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Mathematical Simulation of Bottom Ash Effect and Expanded Polystyrene on the Polystyrene Concrete Properties

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Abstract. Nowadays various light concrete types have many advantages as compared to heavyweight concrete (total structures mass decrease, increased thermophysical properties, less material consumption). Various industrial wastes use such as fly ashes, slag and bottom ash was suggested to enhance the light concretes effectiveness. This is greatly important for a green light concrete production since it is very important to obtain new types of environmentally friendly materials using wastes. The article substantiates the light concrete use and creation with organo-mineral additives based on industrial waste, analysis of the second-order mathematical model describing the bottom ash (BA) amount effect of Vung Ang TPP and expandable polystyrene spheres (EPS) on the light concrete density and compressive strength at the age of 28 days of normal hardening is done. In this work, the BA and EPS amounts varied from 14.5 to 45.5%, respectively, of the cement weight and from 24.5 to 55.5% of the concrete mix volume.

The effect of expanded polystyrene spheres (EPS) and bottom ash (BA) TPP "Vung Ang" amounts as the input parameters on the polystyrene concrete properties (PCP) were investigated in this study. On the one hand, various proportions of BA (14.5, 20, 30, 40 and 45.5%) were blended in concrete mixes as partial weight replacement for Portland cement. On the other hand, EPS amount was replaced by the fresh concrete volume in the range from 24.5% to 55.5%.

Additionally, the central composite design method of Box-Wilson for second order factors was used to predict the EPS and BA effects on the polystyrene concrete properties. The results showed that the proposed regression equations of this mathematical model achieved an adequate prediction accuracy. Hence, the effects of both bottom ash contents and expanded polystyrene spheres on the dry density and 28-day compressive strength of the PSC-specimens were significant. In the future, further investigations have to be carried out to study the quality prediction of green light concrete containing various wastes.

Introduction

One of the ways to develop scientific and technological progress in modern concrete technology is to use mathematical methods to organize experiments by a computer model and practical activities, to process the experimental data and build mathematical processes models to search optimal conditions for the technological process. It has the ability to predict and control not only the concrete mixes properties but also actively effect on the concrete structure formation at all technology stages, and achieve optimal results for the used input product [1, 2].

Experiment planning is a structured process for selecting the experiments number and conditions that are necessary and sufficient to obtain the task with the required accuracy [3, 4]. It is important to consider the following: (1) - The tendency to minimize the number of experiments. (2) - Simultaneous variation of all variables determining the process. (3) - The clear strategy choice that allows making grounded decisions after each series of experiments.

The researches [5, 6] shown that the prior to planning a full-scale experiment in the mathematical models, it is necessary to gather additional information about the input variables and object under study, employing the skills and knowledge obtained in previous studies.

Form the review of published research work, in order to obtain more complete information about the studied objects, in the current investigation the central composite design method was used for two variables when performing modelling experimental objects and predicting the results obtained using tested concrete.

It is evident, the modified light-weight concrete types are multifunctional materials in modern construction with higher strength, lower density and other special properties, as well as used for structural purposes to meet requirements for mechanical strength and become environmentally-friendly materials in the future work [7, 8].

As it is known, expanded polystyrene spheres (EPS) have been used very commonly as the light-weight aggregates in the preparation to produce both the polystyrene and lightweight concretes. It can be not only completely replaced by natural aggregates but also partially replaced by the concrete mixes volume manufacturing structures from lightweight concrete that is an important material in increasing pore volume and reducing the concrete dead-weight in special structures of high-rise buildings in the world cities [9, 10].

On the other hand, results of some published studies [11, 12] have shown the importance of using bottom ash, rice husk ash and fly ash, as well as other industrial waste in the concrete and mortar compositions, which can save a significant amount of energy and cost in cement manufacturing and can improve concrete mechanical and physical properties.

The overarching purpose of the current study has used the Box-Wilson central composite design method for two input factors to predict the effect of EPS and BA (Vietnam) on the dry density and measured the 28-day compressive strength of the polystyrene concrete. Besides, the main properties of the tested specimens also were investigated.

Research Procedure

Materials:

a) In terms of materials and mix design, ordinary Portland cement (SEM 40-Grade and I) (OPC) of “Tam Diep” factory and class-F bottom ash (BA) of TPP "Vung Ang" were used as binder materials. The Portland cement with the specific weight of 3.15 g/cm^3 met the requirements of Russian standard GOST 31108-2016. Besides, the bottom ash with the specific weight of 2.32 g/cm^3, the volume of a natural porous state are 860 kg/m^3 and water demand of 27.8% was used to replace 14.5, 20, 30, 40 and 45.5% cement by mass in this study.

b) the quartz sand (QS) of Lo river, which met the requirements of Russian standard GOST 8736-2014 with the fineness modulus M_K = 2.95, specific gravity and dry density are 2.65 g/cm^3 and 1620 kg/m^3 was used as fine aggregate. Whereas, the expanded polystyrene spheres (EPS) with the size of 2.5 ÷ 5 mm, specific weight and dry density respectively of 0.0181 g/cm^3 and 9.5 kg/m^3 were used as a light-weight aggregate in the concrete mixes preparation and to replace concrete in an amount of 24.5, 30, 40, 50 and 55.5% by the fresh concrete volume.

c) in this work, a considerable amount of type-F superplasticizer (SP) "SR-5000F SilkRoad" (Hanoi-Korea co., Ltd.) with a specific gravity of 1.1 g/cm^3 was used to reduce mixing water content and achieve the desired workability of all concrete mixes.

d) tap water (W) was used as the mixing water for the reference that complied with the requirements of GOST 23732-2011 (Russian Federation standard).

Methods:

On the one hand, this paper will analyze the chemical composition and the grain composition of BA and OPC by laser granulometry method using the BT-9300Z device (China). On the other hand, the calculation method of concrete mixe composition is applied in accordance with the absolute volume method of American Concrete Association [13].

The 28 days compressive strength (f_{cs}, MPa) of the polystyrene concrete was performed by using cubic specimens of 70.7×70.7×70.7 mm as stipulated by GOST 10180-2012 (Russian). Whereas, the dry density of the concrete test is determined by standard BS EN 12390-7:2009 by the above concrete cube samples after 28 days of curing.

In addition, using the Box-Wilson central composite designs method (CCD) for two input factors to create the mathematical models, which depict the BA TPP "Vung Ang" EPS effect on the dry density and compressive strength at age 28 days of polystyrene concrete.

The Box-Wilson Central Composite Design - CCD contains an embedded factorial or fractional factorial design with center points that are augmented with a group of "star points" that allow estimation of the regression equations curvature, as also reported from researches [2, 11, 12]. If the distance from the design space center to a factorial point is ±1 unit for each test factor, the distance from the design space center to a star point is $|\alpha| > 1$. The precise value of α - “star shoulder” depends on certain properties desired for the design and on the number of variables involved. According to the published study [5] for CCD, values of “star shoulder” $\alpha = \sqrt{k}$, where k is the number of the models factors.

2.3 Mixture proportions

Based on the analysis of scientific references [9, 10] and combined with the results from the experimental research, the initial ratios of raw components by weight in concrete mixes to produce polystyrenes concrete are given in table 1.

Table 1. Ratios of raw materials used in the concrete mixes compositions

Ratios	BA (% mass OPC)	EPS (%volume fresh concrete	$\frac{W}{OPC}$	$\frac{QS}{OPC+BA}$	$\frac{SP}{OPC}$	Air volume in concrete
Value	14.5 ÷ 45.5	24.5 ÷ 45.5	0.4	1.2	0.01	2%

Test Results and Discussion

The mathematical method of the experiment planning is aimed at creating mathematical empirical models that depict the influence of input variables on the light concrete properties, considered as output objective functions, which is given in figure 1.

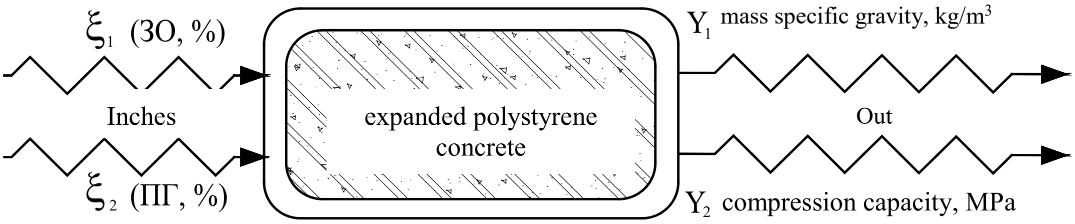

Fig. 1. The structure of the second-order experimental model for two factors

According to the studies [5, 6], the second-order regression equation in this experimental model is shown in equation (1):

$$Y = b_0 + b_1\xi_1 + b_2\xi_2 + b_3\xi_1\xi_2 + b_4\xi_1^2 + b_5\xi^2{}_2 + \Omega, \tag{1}$$

where: Y are the objective functions; ξ_1 and ξ_2 are the input factors; b_0, b_1, b_2, b_3, b_4, and b_5 are the second order regression coefficients; and Ω is a random error that influences the uncontrolled variables [14].

Objective functions description of this experimental model description:

+ Y_1 is the light concrete samples density (kg/m^3) after 28-day of curing.

+ Y_2 is the compressive strength of light concrete (MPa) at the ages of 28-day curing.

Input factors and its limitations were selected as below:

\+ ξ_1 is the BA amount in the range from 14.5% to 45.5% by mass OPC.

\+ ξ_2 is the EPS amount in the range from 24.5% to 55.5% by volume of fresh concrete in PSC-specimens test.

The input variable factors and their variation intervals are shown in table 2.

Table 2. Levels and intervals of the CCD varying factors

Parameter factors	Description factors	Levels varying factors					Intervals varying factors
		-1.414	-1	0	+1	+1.414	
BA amount (%)	ξ_1	14.5	20	30	40	45.5	10% and 5.5%
EPS Amount (%)	ξ_2	24.5	30	40	50	55.5	10% and 5.5%

The number of the CCD experiments for the two factors is indicated by formula (2):

$$N = 2^k + 2\times k + m. \quad (2)$$

where: k is the factors number (k = 2) and m is the trials number repeating at the center (m = 5 as suggested by Williams [1] and Wackerly et al. [2]).

Therefore, $N = 2^2 + 2\times2 + 5 = 13$.

The PSC compositions that calculated following the American Concrete Associate absolute volume method [13] and the central composite rotatable design method of the second-order for two factors are illustrated in table 3. In addition, the PSC density and compressive strength values at 28-day curing are presented in table 4.

Table 3. The second-order planning matrix for two factors and concrete mixes

Trial No.	In terms of variables		Parameter		Concrete mixes compositions (kg/m^3)					
	ξ_1	ξ_2	BA (%)	EPS (%)	OPC	BA	SQ	SP	W	EPS
1	+	+	40	50	307	123	516	6.15	129	9.05
2	-	+	20	50	362	72	522	7.24	130	9.05
3	+	-	40	30	435	174	731	8.71	183	5.43
4	-	-	20	30	513	103	739	10.26	185	5.43
5	+1.414	0	45.5	40	349	169	622	6.98	155	7.24
6	-1.414	0	14.5	40	474	54	634	9.47	158	7.24
7	0	+1.414	30	55.5	274	82	427	5.47	107	10.59
8	0	-1.414	30	24.5	530	159	827	10.60	207	3.89
9	0	0	30	40	402	121	627	8.04	157	7.24
10	0	0	30	40	402	121	627	8.04	157	7.24
11	0	0	30	40	402	121	627	8.04	157	7.24
12	0	0	30	40	402	121	627	8.04	157	7.24
13	0	0	30	40	402	121	627	8.04	157	7.24

Table 4. Average dry density and compressive strength of the PSC samples at 28-day curing

Trial No.	In terms of variables		Average dry density–Y_1 (kg/m^3)				Average compressive strength–Y_2 (MPa)			
	ξ_1	ξ_2	Y_{1j}	$\hat{Y}_{1j}$	$(Y_{1j}-\hat{Y}_{1j})^2$	$(Y_{01j}-\hat{Y}_{01j})^2$	Y_{2j}	$\hat{Y}_{2j}$	$(Y_{2j}-\hat{Y}_{2j})^2$	$(Y_{02j}-\hat{Y}_{02j})^2$
1	+1	+1	959.8	972.1	152	-	6.52	6.3	0.061	-
2	-1	+1	1010.4	1021.9	133.38	-	7.87	7.20	0.446	-
3	+1	-1	1521.5	1534.3	163.05	-	21.45	22.21	0.584	-
4	-1	-1	1515.4	1527.4	144.22	-	26.93	27.27	0.118	-
5	+1.414	0	1305.5	1292.1	179.25	-	11.16	10.82	0.119	-
6	-1.414	0	1334.8	1322.5	151.67	-	14.8	15.05	0.062	-
7	0	+1.414	855.7	843.2	156.67	-	5.15	5.82	0.449	-
8	0	-1.414	1611.2	1598	174.86	-	32.04	31.28	0.577	-
9	0	0	1311.9	1320	65.61	65.61	10.35	9.85	0.248	0.248
10	0	0	1309.8	1320	104.04	104.04	9.85	9.85	0	0
11	0	0	1320.3	1320	0.09	0.09	9.6	9.85	0.064	0.064
12	0	0	1324.5	1320	20.25	20.25	10.11	9.85	0.067	0.067
13	0	0	1335.2	1320	231.04	231.04	9.35	9.85	0.252	0.252
Y_1	$\sum(Y_{1j}-\hat{Y}_{1j})^2=1676.12$		$S_{1d}^2 = 209.52$		$\sum(Y_{01j}-\hat{Y}_{01j})^2=421.03$		$S_{1ll}^2 = 105.26$	$\hat{Y}_{1i} = 1320.3$		
Y_2	$\sum(Y_{2j}-\hat{Y}_{2j})^2=3.045$		$S_{2d}^2 = 0.381$		$\sum(Y_{02j}-\hat{Y}_{02j})^2=0.63$		$S_{2ll}^2 = 0.158$	$\hat{Y}_{2i} = 9.852$		

The mathematical regression equation for this experimental model description: The fitting results for each second-order regression equations with the acceptable coefficient of correlation values are shown in equations (3) and (4), according to the calculated and analyzed results obtained by the Matlab program.

For the dry density of PSC samples with $R^2 = 0.9972$ and Adj. $R^2 = 0.9951$:

$$Y_1 = 1320 - 10.74\xi_1 - 266.9\xi_2 - 6.351\xi_1^2 - 14.17\xi_1\xi_2 - 49.71\xi_2^2 . \tag{3}$$

For the compressive strength of PSC samples with $R^2 = 0.9962$ and Adj. $R^2 = 0.9936$:

$$Y_2 = 9.852 - 1.497\xi_1 - 9.003\xi_2 + 1.54\xi_1^2 + 1.033\xi_1\xi_2 + 4.349\xi_2^2. \tag{4}$$

According to [4-6], the regression equations adequacy is checked by means of the Fisher criterion. Which calculated value is the following ratio (5):

$$F_0 = \frac{S_d^2}{S_{ll}^2}, \tag{5}$$

where S_{ll}^2 is variance estimates the experiment reproducibility, determined by equation (6):

$$S_{ll}^2 = \frac{\sum_{j=1}^{m}\left(Y_{oj} - \hat{Y}_o\right)^2}{m-1}, \tag{6}$$

where m is the number of repeated experiments at the center (m = 5), Y_{oj} - the obtained value of the i-th experiment at the center and $\hat{Y}_0$ is the average value of m experiments at the center.

S_d^2 is the estimation of the inadequacy dispersion, determined by equation (7):

$$S_d^2 = \frac{\sum_{j=1}^{N}\left(Y_j - \hat{Y}_j\right)^2}{N-B}, \tag{7}$$

Where: *B* is the coefficient numbers of the second-order regression equation that were significant (B = 6), Y_j is the observed value of the *i*-th experiment, and $\hat{Y}_j$ is the obtained value of the experimental function in accordance with the *i*-th experiment, $F_\alpha(f_1, f_2)$ is the Fisher criterion value, obtained from the references data [15], with a significant level of $\alpha = 0.05$; f_1 is the number of freedom degrees for the residual variance $(f_1 = N - B = 13 - 6 = 7)$; f_2 is the number of freedom degrees for estimating the observed variance $(f_2 = m - 1 = 5 - 1 = 4)$. Therefore, $F_{0.05}(7, 4) = 6.0942$.

For the regression equation (3): $S_d^2 = 209.52$ and $S_{ll}^2 = 105.26$. (refer with Table 4).

Then $F_0 = \frac{S_d^2}{S_{ll}^2} = \frac{209.52}{105.26} = 1.9905$. As $F_0 = 1.9905 < F_{0.05}(7, 4) = 6.0942$, this experimental model described by equation (3) was adequate.

For the regression equation (4): $S_d^2 = 0.381$ and $S_{ll}^2 = 0.158$. (refer with Table 4).

Then $F_0 = \frac{S_d^2}{S_{ll}^2} = \frac{0.381}{0.158} = 2.4114$. As $F_0 = 2.4114 < F_{0.05}(7, 4) = 6.0942$, this experimental model described by equation (4) was adequate.

The quadratic response surface analysis results of the regression equations (3) and (4) with the correlation coefficients (R^2), respectively, 0.9972 and 0.9962 indicated that both the contents of bottom ash and expanded polystyrene spheres were significant.

By using the Matlab program, the images of response surface and corresponding contour plot of the regression equations (3) and (4) are given in Figures 1 and 2.

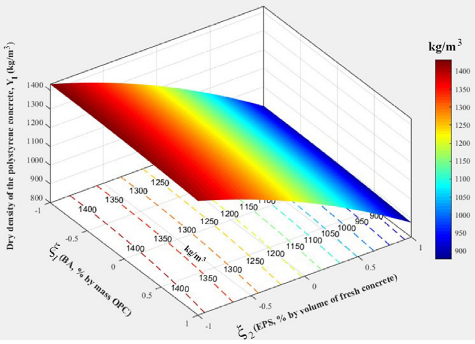

Fig. 1. The image of a three-dimensional response surface and corresponding contour plot of the regression equations (3)

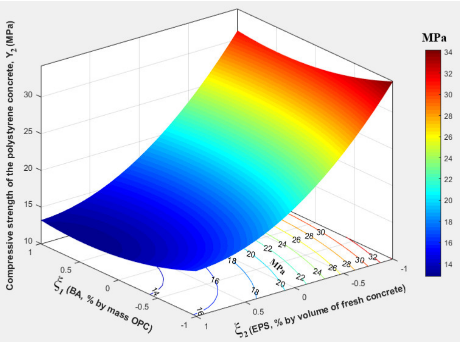

Fig. 2. The image of a three-dimensional response surface and corresponding contour plot of the regression equations (4)

The density of PSC samples complied with BS EN 12390-7:2009 containing different BA and EPS contents were in the range of 855.7 ÷ 1611.2 kg/m^3 (refer with Table 4). While, the compressive strength of polystyrene concrete is decreased at both the BA and EPS contents were increased in the concrete mixes. For example, the average compressive strength for the concrete mixe (30% BA + 24.5% EPS) was 32.04 MPa at 28-day age and this decreased to 5.15 MPa for the mix containing 30% BA + 55.5% EPS at the same age; the decrease in strength was about 83.93%.

Summary

1. Bottom ash is the potentially viable material to replace Portland cement as a mineral additive, while expanded polystyrene spheres were used as a light-weight aggregate to produce green ligh concrete in Vietnam.

2. Using the Box-Wilson Central Composite Design with the help of Matlab software second-order regression equations (3) for dry density and (4) for 28-day compressive strength of polystyrene concrete were obtained as well as images of the surface response and corresponding contour plot, which were shown in Figures 1 and 2. These proposed equations adequately described the Y_1 dry density dependence and compressive strength at age 28 days, the Y_2 tested specimens on two input factors, including ξ_1 – the BA TPP "Vung Ang" amount and ξ_2 – the EPS amount in this investigation.

3. In the future, further investigations have to be carried out to study the ways where bottom ash as a natural fine aggregate replacement and expanded polystyrene waste as a lightweight aggregate in concrete, which affects the rheological properties of fresh concrete, mechanical and durability properties of hardened mass.

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