Journal of Southeast University (English Edition) Vol. 22, No. 4, pp. 549 – 552 Dec. 2006 ISSN 1003—7985

Prediction of compressive strength of cement mortars with fly ash and activated coal gangue

Zhou Shuangxi[1, 2] Chen Yimin[1] Zhang Wensheng[1]

([1] China Building Materials Academy, Beijing 100024, China)

([2] School of Civil Engineering and Architecture, East China Jiaotong University, Nanchang 330013, China)

Abstract: The pozzolanic activity of coal gangue, which is calcining at 500 to 1 000 ℃, differs distinctly. The simplex-centroid design with upper and lower bounds of component proportion is adopted to study the compressive strength of mortars made with ternary blends of cement, activated coal gangue and fly ash. Based on the results of a minimum of seven design points, three special cubic polynomial models are used to establish the strength predicating equations at different ages for mortars. Five experimental checkpoints were also designed to verify the precision of the equations. The most frequent errors of the predicted values are within 3%. A simple and practical way is provided for determining the optimal proportion of two admixtures when they are used in concrete.

Key words: thermal activated coal gangue; simplex-centroid design; predicating equation; compressive strength

Coal gangue is a waste residue resulting from the process of coal mining and coal washing, and it is currently one of the greatest contribution to industrially discharged solid waste in our country. Generally, coal gangue comprehensive discharge capacity makes up 15% to 20% of the output of raw coal. Statistics, according to national state economic and trade commissions, show that the annual emission of coal gangue in our country is near to 10^8 t[1], which now amounts to an accumulation of more than 3×10^9 t, covering an area of 1 200 km^2.

Because of varying chemical composition, its mineral composition is relatively complex. Its major composition, normally, is silicon and aluminum. Its main mineral composition consists of clay mineral, followed by primary minerals, such as quartz, anorthite, siderite, pyrite and calcite. Many studies show that the cementitious property of raw coal gangue is very weak because this kind of coal gangue has a steady crystal structure: atoms, ions and members, etc. are put according to certain laws by order. Even if its chemical composition is proper, its pozzolanic activity is low[2], but coal gangue has certain activities after calcining at a certain temperature.

The usage of activated coal gangue or fly ash in concrete can lead to many technical advantages[3]. When the two mineral admixtures are used together, better results can always be achieved[4]. In fact, high performance concrete with the principal characteristics of strength, dimensional stability, impermeability, and high workability can also be produced with mineral additives. A rational way with better accuracy and a minimum of test mixes should be found to evaluate the strength effect of the ternary blends.

There are a few ways to study the strength effect of the ternary blends. The entire simplex-centroid design used by Douglas et al. is encouraging[5]. The complex-centroid design is also used in other fields; for example, Standish et al. once used it on porosity calculations of ternary mixtures of particles.

However, the proportions of cement, activated coal gangue and fly ash in the ternary blends should have upper and lower bounds in order to meet the requirements for early strength of concrete. Either fly ash or activated coal gangue, may hydrate only when $Ca(OH)_2$, which is released by cement hydration, exists. The strength-predicting equation of mortars with mineral additives by the simplex-centroid design with upper and lower bounds is established in this paper.

According to Ref. [6], the upper and lower bounds are as follows: the cement is 40% to 100%; the activated coal gangue and the fly ash are 0 to 40%.

1 Theory

The simplex-lattice design was introduced by Scheffe in 1958. Based on the simplex-lattice design, some modified designs have been developed, including the simplex-centroid design[7].

In the simplex-centroid design, let n be the num-

Received 2006-01-06.

Foundation item: The National Basic Research Program of China (973 Program) (No. 2000CB610703).

Biographies: Zhou Shuangxi (1973—), male, graduate; Chen Yimin (corresponding author), male, doctor, professor, chenym3@163.com.

ber of components and x_i the proportion of the components in a mixture, then there are constraints:

$$x_i \geqslant 0 \qquad i = 1, 2, \ldots, n$$
$$x_1 + x_2 + x_3 + \ldots + x_n = 1 \tag{1}$$

In the simplex-centroid design, $2^n - 1$ measurements are taken, where n stands for the number of pure components. A polynomial which has as many coefficients as the number of measured points in this design is adopted to regress the relationship between any component proportions and the corresponding response:

$$Y = \sum_{1 \leqslant i \leqslant n} \beta_i x_i + \sum_{1 \leqslant i \leqslant j \leqslant n} \beta_{ij} x_i x_j + \sum_{1 \leqslant i \leqslant j \leqslant k \leqslant n} \beta_{ijk} x_i x_j x_k + \ldots + \beta_{12\ldots n} x_1 x_2 \ldots x_n \tag{2}$$

If the mixture is composed of three components, then

$$Y = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{123} x_1 x_2 x_3 \tag{3}$$

For the case of lower bounds, we can transform it into the entire simplex-centroid design by the pseudo-components as follows.

Let $a_i \geqslant 0$ be the lower bound for component i, and let $L = \sum_{I=1}^{n} a_i$. Note that a_i can be zero for some components and L must be less than 1, because otherwise there would be no region satisfying the constraints. The pseudo-components $x_i^* = \dfrac{x_i - a_i}{1 - L}$ are linear transformations of the original components such that there are no constraints on the pseudo components. All the techniques for modeling over the entire simplex can be used with the pseudo-components. Once a design has been chosen in the pseudo-components, the setting of the original components can be obtained by

$$x_i = a_i + (1 - L) x_i^* \tag{4}$$

In the ternary blends of mortars, the proportion bounds of cement, activated coal gangue and fly ash are $0.4 \leqslant x_1 \leqslant 1.0$, $0 \leqslant x_2 \leqslant 0.4$, $0 \leqslant x_3 \leqslant 0.4$, respectively. According to the design discussed above, seven design points are obtained (see Tab. 1). Based on the results of the seven design points, the compressive strength equations of mortars made with Portland cement, activated coal gangue and fly ash blends can be regressed by special cubic polynomial models.

Tab. 1 Seven test points for mortars of ternary blends

Number	x_1	x_2	x_3
1	1.00	0.00	0.00
2	0.90	0.10	0.00
3	0.80	0.10	0.10
4	0.70	0.30	0.00
5	0.70	0.00	0.30
6	0.60	0.20	0.20
7	0.50	0.35	0.15

2 Materials and Test

The 52.5R Portland cement produced by Huaxin Cement Plant in Hubei Province was used in all the mortar mixtures. The original coal gangue was obtained from Xuzhou Coal Mine. The fly ash produced in Shijingshan Power Plant was used. Their chemical composition characteristics are described in Tab. 2. The XRD patterns of the mine compositions of cement clinker and original coal gangue are shown in Fig. 1.

Tab. 2 Chemical composition of cementitious materials

Chemical composition	Component proportion/%		
	w(cement)	w(coal gangue)	w(fly ash)
SiO_2	21.06	43.97	42.85
Al_2O_3	6.04	27.72	41.26
Fe_2O_3	3.63	1.92	4.32
CaO	63.98	0.6	3.89
MgO	2.67	5.02	0.56
SO_3	2.25	0.45	0.16
Density/(g m^{-3})	3.15	2.43	2.14

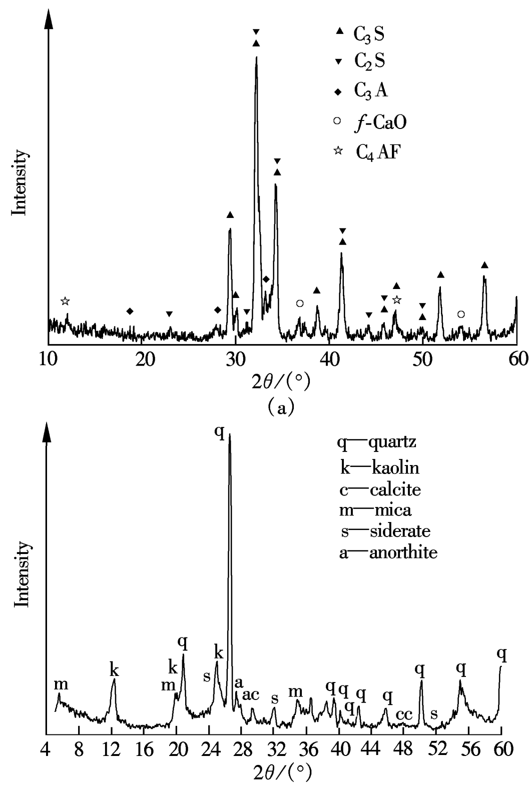

Fig. 1 XRD patterns of the mine compositions. (a) Cement clinker; (b) Xuzhou original coal gangue

Fig. 2 shows the particle size accumulative distribution total of cement, activated coal gangue and fly ash calculated by Opeik laser size analysis.

The mortar specimens were prepared according to GB/T 17671—1999, which specifies a water to cementitious material ratio of 0.5 and a sand to cementitious

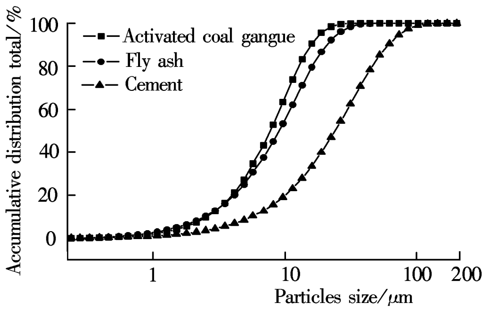

Fig. 2 Particle size accumulative distribution total of cement, activated coal gangue and fly ash

material ratio of 3 by weight.

The mortars were cast into 40 mm × 40 mm × 160 mm molds, which were stored at (20 ± 2) ℃ and relative humidity > 98%. The specimens were demolded after 24 h and left in the moist curing room until compressive measurement was carried out after 3 or 28 d.

The compressive strength of cement pastes was tested after adding different thermal activated coal gangues, calcining at temperatures from 500 to 1 000 ℃, with a mass fraction of 30% Portland cement. The component proportions and compressive strengths are listed in Tab. 3.

Tab. 3 Component proportions and compressive strength of cement mortars with activated coal gangue

Number	Calcining temperature/℃	Component proportion/%		Compressive strength/MPa	
		w(cement)	w(coal gangue)	3 d	28 d
1		100	0	39.8	64.0
2	500	70	30	16.9	47.0
3	550	70	30	19.7	48.3
4	600	70	30	20.8	50.3
5	650	70	30	21.3	54.0
6	700	70	30	22.7	56.7
7	750	70	30	24.4	58.9
8	800	70	30	27.6	61.6
9	850	70	30	27.1	61.1
10	900	70	30	26.4	59.8
11	950	70	30	23.5	57.2
12	1 000	70	30	22.3	56.4

In the ternary blends of mortars, the proportion bounds of cement, activated coal gangue (activated at 800 ℃) and fly ash are listed in Tab. 1.

In the simplex-centroid design, the component proportion and compressive strength of mortars of blended cement mortars with activated coal gangue (activated at 800 ℃) are listed in Tab. 4.

The strength-predicating equations can be established by solving three seven-variable linear equations. The compressive strength at different ages of any mortar of the ternary blends can be obtained by putting the component proportions into the corresponding cubic polynomial models.

Tab. 4 Component proportions and compressive strength of mortars with ternary blends

Number	Component proportion/%			Compressive strength/MPa	
	w(cement)	w(activated coal gangue)	w(fly ash)	3 d	28 d
1	100	0	0	39.8	64.0
2	90	10	0	37.4	63.5
3	80	10	10	31.5	61.7
4	70	30	0	27.6	61.6
5	70	0	30	24.9	60.8
6	60	20	20	23.0	58.0
7	50	35	15	19.6	52.3
8	0.9	0	10	34.2	59.4
9	80	20	0	34.0	61.3
10	70	15	15	26.5	60.9
11	60	30	10	22.7	57.7
12	50	25	25	20.9	52.1

3 Results and Discussion

From Tab. 3, the results show that the calcining temperature of coal gangue affects its pozzolanic activity. The cementitious properties of coal gangue will be enhanced along with the increase of calcining temperature, but to some extent, they will be reduced. The appropriate activated temperature is 800 ℃ to Xuzhou coal gangue for achieving high pozzolanic activity.

To 3 d, the strength-predicating equation is as follows:

$$Y = 39.8x_1 - 59.2x_2 - 35.0x_3 + 83.3x_1x_2 + 35.9x_1x_3 + 502.9x_2x_3 - 686.0x_1x_2x_3 \quad (5)$$

To 28 d, the strength-predicating equation is as follows:

$$Y = 64.0x_1 + 45.5x_2 + 130.1x_3 + 15.0x_1x_2 - 109.7x_1x_3 - 570.4x_2x_3 + 777.2x_1x_2x_3 \quad (6)$$

From Tab. 4, the results show that the compressive strength at 3 or 28 d of mortars with water to cementitious material ratio of 0.5 is almost proportional to the proportions of the Portland cement. The contribution of activated coal gangue (activated at 800 ℃) on the strength of 3 d is larger than that of fly ash.

The strength-predicting equations based on 1 to 7 tests mixes are listed in Eqs. (5) and (6), where x_1, x_2, and x_3 are mass fractions of the Portland cement, activated coal gangue and fly ash, respectively. On the basis of the strength-predicating equations, we can calculate the compressive strengths of mortars of ternary blends with component proportions satisfying specific bounds. The comparison of the predicted values and experimental values for the checkpoints numbered 8 to 12 are shown in Tab. 5. It can be also seen that the accuracy of most predicted values is 97% or better.

Tab. 5 Predicted and experimental compressive strength values of checkpoints MPa

Number	Experimental values		Predicted values	
	3 d	28 d	3 d	28 d
8	34. 2	59. 4	35. 6	60. 7
9	34. 0	61. 3	33. 3	62. 7
10	26. 5	60. 9	27. 8	60. 1
11	22. 7	57. 7	23. 5	58. 2
12	20. 9	52. 1	21. 2	53. 7

4 Conclusions

1) The calcining temperature of coal gangue affects its pozzolanic activity and the optimum calcining temperature of coal gangue used is about 800 ℃ in the present study.

2) The simplex-centroid design with upper and lower bounds of component proportions can be used to study the compressive strengths of blended cement mortars with activated coal gangue and fly ash. Based on the results of the minimum of seven design points, the strength-predicating equations can be established.

3) At different ages the compressive strengths of mortars of blended cement can be calculated, which are accurate according to experiment results.

References

[1] National State Economic and Trade Commission. Policy point of coal gangue utilization[J]. *Coal Clean Technology*, 2000, **6**(1): 56. (in Chinese)

[2] Li Dongxu, Song Xuyan, Gong Chenchen, et al. Research on cementitious behavior and mechanism of composite cement with coal gangue[J]. *Journal of the Chinese Ceramic Society*, 2004, **32**(3): 358 − 363. (in Chinese)

[3] Aitcin Pierre-Claude. Cements of yesterday and today concrete of tomorrow [J]. *Cement and Concrete Research*, 2000, **30**(9): 1349 − 1359.

[4] Shen D S, Mao Z E. *High quality fly ash concrete*[M]. Shanghai: Shanghai Science and Technology Press, 1992. 54 − 57. (in Chinese)

[5] Douglas E, Pouskouleli G. Prediction of compressive strength of mortars made with Portland cement-blast furnace slag-fly ash blends [J]. *Cement and Concrete Research*, 1991, **21**(4): 523 − 534.

[6] Wang Dehuai, Chen Zhaoyuan. On prediction compressive strengths of mortars with ternary blends of cement, GGBFS and fly ash [J]. *Cement and Concrete Research*, 1997, **27**(4): 488 − 493.

[7] Wadsworth Harrison M. *Handbook of statistical methods for engineers and scientists*[M]. McGraw-Hill, Inc, 1990.

掺活化煤矸石粉、粉煤灰水泥砂浆抗压强度预测

周双喜[1,2] 陈益民[1] 张文生[1]

([1] 中国建筑材料科学研究总院,北京 100024)
([2] 华东交通大学土木工程学院,南昌 330013)

摘要:煤矸石经不同的温度(500 ~ 1 000 ℃)热活化后,其辅助胶凝性能相差很大. 为了研究双掺活化煤矸石与粉煤灰对水泥强度性能的影响,运用单纯形-中心设计方法,并确立各组分的上下限,通过 7 组砂浆实验,得出活化煤矸石粉、粉煤灰多元复合水泥不同龄期强度数学模型,并利用 5 组砂浆实验,对强度预测方程的精确性进行了研究. 实验结果表明方程的计算值与实验测量值相差很小,误差范围在 3% 以下. 为配制多种混合材的复合水泥最优配比提供了一个简单实用的方法.

关键词:热活化煤矸石;单纯形-中心设计;预测方程;抗压强度

中图分类号:TQ172