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Analysis of the relationship between particle size distribution of α-calcium sulfate hemihydrate and compressive strength of set plaster—Using grey model

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ABSTRACT

Particle size distribution (PSD) is one of the important factors associated with the strength property of cementitious materials. However, the relationship between PSD of α-calcium sulfate hemihydrate (α-HH) and compressive strength of set plaster is not well known. The plaster system could be regarded as a grey system and a grey model was developed to explore the relationship. The grey model shows that the compressive strength is derived from the combined action of each particle fraction, which could be divided into two groups. One works with positive effect: the particle fractions of 0–20 μm, 20–50 μm and 90–140 μm. The other works with negative effect: the particle fractions of 50–90 μm and >140 μm. Variations of the compressive strength with the increment of specific particle fractions, which result from actions of particles on the hydration rate and the characteristics of pore structure, are in general agreement with the results given by the grey model. The availability of the grey model is restricted by the water–hemihydrate weight ratio (W/H) giving standard consistency of α-HH paste. The results indicate that the grey model could provide a potential method to evaluate the relationship.

1. Introduction

Particle size distribution (PSD) of cementitious materials affects the packing density [1] and the hydration process of powders [2–4], and thus plays a great role in characteristics of the materials, such as setting time [3], water requirement for standard consistency [5], fluidity [6], microstructure [4,7] and strength property [5,8]. Many efforts have been concentrated on illustrating the relationship between PSD and compressive strength in cement and concrete [9–11]. PSD was usually characterized by specific surface area, sieve residue of certain particle sizes, characteristic diameter and distribution width when it was correlated with compressive strength [5,9,12]. The relationship has been mostly determined qualitatively. In fact, the quantitative analysis is more attractive. Zhang and Napier-Munn [8] and Tsivilis and Parissakis [13] respectively provided models involving PSD and chemical composition to predict the compressive strength. α-Calcium sulfate hemihydrate (α-HH), another important class of cementitious materials, has been widely applied in precision instrument moulds, ceramics, industrial arts and architecture. The PSD of α-HH is believed to be one of the most important parameters that control the hydration and hardening process of plaster, and is helpful in allowing us to understand the compressive strength of set plaster. However, the effect of the PSD on the compressive strength of set plaster is still obscure. Factors influencing the strength property are so complicate that no precise model has been established yet.

A grey system is defined as the one in which partial information is known and the remaining is unknown [14]. Grey system theory has been employed in cement material to analyze the relationship between PSD and compressive strength. Jiang and Yan [15] evaluated the influence of PSD of fly ash on the compressive strength of cement using grey correlation analysis and a grey model. Zhang and Zhang [10] analyzed the effect of PSD of slag powder on the compressive strength of cement using grey correlation analysis. The plaster system can also be regarded as a grey system as this relationship is concerned. Thus, the grey model, which is successful in the analysis for a grey system, is expected to help to explore such a relationship in plaster.

In this study, experiments were carried out to investigate the effect of PSD on the compressive strength of α-HH based set plaster, focusing on the establishment and application of a grey model. The hydration rate of α-HH and the characteristics of pore structure of set plasters with different PSDs were determined to elucidate the grey model. Such a study will contribute to a better understanding on the preparation of paste from α-HH based plaster and other cementitious materials.

2. Methodology

2.1. Establishment of a grey model

A grey model (GM (1, N) model) is a dynamic model which could be employed to illustrate the impact of influence factors $\{X_2^{(0)}(k)\}$, $\{X_3^{(0)}(k)\}$, …, $\{X_N^{(0)}(k)\}$ ($k=1, 2, …, n$) on the main factor $\{X_1^{(0)}(k)\}$. By

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normalization operation of $\{X_i^{(0)}(k)\}$ ($i=1, 2, \ldots, N$), the factors become

$$\{x_1^{(0)}(k)\}, \{x_2^{(0)}(k)\}, \ldots, \{x_N^{(0)}(k)\}$$

where $x_i^{(0)}(k) = X_i^{(0)}(k)/\overline{X_i}$, $\overline{X_i} = \frac{1}{n}\sum_{k=1}^{n} X_i^{(0)}(k)$, i is the sequence number of factors, and n is the amount of samples used for model establishment ($n \geq N+1$, in this study $n=N+1$). To lower the simulation error of the GM (1, N) model, the array of main factor is arranged in an increasing sequence.

The grey differential equation form of the GM (1, N) model is as follows [16–18]:

$$x_1^{(0)}(k) + az_1^{(1)}(k) = \sum_{i=2}^{N} b_i x_i^{(1)}(k), \quad (1)$$

where

$$x_i^{(1)}(k) = \sum_{m=1}^{k} x_i^{(0)}(m) = x_i^{(0)}(k) + x_i^{(1)}(k-1), \quad (2)$$

$$z_1^{(1)}(k) = 0.5x_1^{(1)}(k) + 0.5x_1^{(1)}(k-1), \quad (3)$$

$2 \leq k \leq n$, a and b_i are coefficients.

Eq. (1) can be rewritten as

$$x_1^{(0)}(k) + 0.5a(x_1^{(1)}(k) + x_1^{(1)}(k-1)) = \sum_{i=2}^{N} b_i x_i^{(1)}(k), \quad (4)$$

$$\Rightarrow x_1^{(0)}(k) + 0.5a(2x_1^{(1)}(k-1) + x_1^{(0)}(k)) = \sum_{i=2}^{N} b_i x_i^{(1)}(k), \quad (5)$$

$$\Rightarrow x_1^{(0)}(k) = \sum_{i=2}^{N} \beta_i x_i^{(1)}(k) - \alpha x_1^{(1)}(k-1), \quad (6)$$

where $\beta_i = b_i/(1+0.5a)$, $\alpha = a/(1+0.5a)$. Let $k=j-1$, then

$$x_1^{(0)}(j-1) = \sum_{i=2}^{N} \beta_i x_i^{(1)}(j-1) - \alpha x_1^{(1)}(j-2). \quad (7)$$

Let $k=j$, then

$$\begin{aligned} x_1^{(0)}(j) &= \sum_{i=2}^{N} \beta_i x_i^{(1)}(j) - \alpha x_1^{(1)}(j-1) \\ &= \sum_{i=2}^{N} \left[\beta_i x_i^{(1)}(j-1) + \beta_i x_i^{(0)}(j)\right] - \alpha x_1^{(1)}(j-1) \\ &= \sum_{i=2}^{N} \beta_i x_i^{(1)}(j-1) + \sum_{i=2}^{N} \beta_i x_i^{(0)}(j) - \alpha x_1^{(1)}(j-2) - \alpha x_1^{(0)}(j-1) \\ &= x_1^{(0)}(j-1) + \sum_{i=2}^{N} \beta_i x_i^{(0)}(j) - \alpha x_1^{(0)}(j-1). \end{aligned}$$

So

$$x_1^{(0)}(k) = \sum_{i=2}^{N} \beta_i x_i^{(0)}(k) + (1-\alpha)x_1^{(0)}(k-1) \ (k \geq 3). \quad (8)$$

Values of a and b_i ($i=2, 3, \ldots, N$) are given using least square method, $\hat{\boldsymbol{a}} = (\boldsymbol{B}^T\boldsymbol{B})^{-1}\boldsymbol{B}^T\boldsymbol{y}_N$, where

$$\hat{a} = \begin{bmatrix} a \\ b_2 \\ \cdots \\ b_N \end{bmatrix}, z_1^{(1)} = \begin{bmatrix} z_1^{(1)}(2) \\ z_1^{(1)}(3) \\ \cdots \\ z_1^{(1)}(n) \end{bmatrix}, \boldsymbol{B} = \begin{bmatrix} -z_1^{(1)}(2) & x_2^{(1)}(2) & \cdots & x_N^{(1)}(2) \\ -z_1^{(1)}(3) & x_2^{(1)}(3) & \cdots & x_N^{(1)}(3) \\ \cdots & \cdots & \cdots & \cdots \\ -z_1^{(1)}(n) & x_2^{(1)}(n) & \cdots & x_N^{(1)}(n) \end{bmatrix}, \boldsymbol{y}_N = \begin{bmatrix} x_1^{(0)}(2) \\ x_1^{(0)}(3) \\ \cdots \\ x_1^{(0)}(n) \end{bmatrix}. \quad (9)$$

The values of b_i denote the influencing degree of the factors $\{x_2^{(0)}(k)\}$, $\{x_3^{(0)}(k)\}$, …, $\{x_N^{(0)}(k)\}$ on the main factor $\{x_1^{(0)}(k)\}$. Then, simulated values of $x_1^{(0)}(k)$ expressed as $\widehat{x_1^{(0)}}(k)$ can be calculated by substituting α and β_i into Eq. (8):

$$\widehat{x_1^{(0)}}(k) = \sum_{i=2}^{N} \beta_i x_i^{(0)}(k) + (1-\alpha)x_1^{(0)}(k-1)(3 \leq k \leq n). \quad (10)$$

Simulated values of $X_1^{(0)}(k)$ expressed as $\widehat{X_1^{(0)}}(k)$ can be determined by

$$\widehat{X_1^{(0)}}(k) = \overline{X_1}\,\widehat{x_1^{(0)}}(k) = \overline{X_1}\left(\sum_{i=2}^{N} \beta_i x_i^{(0)}(k) + (1-\alpha)x_1^{(0)}(k-1)\right)(3 \leq k \leq n), \quad (11)$$

where $\overline{X_1}$ is the mean value of $X_1^{(0)}(k)$ ($1 \leq k \leq n$).

Simulation errors of a GM (1, N) model can be calculated as

$$\begin{aligned} \varepsilon(k) &= X_1^{(0)}(k) - \widehat{X_1^{(0)}}(k), \\ \Delta_k &= |\varepsilon(k)|/X_1^{(0)}(k), \\ \overline{\Delta} &= \frac{1}{n-2}\sum_{k=3}^{n} \Delta_k, \end{aligned} \quad (12)$$

where $\varepsilon(k)$, Δ_k and $\overline{\Delta}$ denote the residual error, relative error and average relative error, respectively.

2.2. Prediction by a grey model

Values of $X_1^{(0)}(k)$ ($k>n$) can be predicted by substituting values of $x_i^{(0)}(k)$ into the GM (1, N) model (Eq. (11)):

$$\widehat{X_1^{(0)}}(k_m) = \overline{X_1}\left(\sum_{i=2}^{N} \beta_i x_i^{(0)}(k) + (1-\alpha)x_1^{(0)}(m)\right)(k > n, m = 2, 3, \cdots, n) \quad (13)$$

where $\widehat{X_1^{(0)}}(k_m)$ denotes the predicted values of $X_1^{(0)}(k)$ under different values of m, so the mean value which is used to denote the predicted result of $X_1^{(0)}(k)$ is

$$\overline{\widehat{X_1^{(0)}}(k)} = \frac{1}{n-1}\sum_{m=2}^{n} \widehat{X_1^{(0)}}(k_m). \quad (14)$$

Prediction errors of the GM (1, N) model can be calculated as

$$\begin{aligned} \varepsilon(k) &= X_1^{(0)}(k) - \overline{\widehat{X_1^{(0)}}(k)}, \\ \Delta_k &= |\varepsilon(k)|/X_1^{(0)}(k). \end{aligned} \quad (15)$$

3. Materials and methods

The raw material is a commercial product prepared from natural gypsum mineral by autoclaving method (Jinxin Construction Material Co. Ltd., Shandong, China). The unground powder was numbered as S0. DSC/TG curves (Fig. 1) confirm plaster S0 to be α-HH, because the DSC pattern shows an endothermic peak at 163.0 °C followed by an exothermic peak at 172.4 °C, and the crystal water content is about 6.45%. PSD of plaster S0 was tested by a laser particle size analyzer (Mastersizer 2000, Malvern, England) after dispersing plaster in anhydrous ethanol with an ultrasonic bath, as shown in Fig. 2a and Table 1. According to the characteristics of the PSD of plaster S0 (Table 1), the size ranges of particles were classified into five groups: 0–20 μm, 20–50 μm, 50–90 μm, 90–140 μm and >140 μm.

Plasters with different PSDs were obtained by a laboratory-scale ball mill and a vibrating screen. Plasters S6, S12, S13 and S14 were