining uncertain and observational data (experimental data) with models from different sources and quantifying uncertain information about the obtained model. Bayesian inferences enable the combination of uncertain and incomplete information (observational data) with models from different sources and provide probabilistic information about the accuracy of the material design model. The MSVM, an excellent machine learning, not only characterizes the relationship between input and the multi-outputs but also deals with the correlation between different outputs. In this study, the Bayesian inference was employed to quantify the uncertainty during material design of the cement grouting material. To characterize the relationship between the formula of cement grouting material and their properties, the MSVM was used to approximate the complex and nonlinear function based on the design of laboratory experiments. Based on this, a novel framework was developed to evaluate the uncertainty during material design by combing the MSVM, Bayesian inference, and laboratory experiments, as illustrated in Fig. 1.

2 Materials and Methods

2.1 Materials

Shanlv P. O. 42.5R cement, accelerating agent, early strength water-reducing agent, and UEA expansion agent, are adopted to prepare the grouting material in this study. Their basic properties are presented in Tables 1, 2, 3, and 4, respectively. The sample preparation process of the grouting material is illustrated in Fig. 2.

2.2 Bayesian Inference

As previously mentioned, the properties of the cement grouting material are uncertain because of the uncertainty of the hydration reaction and spatial distribution of the components. The joint probability density function (PDF) is adopted to characterize the uncertain parameters, regarded as random variables X. The property information of the cement grouting material was obtained on the different formulas by laboratory experiments. When the cement grouting material uses a new formula, and the related properties are available, these can be useful to modify the formula to improve the material performance. The well-known Bayes's rule enables one to update the formula based on the properties of the material. The updating model can be presented as follows:

$$p(\theta|y) = \frac{L(y|\theta)p(\theta)}{p(y)} \tag{1}$$

where $p(\theta)$ is the prior statistical properties of the material formula, which denotes the initial information of the unknown parameters θ before obtaining the new information. $L(y|\theta)$ denotes the likelihood function, which is the knowledge obtained based on some tests or observations (laboratory data (y) on the formula of the materials (θ)). $p(y)$ denotes the model evidence and can be obtained using $p(y) = \int L\left(y|\theta\right)p(\theta)d\theta$, which is generally a normalizing constant. $p(\theta|y)$ is the posterior statistical information of the material formula updated by laboratory data which synthesizes both the subjective estimation and the observed information.

When performing Bayesian inferences, the full posterior joint distribution needs to be computed over a set of random variables. This study aimed to determine the material formula based on the test information of the input variables. Assuming that the observed data are conditionally independent given θ, the following equation can determine the posterior updating information:

$$p\left(\bar{y}|y\right) = \int_{\theta} p\left(\bar{y}|\theta\right)p\left(\theta|y\right)d\theta \tag{2}$$

where $\bar{y}$ denotes the updated component. In practice, it is difficult to calculate the intractable integrals due to the complexity and high dimensionality of $p\left(\bar{y}|\theta\right)$ or $p\left(\theta|y\right)$, and it is impossible to obtain an analytical solution for the integral. In this case, we proceed with sampling techniques based on the Markov Chain Monte Carlo (MCMC) method.

The MCMC approach is a powerful technology to approximate the integration (Eq. 2) by combining the Monte Carlo integration and Markov chains. A Markov chain is a sequential random model of transition from one state to another, in which the next state of the chain is based on the previous state. Samples are taken from distributions using Markov chains whose integral purpose is to perform the approximation completed by Monte Carlo integrals. The Markov chain eventually converges to a posterior distribution $p\left(\theta|y\right)$. This study used the Metropolis–Hastings (MH) algorithm to simulate samples from a probability distribution based on prior distributions and full joint density function for each variable. The procedure of the MH algorithm is presented in Fig. 3. More details can refer to Lynch's study (Lynch,

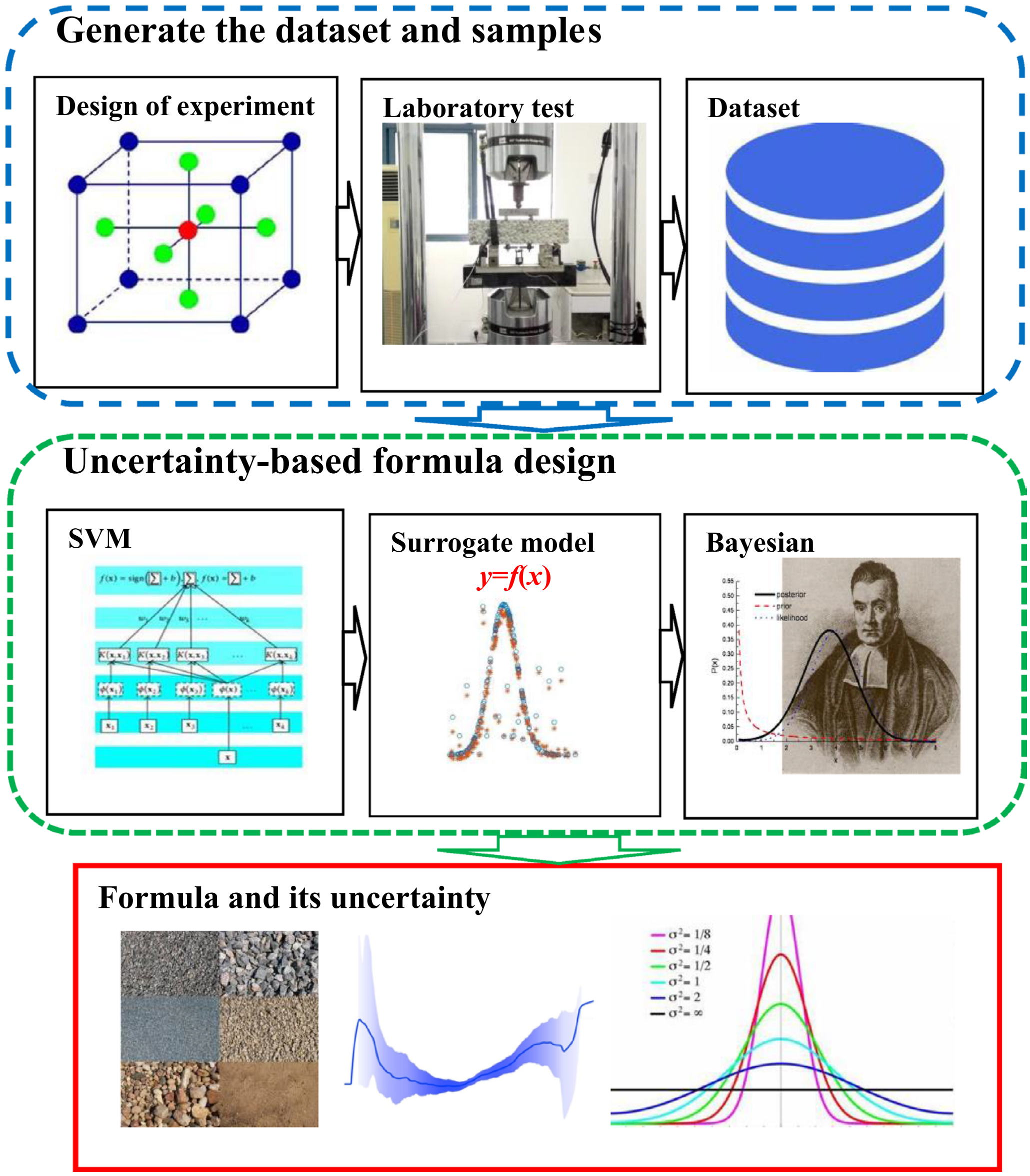

Fig. 1 Framework of the developed method

Table 1 Basic properties of the cement

Stability	Setting time (min)		Flexural strength (MPa)		Compressive strength (MPa)	
	Initial	Permanent	3 days	28 days	3 days	28 days
Qualification	170	210	5.7	8.9	30.0	53.6

2007). The detailed procedure of the MH algorithm is as follows:

- Step 1: Initialize the sample value for each uncertainty variable;
- Step 2: Compute a proposal sample based on the proposal distribution;

Table 2 Basic properties of the water reducing agent

Water reduction (%)	Density (g/cm^3)	Chloride ion content (%)	Alkali content (%)	Bleeding rate (%)	Compressive strength ratio (%)	
					7 days	28 days
21.2	1.031	0.21	3.5	30	150	135

Table 3 Basic properties of the accelerating agent

Setting time (min)		Fineness (%)	Water content (%)	28d compressive strength ratio (%)
Initial setting	Permanent Setting			
2–3	8–10	11.6	1.7	75

- Step 3: Determine the acceptance probability according to the acceptance function based on the full joint density;
- Step 4: Accept or reject the candidate samples according to the acceptance probability; and
- Step 5: If the sample number meets, it ends, or else Go to Step 2.

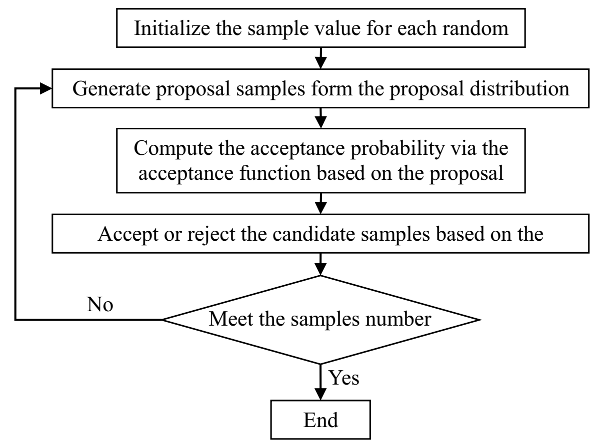

Fig. 3 Procedure of the Bayesian inference

2.3 Multioutput Support Vector Machine (MSVM)

Suppose the observable output is a vector to be predicted with a Q variable, i.e., $y \in R^Q$, a multidimensional approximation problem needs to be determined via solving the weight vector w_j and b_j ($j = 1, 2,..., Q$) for every output. The multi-output support vector machine is introduced by Tuia et al. (2011) to solve the above multidimensional case, as expressed in the following equation:

$$L_P(\mathbf{W},\mathbf{b}) = \frac{1}{2}\sum_{j=1}^{Q}\left\|\mathbf{W}^j\right\|^2 + C\sum_{i=1}^{N}L(\mathbf{u}_i) \tag{3}$$

where $\mathbf{W}$ denotes a vector $[W_1,..., W_Q]$, $\mathbf{b}$ denotes a vector $[b_1, ..., b_Q]$, C, which is a constant, denotes the penalty factor and must be larger than zero, $\mathbf{u}_i$ is the approximation error:

Table 4 Basic properties of the expansion agent

Chemical composition				Fineness		
Magnesium oxide (%)	Water content (%)	Total alkali content (%)	Chloride ion (%)	Specific surface area (m$^2 \times$ kg^{-1})	0.08 mmmaterial retained (%)	1.25 mmmaterial retained (%)
2.661	0.80	0.15	0.01	333	7.0	0.31

Fig. 2 Sample preparation process

$$\mathbf{u}_i = \|e_i\|, e_i = y_i - \phi(x_i)\mathbf{W} - \mathbf{b} \tag{4}$$

$$L(u) = \begin{cases} 0 & u < \varepsilon \\ u^2 - 2u\varepsilon + \varepsilon^2 & u \geq \varepsilon \end{cases} \tag{5}$$

where ε denotes the accuracy of MSVM regression, y_i is the ith sample output, and $\phi(x_i)$ is the feature function presented using kernel function later. The optimization problem is solved by an iterative reweighted least-squares (IRWLS) algorithm, and each iteration (t) depends on the previous solution ($\mathbf{W}^t$ and $\mathbf{b}^t$) until the optimal solution is obtained. A first-order Taylor expansion of $L(u)$ over the previous solution is used to construct the IRWLS procedure for approximating Eq. 3 in the following form:

$$L_P(\mathbf{W}, \mathbf{b}) \approx L''_P(\mathbf{W}, \mathbf{b}) = \frac{1}{2}\sum_{j=1}^{Q}\left\|\mathbf{W}^j\right\|^2 + \frac{1}{2}\sum_{i=1}^{1} a_i u_i^2 + \tau \tag{6}$$

where

$$a_i = \begin{cases} 0 & u_i^k < \varepsilon \\ 2C\left(u_i^k - \varepsilon\right)u_i^k & u_i^k \geq \varepsilon \end{cases} \tag{7}$$

where τ denotes a sum of constant terms, which is independent on either $\mathbf{W}$ or $\mathbf{b}$ and presents the same value and their gradient as $Lp(\mathbf{W},\mathbf{b})$ for $\mathbf{W} = \mathbf{W}^k$ and $\mathbf{b} = \mathbf{b}^k$. It shows that the optimization problem (Eq. 12) is a weighted least squares problem in which the weights depend on the previous solutions and contain knowledge of all components of each $\mathbf{y}_i$. Once $\mathbf{W}^k$ and $\mathbf{b}^k$ are determined, the optimization problem corresponding to Lp(W,b) can be transformed into finding the optimal solution of $L''_p(\mathbf{W},\mathbf{b})$. The following equations can be obtained based on the representer theorem (Schölkopf & Smola, 2002) and SVM theory:

$$\begin{cases} \begin{bmatrix} \mathbf{K} + \mathbf{D}_a^{-1} & 1 \\ a^T\mathbf{K} & 1^T \end{bmatrix} \begin{bmatrix} \beta^j \\ b^j \end{bmatrix} = \begin{bmatrix} \mathbf{y}^j \\ a^T\mathbf{y}^j \end{bmatrix} (j = 1, 2, \cdots, k) \\ \mathbf{K} = K(x_i, x_j) \\ \mathbf{D}_a = a_i\delta(i-j) \\ \mathbf{y}^j = [y_i^j, \cdots, y_N^j] \end{cases} \tag{8}$$

where $\mathbf{K}$ denoted the kernel matrix, 1 is an all-one column vector, and δ is the Dirac function.

$\mathbf{W}^s$ and $\mathbf{b}^s$ will be determined by solving Eq. 8. To determine $\mathbf{W}^{t+1}$ and $\mathbf{b}^{t+1}$, a descending direction $\mathbf{P}^t$ is established as expressed in Eqs. 9 and 10:

$$\begin{bmatrix} \mathbf{W}^{t+1} \\ \left(\mathbf{b}^{t+1}\right)^T \end{bmatrix} = \begin{bmatrix} \mathbf{W}^t \\ \left(\mathbf{b}^t\right)^T \end{bmatrix} + \eta^t\mathbf{P}^t \tag{9}$$

$$\mathbf{P}^t = \begin{bmatrix} \mathbf{W}^s - \mathbf{W}^t \\ \left(\mathbf{b}^s - \mathbf{b}^t\right)^T \end{bmatrix} \tag{10}$$

where η^t is determined based on a back-tracking algorithm by initializing $\eta^t = 1$:

$$\eta^t = \xi\eta^t \tag{11}$$

where ξ denotes a constant and is less than 1. Fig. 4 lists the detailed flowchart of the MSVM. The followings are the procedures of the MSVM algorithm.

- Step 1: Initialization t, W^t, b^t.
- Step 2: Determine u_i and a_i based on Eqs. 4 and 7.
- Step 3: Compute $\mathbf{W}^s$ and $\mathbf{b}^s$ using Eq. 8.
- Step 4: Set $\eta^t = 1$, compute the descending direction using Eq. 10.
- Step 5: Obtain the next step solution using Eq. 9.
- Step 6: If $Lp(\mathbf{W}^{t+1},\mathbf{b}^{t+1}) > Lp(\mathbf{W}^t,\mathbf{b}^t)$ then set $\eta^t = \xi\eta^t$, and Go to Step 5.
- Step 7: If $||\mathbf{u}_i^t||$ or t meets the convergence condition, then End, Else Set $t = t + 1$, Go to Step 2.

3 Laboratory Experiment

In this study, the orthogonal experiment method (Ren et al., 2019) is adopted to determine the target cement grouting material. Four test factors (water–cement ratio, content of expansion agent, content of water reducing agent, and content of accelerating agent) are determined for the orthogonal experiments in this study. Four test levels are selected for each test factor. Considering the recommended content of the water reducing agent, accelerating agent, and expansion agent by the manufacturers are 1.2–1.4%, 2.0–2.5%, and 7.0–8.0%, respectively, the test levels of the three additives are determined to '1.0–1.2–1.4–1.6%', '1.5–2.0–2.5–3.0%', and '6.0–7.0–8.0–9.0%'. Moreover, to determine the test level of water–cement ratio and balance the time cost, laboratory tests listed in Table 5 are implemented. Owing to the fluidity criteria of the cement grouting material being 9–13 s (CAECS, 2019), the test level of the water–cement ratio is determined to '0.50–0.53–0.56–0.60'.

Table 6 presents the scheme generated by orthogonal experimental design. The fluidity, flexural and compression strength (1 day, 3 days, and 7 days), and shrinkage rate (7 days and 28 days) were tested to investigate

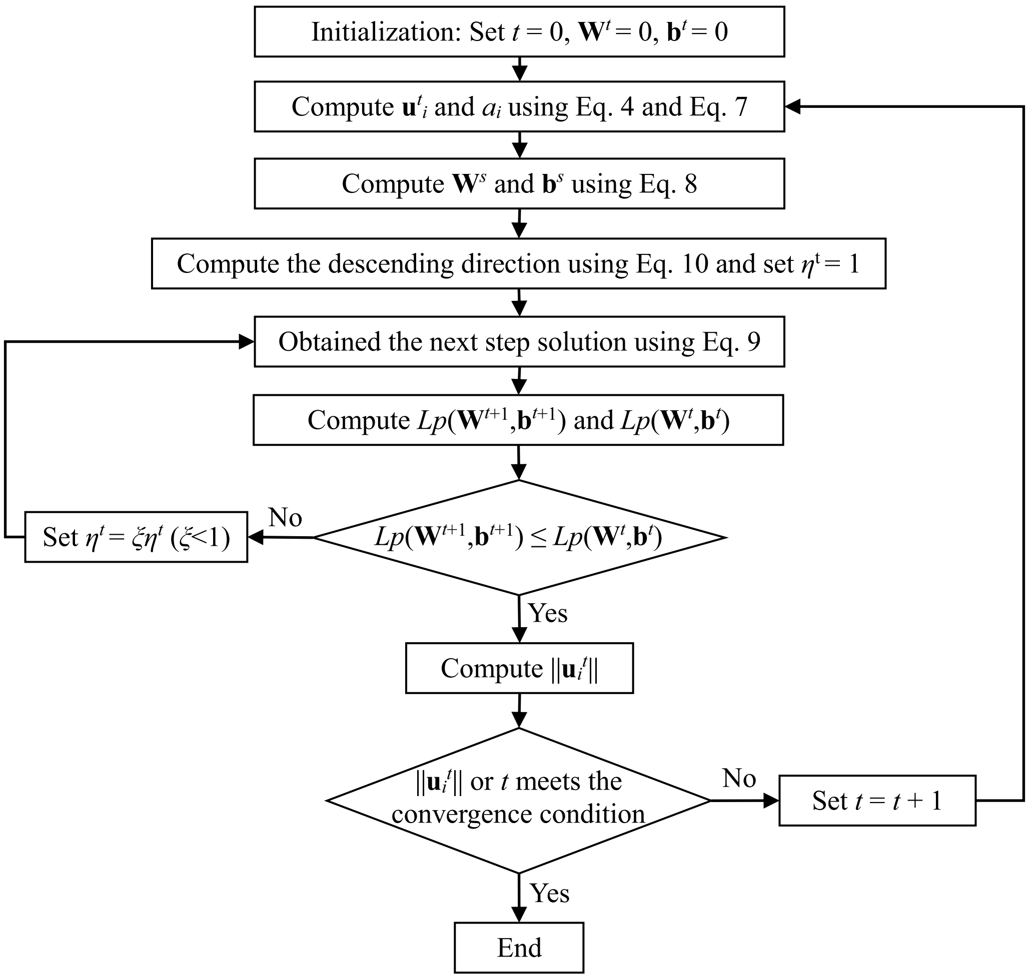

Fig. 4 Procedure of the MSVM

Table 5 Laboratory test for determining test level of water–cement ratio

Water–cement ratio	Expansion agent (%)	Water reducing agent (%)	Accelerating agent (%)	Fluidity (s)
0.45	7.5	1.3	2.25	22.7
0.50				15.3
0.55				12.1
0.60				9.7
0.65				6.9

physical and mechanical properties of the grouting materials. All the tests are implemented following the Chinese specification (MTPPC, 2020). The average values of test results are listed in Table 7. Six samples are successfully experimented for each condition, and all the data are used for the uncertainty analysis.

It should be explained that the analysis process of formula determination is complex in the orthogonal experimental method, which can be found in our previous study (Ren et al., 2021a, 2021b) and not described in this paper. The formula determined by the orthogonal experimental method is listed in Table 8. The engineering properties of the proposed formula are presented in Table 9. O-1 and O-2 are the two optimized formulas of the cement grouting material based on the orthogonal experimental method. The optimized criteria for the proposed formula are according to the Chinese standard (CAECS, 2019), as shown in Table 9. The fluidity must range from 9 to 13 s. As far as the flexural and compressive strength is concerned, the higher the better. The shrinkage rate should be lower than 0.5%.

Table 6 Test scheme based on experimental design

No.	Water–cement ratio	Expansion agent (%)	Water reducing agent (%)	Accelerating agent (%)	Orthogonal combination
1	0.50	6.0	1.0	1.5	$A_1B_1C_1D_1$
2	0.50	7.0	1.2	2.0	$A_1B_2C_2D_2$
3	0.50	8.0	1.4	2.5	$A_1B_3C_3D_3$
4	0.50	9.0	1.6	3.0	$A_1B_4C_4D_4$
5	0.53	8.0	1.0	2.0	$A_2B_3C_1D_2$
6	0.53	9.0	1.2	1.5	$A_2B_4C_2D_1$
7	0.53	6.0	1.4	3.0	$A_2B_1C_3D_4$
8	0.53	7.0	1.6	2.5	$A_2B_2C_4D_3$
9	0.56	9.0	1.0	2.5	$A_3B_4C_1D_3$
10	0.56	8.0	1.2	3.0	$A_3B_3C_2D_4$
11	0.56	7.0	1.4	1.5	$A_3B_2C_3D_1$
12	0.56	6.0	1.6	2.0	$A_3B_1C_4D_2$
13	0.60	7.0	1.0	3.0	$A_4B_2C_1D_4$
14	0.60	6.0	1.2	2.5	$A_4B_1C_2D_3$
15	0.60	9.0	1.4	2.0	$A_4B_4C_3D_2$
16	0.60	8.0	1.6	1.5	$A_4B_3C_4D_1$

4 Uncertainty Analysis of Material Design

4.1 Process

In this study, a novel framework was developed to evaluate the certainty of the cement grouting material by combing the Bayesian inference, MSVM, and laboratory experiments. The laboratory experiment (orthogonal experiments used in this study) was used to obtain the combination of the material component based on the material formula to generate the data set for the MSVM. The MSVM was adopted to approximate the complex and nonlinear function between the material formula and the related properties based on the data set. Finally, the Bayesian inference was used to obtain the rational formula of civil material based on the code requirement by considering the uncertainty.

The detailed process of the developed method is as follows, as shown in Fig. 5.

- Collect the engineering and code requirements, such as the raw materials, formula theory, experimental method, performance standard, etc.
- Implement the laboratory experiments of the cement grouting material according to experimental design, and establish the data set composed with laboratory data.
- Obtain the surrogate model based on the data set using the MSVM.

Table 8 Formula of the cement grouting material based on the orthogonal method

No.	Water–cement ratio	Water reducing agent (%)	Accelerating agent (%)	Expansion agent (%)
O-1	0.53	1.0	2.0	9.0
O-2	0.56	1.2	2.5	8.0

Table 7 Result based on the test scheme (Ren et al., 2021a, 2021b)

No.	Fluidity (s)	Flexural strength (MPa)			Compressive strength (MPa)			Shrinkage rate (%)	
		1 day	3 days	7 days	1 day	3 days	7 days	7 days	28 days
1	14.1	2.5	9.1	13.0	10.3	29.0	40.0	0.047	0.138
2	14.7	2.6	9.4	11.6	10.9	29.3	38.6	0.038	0.133
3	17.5	2.8	9.7	12.6	12.7	30.1	39.0	0.030	0.127
4	20.0	2.9	10.0	13.7	12.6	30.4	43.9	0.024	0.121
5	12.8	2.7	8.6	10.7	11.1	27.6	34.9	0.035	0.117
6	13.1	2.6	7.8	10.7	9.6	26.2	35.7	0.027	0.111
7	14.7	3.1	8.9	11.6	12.1	28.6	36.0	0.041	0.139
8	14.3	2.8	8.2	11.3	10.1	27.3	37.0	0.030	0.126
9	9.2	3.1	8.1	10.9	11.0	26.2	34.9	0.021	0.101
10	10.8	3.4	8.2	10.0	10.5	26.7	34.4	0.017	0.107
11	11.1	2.8	7.2	9.1	9.3	25.7	31.4	0.022	0.112
12	11.8	2.9	7.3	10.0	9.4	26.0	35.4	0.031	0.119
13	8.8	2.7	6.2	8.2	9.0	21.8	28.8	0.027	0.109
14	10.0	2.3	5.5	7.1	7.3	21.8	28.7	0.026	0.106
15	9.9	2.2	5.3	6.9	6.1	20.7	26.5	0.010	0.096
16	10.5	2.0	5.0	6.5	5.7	20.7	27.4	0.008	0.096

Table 9 Engineering properties of the proposed formula

No.	Fluidity (s)	Flexural strength (MPa)			Compressive strength (MPa)			Shrinkage rate (%)	
		1 day	3 days	7 days	1 day	3 days	7 days	7 days	28 days
O-1	12.9	2.7	8.4	11.1	10.8	27.1	35.9	0.018	0.121
O-2	10.4	3.4	8.2	10.7	10.9	26.0	34.4	0.021	0.108
Requirement	9–13	–	–	≥ 2	–	–	≥ 10	–	< 0.5

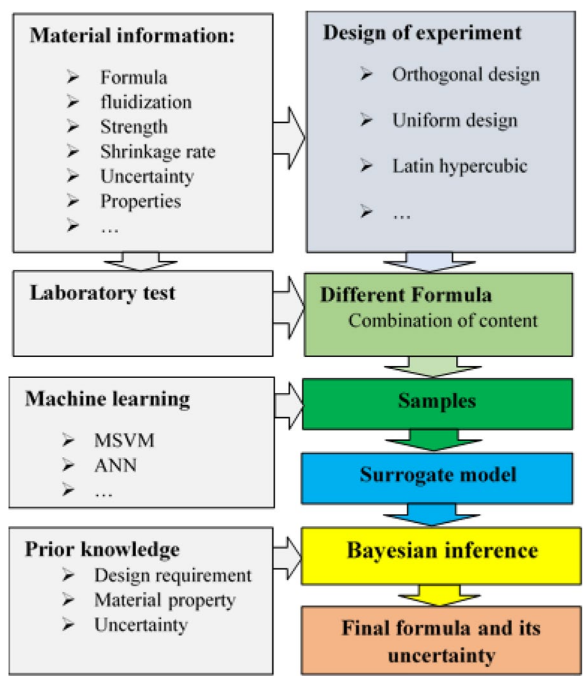

Fig. 5 Flowchart of the developed method

- Call the Bayesian inference and obtain the uncertainty evaluation based on the code requirement.

4.2 Results and Discussion

Once obtained the data sets (Tables 6 and 7), the MSVM algorithm was built using the algorithm introduced in Sect. 2.3. The predicted properties of the MSVM model are shown in Fig. 6. It implies that the MSVM model characterizes the physical and mechanical properties well using the data sets obtained based on laboratory experiments. The MSVM model can be regarded as a surrogate model which replaces the costly and time-consuming.

When the surrogate model was obtained via the MSVM (Fig. 5), the Bayesian inference was utilized to analyze the uncertainty of the data sets (laboratory experiments). In this study, the Markov Chain Monte Carlo (MCMC) method was selected to implement the Bayesian inference. Fig. 7 shows the MCMC of the test factors using the Bayesian inference process. Owing to the parameters of the MCMC method tend to be generated in the interval which is more likely to obtain target output values (i.e., the expected properties in this study) based on the surrogate model, the possibility that obtains acceptable properties is larger when the frequencies of the design factors reach a high level. For the proposed cement grouting material in this study, the target output values are that: the fluidity ranges from 9 to 13 s, the 1-day and 3-day strength are as high as possible, the 7-day flexible and compressive strength are higher than 2 MPa and 30 MPa, and the shrinkage rate is lower than 0.5%, according to the standard in the Chinese specification '*Technical Specification for Road Semi-Flexible Pavement*' (CAECS, 2019).

When a series of design factors with a high frequency are selected to constitute the formula, the prepared cement grouting material is more likely to provide a better performance and is not easy to appear performance fluctuation. Selecting a design factor with a low frequency will cause an increased possibility of suboptimal performance appearing. In other words, performance fluctuation will tend to appear in the formula containing the design factor with a low frequency. For instance, water–cement ratio and accelerating agent content are the critical factors for the early strength of the cement grouting material (Ren et al., 2021a, 2021b). Compared with the O-1 and O-2 (see Table 9), the frequencies when the accelerating agent content and water–cement ratio are equal to 2.5% and 0.56 for the O-2 are higher than the frequencies when the accelerating agent content and water–cement ratio are equal to 2.0% and 0.53 for the O-1, respectively. As a result, the 1-day strength of the O-2 is higher than the O-1. However, from a view of the frequency, the optimal content of the water reducing agent and the accelerating agent is not equal to the formula O-1 and O-2. To determine the optimal formula based on the uncertainty analysis, Fig. 8 plots the probability of each design factor via the Markov Chain shown in Fig. 7.

According to Fig. 8, the design factors corresponding to the highest probability are selected to constitute the formula (UF), as shown in Table 10. Moreover, Table 11 and Fig. 9 presents the properties and the

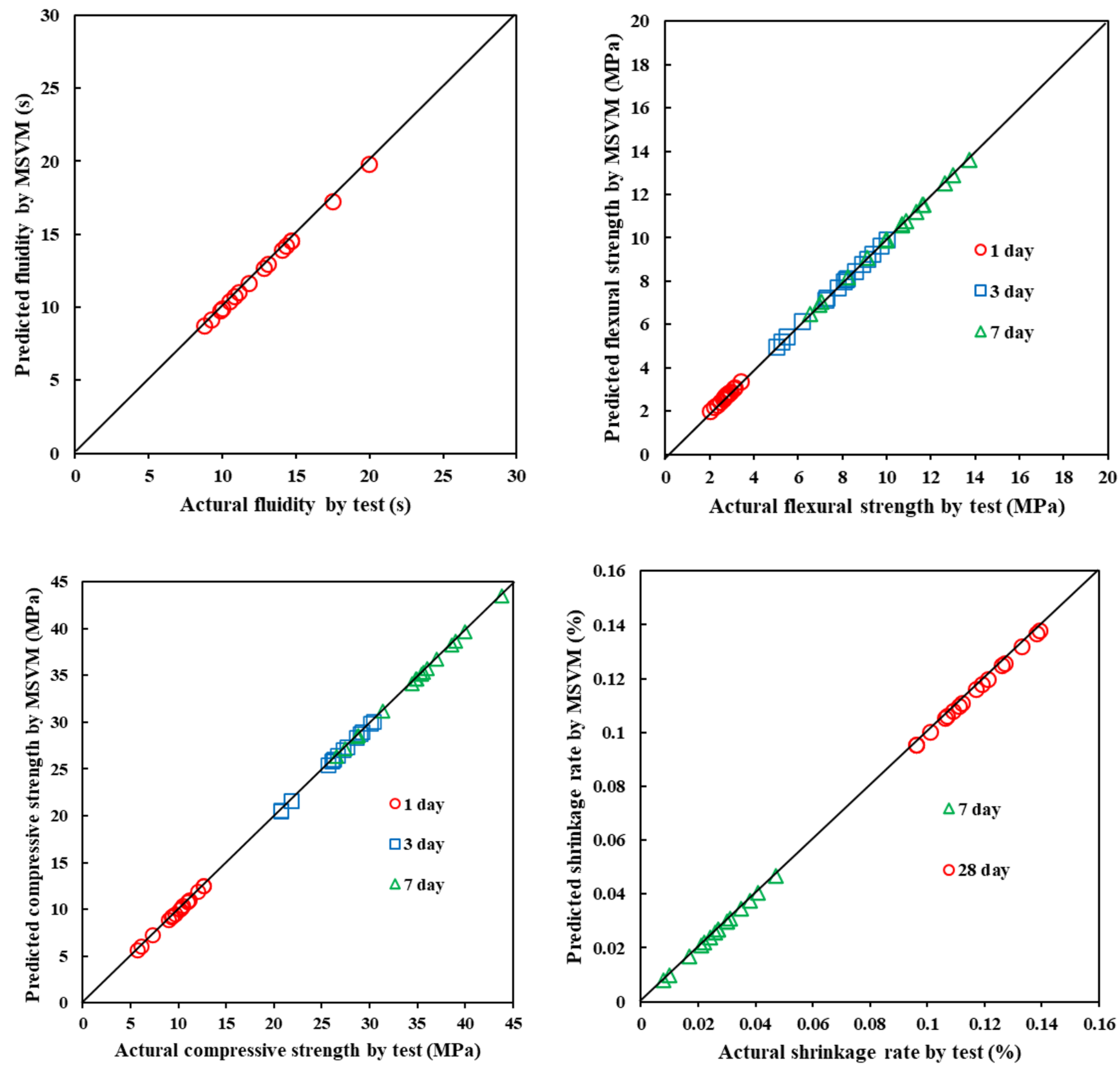

Fig. 6 Predicted performance of the proposed model

corresponding coefficient of variations of the cement grouting material with the orthogonal-based formula (O-1 and O-2) and the uncertainty-based formula (UF) via laboratory experiments. The performance standard of cement grouting material is from the Chinese specification '*Technical Specification for Road Semi-Flexible Pavement*' (CAECS, 2019). The coefficient of variation (CV) can be calculated via Eq. (12):

$$CV = \sigma/\mu \times 100\% \tag{12}$$

where σ is the standard deviation and μ is the average value.

As shown in Table 11 and Fig. 9, it can be found that the strengths of the UF at different curing ages are higher than the O-1 and O-2, especially for the early strength. The flexural and compressive strength at different curing ages is on average 1.16 and 1.12 times higher than the O-1 and O-2, respectively. The 1-day flexural and compressive strength is 1.27 and 1.17 times higher than the O-1 and O-2, respectively. It shows that the formula UF can provide improved strength. Moreover, the CVs of the flexural and compressive strength of the formula UF at different curing ages on average decrease 29.6% and 28.2%, respectively, compared to the O-1 and O-2, implying that the formula UF has better performance stability. Moreover, due to the fluidity being tested before the curing and is less affected by the uncertainty of hydration reaction, the water–cement

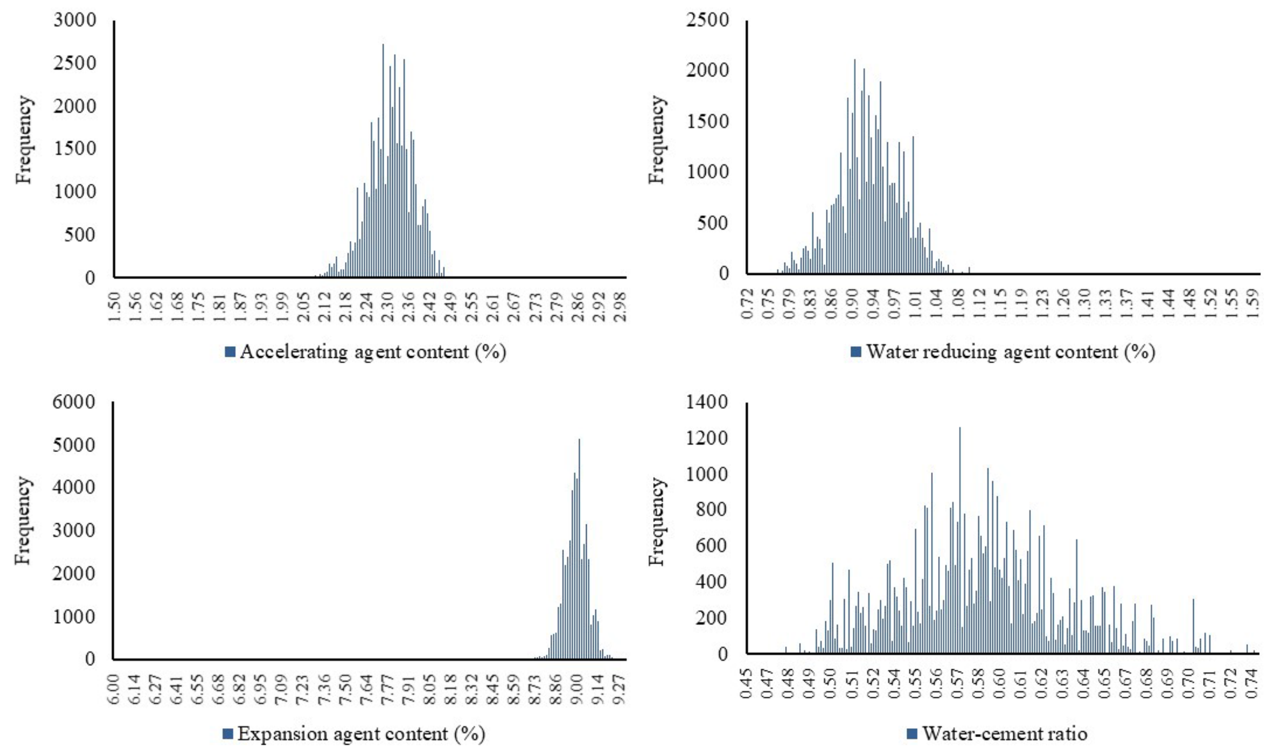

Fig. 7 Markov Chain of different design factors

ratio is the most important factor for the fluidity. As shown in Fig. 7, the water–cement ratio has the highest probability when it is equal to 0.56. Hence, the fluidity of the UF is similar to the O-2 and is 17.8% lower than the O-1, because the water–cement ratio of the UF and O-2 both are 0.56, while the water–cement ratio of the O-1 is 0.53. The above proves the worth of the uncertainty inspection for material design using the proposed method in this study. In addition, the difference in the 7-day shrinkage rate of the O-1, O-2, and UF is very limited, because the contents of the expansion agent in the three formulas all reach a high level (> 8.0%). The difference in the 28-day shrinkage rate of the three formulas may be originated from experimental error, because the test results of shrinkage rate usually have a high divergence. In the Chinese test standard (MTPPC, 2020), the allowable test error of shrinkage rate is 15%, which is higher than the difference in the 28-day shrinkage rate of the three formulas.

5 Summary and Conclusions

In this study, design optimization of the cement grouting material used in semi-flexible composite mixture is implemented based on the uncertainty analysis by combining the Multioutput support vector machine (MSVM), Bayesian inference, and experimental tests. The following specific conclusions were drawn from the results.

- The surrogate model based on the MSVM was employed to construct the complex and nonlinear relationship between the properties of cement grouting material and its formulas, which was in good agreement with the laboratory experiment results. It provided an effective way to improve the efficiency of material design.
- The Bayesian inference with the Markov Chain Monte Carlo method is used to obtain the probability of different design factors to evaluate the uncertainty during material design.
- An optimized formula of the cement grouting material is proposed based on the uncertainty analysis to provide improve performance and stability. Composed to the formula determined by traditional orthogonal design method, the early strength in the case of using the proposed optimized formula improves 1.17–1.27 times, while the coefficient of variable decreases nearly 30%.

The developed novel framework provides a helpful, valuable, and promising tool for evaluating the

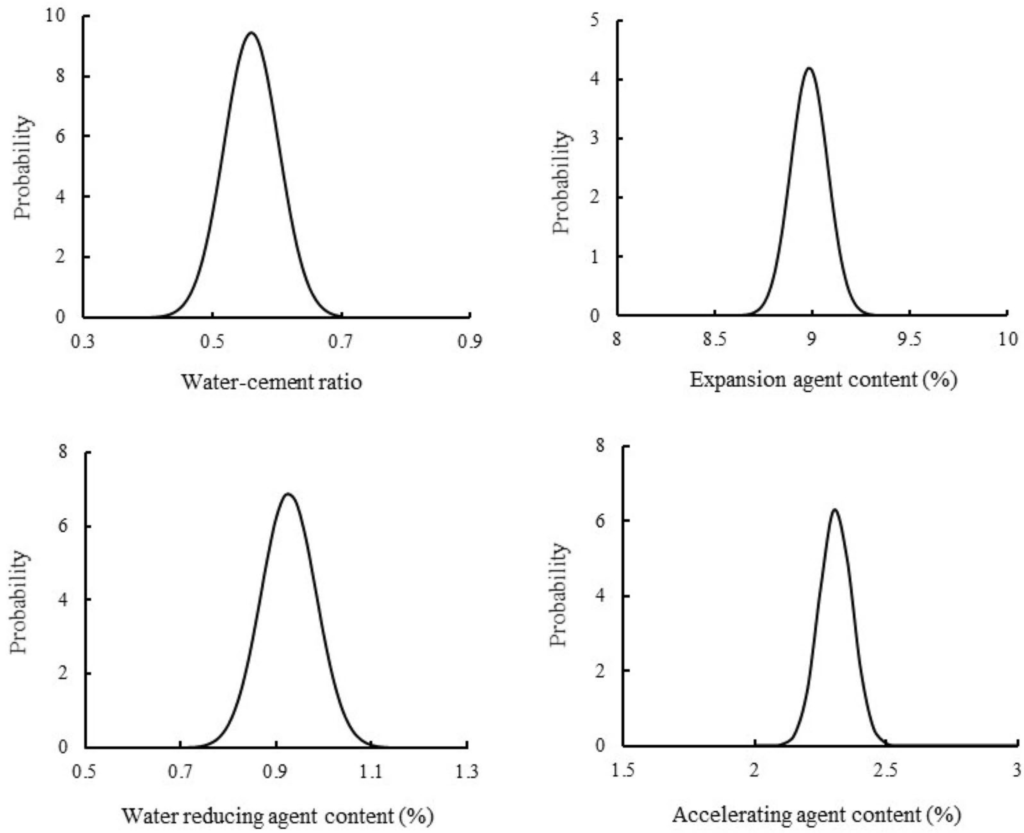

Fig. 8 Probability of different design factors

Table 10 Formulas of the cement grouting material based on different methods

No.	Water–cement ratio	Water reducing agent (%)	Accelerating agent (%)	Expansion agent (%)
O-1	0.53	1.0	2.0	9.0
O-2	0.56	1.2	2.5	8.0
UF	0.56	1.0[a]	2.3	9.0

[a] Owing to the lowest content of water reducing agent is 1.0% in the laboratory experiments, the content of water reducing agent is selected as 1.0% rather than 0.93%

Table 11 Properties (PV) and coefficient of variation (CV) of different formulas

Type	Fluidity	Flexural strength			Compressive strength			Shrinkage rate	
		1 day	3 days	7 days	1 day	3 days	7 days	7 days	28 days
O-1									
PV	12.9 s	2.7 MPa	8.4 MPa	11.1 MPa	10.8 MPa	27.1 MPa	35.9 MPa	0.018%	0.121%
CV	8.1%	11.1%	8.8%	6.9%	8.7%	6.6%	5.1%	9.7%	6.7%
O-2									
PV	10.4 s	3.4 MPa	8.2 MPa	10.7 MPa	10.9 MPa	26.0 MPa	34.4 MPa	0.021%	0.108%
CV	7.6%	10.9%	8.3%	7.0%	8.3%	6.1%	5.4%	9.0%	7.1%
UF									
PV	10.6 s	3.9 MPa	9.7 MPa	12.1 MPa	12.1 MPa	28.9 MPa	38.1 MPa	0.018%	0.109%
CV	7.7%	7.1%	6.2%	5.3%	4.6%	4.6%	4.7%	9.1%	6.1%

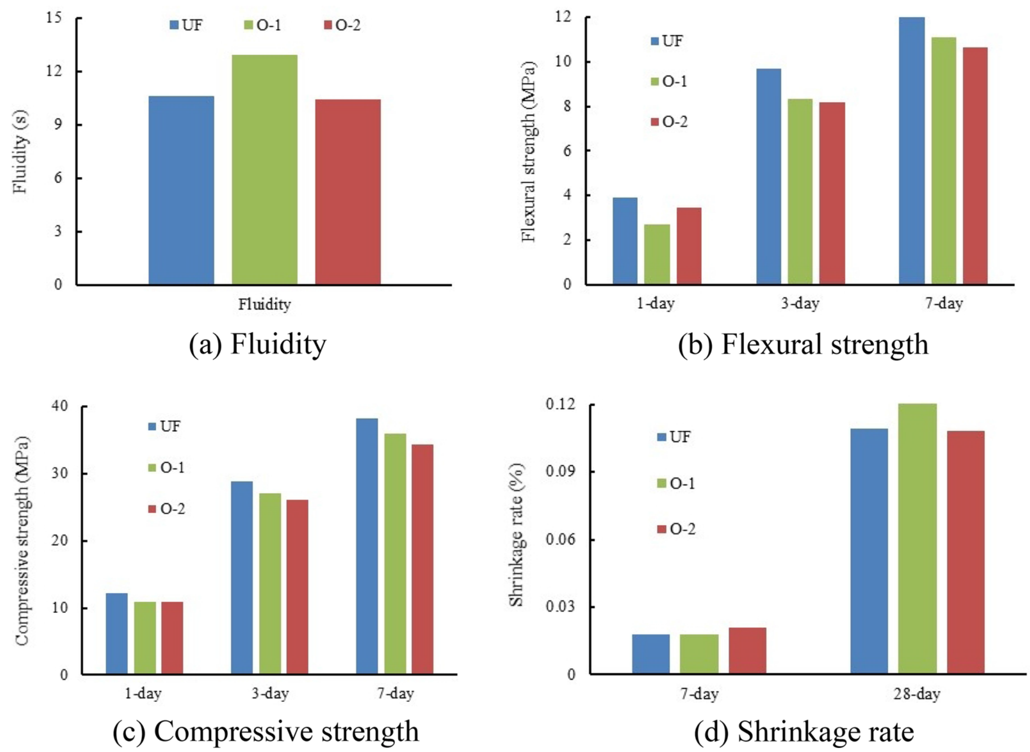

Fig. 9 Engineering properties of different formulas

reliability of material design of the cement grouting material considering the uncertainty. It is beneficial to alleviate the uncertainty effect during material design and reduce the potential risk in engineering.

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Author contributions
JR: conceptualization, formal analysis, funding acquisition, and writing—review and editing. MW: data collection and validation. LZ: methodology, and review and editing. ZZ: test and validation. JW: test and data collection. JC: data collection and validation. HZ: conceptualization, methodology, software, validation, and writing—original draft. All authors read and approved the final manuscript.

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Availability of data and materials
All data are provided in the results section.

Declarations

Ethics approval and consent to participate
The authors state that the research was conducted according to ethical standards.

Consent for publication
The authors consent for publication.

Competing interests
The authors declare that they have no competing interests in this work.

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