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Prediction of product parameters of fly ash cement bricks using two dimensional orthogonal polynomials in the regression analysis

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Abstract. This paper focuses on the application of two dimensional orthogonal polynomials in the regression analysis for the relationship of product parameters viz. compressive strength, bulk density and water absorption of fly ash cement bricks with other process parameters such as percentages of fly ash, sand and cement. The method has been validated by linear and non-linear two parameter regression models. The use of two dimensional orthogonal system makes the analysis computationally efficient, simple and straight forward. Corresponding co-efficient of determination and F-test are also reported to show the efficacy and reliability of the relationships. By applying the evolved relationships, the product parameters of fly ash cement bricks may be approximated for the use in construction sectors.

Keywords: fly ash; cement; brick; modeling; orthogonal polynomials; regression; compressive strength.

1. Introduction

At present over 150 million tones of fly ash is being produced from thermal power stations all over India. Efforts have been made during the past few decades to utilize this waste in the production of various building materials (Dattatreya, *et al.*, 2002, Rajamane, *et al.*, 2007, Li and Wu 2005). Flyash has also been used in calcium silicate and lime based autoclaved bricks (Mohan, *et al.*, 1998, National 1990, Cicek and Tanriverdi 2007). Calcium silicate bricks popularly known as sand lime bricks are one of the most promising alternative building materials in which fly ash is used. Now-a-days in spite of using lime, cement is also being used to make fly ash bricks extensively.

The production of fly ash cement bricks consist of four main operations viz. (a) preparation of raw materials (b) mixing (c) shaping or pressing, and (d) curing. The ultimate strength of these bricks depends upon various factors such as (i) characteristics of raw materials (ii) moulding pressure and (iii) duration of curing. First, a small quantity of water is added in the mixture and mixed properly. Then it is filled in the moulds of the brick making machine and bricks are manufactured by using vibro-compaction technique. The bricks are taken off the table and water cured in normal atmospheric pressure for twenty eight days. Then the bricks are ready for use.

Often experimental investigations are used for finding the product parameters of fly ash bricks. Yeh (1998) and Wang and Ni (2000) have used neural networks with 2 layer and 3 layer back propagation networks for predicting compressive strength of cementitious systems. Hossain, *et al.*

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(2006) used artificial neural network model for the strength prediction of fully restrained RC slabs subjected to membrane action. (Mandal and Roy 2006) trained Back propogation Neural Network of different configurations of the sand mix for molasses cement sand systems. Results obtained from these networks are analysed and compared with those obtained from regression equations and experiments. These can predict properties without concerning how component work and deals with discrete data. However, it needs a large amount of experimental data to obtain a reliable system. Further it does not present quantitative relationship between material properties and components. Some investigators (Douglas and Pousk 1991, Wang and Chen 1997) have also used statistical based lattice design in fly ash cement mortars. Recently the present author with his co-authors (Project completion report on 'Development of software for assessment of physical properties of building bricks' CBRI, Roorkee, 2004, Chakraverty, *et al*. 2004, Chakraverty and Panigrahi 2005) has used regression analysis for linear and non-linear analysis for product parameters of cement/ lime fly ash bricks. Cheng (2006) proposed two methodologies, parameter-trend-regression and four-parameter-optimisation methodologies which makes the prediction of concrete strength more convenient. Freidin (2005) has studied influence of oil shale flyash on compressive strength of cementless building components and estimated the strength by regression analysis and analysis of variances. A software (Chakraverty and Panigrahi 2005) related to the physical parameters of fly ash lime bricks has also been developed. Recently, a mathematical model for strength and porosity of mortars made with ternary blends of ordinary Portland cement (OPC), ground rice husk ash (RHA) and classified fly ash (FA) is presented by Rukzon and Chindaprasirt (Rukzon Chindaprasirt 2008). Equations are proposed by Ramadoss and Nagamani (2008) applying statistical methods to predict 28-day compressive strength of high-performance fiber reinforced concrete (HPFRC) effecting the fiber addition in terms of fiber reinforcing index.

In the present investigation a numerically efficient methodology in term of two dimensional orthogonal polynomials in the regression analysis has been proposed for easy assessment of product parameter when it depends upon more than one variable. The one dimensional orthogonal polynomials may be used for one parameter model only and those are simple to generate by using well known recurrence relation. The investigators conducted experiments with various percentages of fly ash, sand and cement for making bricks under an ongoing task force mission mode project of CSIR, INDIA. The corresponding product parameters in particular compressive strength, water absorption and bulk density of these bricks are experimentally obtained. The fly ash samples and sand used are collected from NTPC, Dadri, New Delhi. Present study uses the experimental data obtained from these experiments for developing mathematical relationships of the product parameters of fly ash cement bricks with the process parameters namely, percentages of fly ash and cement etc.

In the following paragraphs two dimensional orthogonal polynomials are discussed to use in the regression analysis which shows a computationally efficient procedure for the evolved relationships.

2. Mathematical descriptions

2.1. Two parameter model

In the present methodology, the data from the experiments as discussed above have been used. First, usual regression analysis has been done to get polynomial equations with the hope to get desired product parameter.

2.2. Establishing the regression model

Let us consider that Z is the desired product parameter, which depends upon the process parameters. Then the two parameter model may be written as follows

$$Z=\sum_{k=0}^{n} C_k x^{lk} y^{mk} \tag{1}$$

Where Z is the product parameter, for example the compressive strength (or Bulk Density or Water Absorption), x and y are respectively the percentages of flyash and cement required in making the bricks. The notations C_k are n+1 constants and the corresponding values of lk and mk are given in Table 1.

In order to obtain 1st order polynomial relation of two parameters, the value of k in Table 1 is taken from 0 to 2 and for 2nd order k varies from 0 to 5. Similarly for 3rd order polynomial k varies from 0 to 9. In the same way for getting nth order polynomial the variation of k will be from 0 to n.

Therefore the 1st order, 2nd order and 3rd order polynomials in two parameters may respectively be written as

$$Z=C_0+C_1x+C_2\,y$$
$$Z=C_0+C_1x+C_2y+C_3x^2+C_4xy+C_5\,y^2$$
$$Z=C_0+C_1x+C_2y+C_3x^2+C_4xy+C_5y^2+C_6x^3+C_7x^2y+C_8\,xy^2+C_9y^3$$

Here it is to be noted that the third parameter i.e. sand is a dependent variable of x and y (i.e. 100 - x - y). Now by writing the above equations for each set of data, say N, the error term may be written as

$$E=\sum_{i=1}^{N}\left[Z_i-\sum_{k=0}^{n} C_k x_i^{lk} y_i^{mk}\right]^2 \tag{2}$$

As per the least square approach (Daouglas and George 1999, Gerald CF and Wheatley PO Applied Numerical analysis, Addison Wesley, 1999, Bhat and Charkaverty 2004), E is differentiated with respect to C_k and equated to zero in order to get k+1 unknowns C_k. Following are the corresponding equations

$$\frac{\partial E}{\partial C_K}=\left\{\sum_{i=1}^{N}\left[Z_i-\left(\sum_{k=0}^{n} C_k x_i^{lk} y_i^{mk}\right)\right]\right\}\times(-x_i^{lk} y_i^{mk})=0 \tag{3}$$

Eq. (3) gives a matrix equation which can be solved for the unknowns C_k. Approximated values of Z for the 1st order, 2nd order and 3rd order can be obtained by substituting the values of these constants in the polynomial equation. However it is known that the higher order polynomial equation gives better accuracy in comparison to lower order polynomial equation. But the higher order polynomial equation is not computationally efficient and some time gives absurd results due to rounding off and ill conditions of the system thereby giving numerical instability. So in the following paragraph a procedure in term of orthogonal system is presented to overcome these difficulties. Moreover the computations become easier and also the numerical relationships give good representation of the model.

2.3. Establishing the orthogonal system

Here the two parameter analysis of the problem has been presented through the use of two dimensional orthogonal system (Singh and Chakraverty 1994) in the regression model. Let us suppose that the product parameter Z for the two parameter model is described as follows

$$Z = \sum_{k=0}^{n} C_k \phi_k(x,y) \tag{4}$$

where $\phi_k(x,y)$ are the two dimensional orthogonal polynomials and n depends upon the order of the polynomial that is to be considered for the analysis. The n+1 unknown constants C_k are to be determined by the analysis. It is to be noted here that there exists no recurrence relation for generating the two dimensional orthogonal polynomials as it is available for one dimensional case. So here, these are generated numerically by using Gram Schmidt orthogonalization procedure (Bhat and Chakraverty 2004, Singh and Chakraverty 1994) as follows

$$\phi_0(x,y) = f_0(x,y) \tag{5}$$

$$\phi_k(x,y) = f_k(x,y) - \sum_{j=0}^{k-1} \alpha_{kj}\phi_j(x,y), \quad k = 1,\ldots\ldots n \tag{6}$$

Where $\alpha_{kj} = \dfrac{\sum_{i=1}^{N} f_k(x_i,y_i) \times \phi_j(x_i,y_i)}{\sum_{i=1}^{N} [\phi_j(x_i,y_i)]^2}$ and

$f_k(x_i,y_i) = x_i^{lk} y_i^{mk}$

The values of lk and mk are again incorporated in Table 1 and N is the number of data used in the analysis.

After obtaining the two dimensional orthogonal polynomials as above the usual error term E may be written as

$$E = \sum_{i=1}^{N}\left[Z_i - \sum_{k=0}^{n} C_k \phi_k(x_i,y_i)\right]^2 \tag{7}$$

As per the least square approach, E is differentiated with respect to C_k and equated to zero in order to get n+1 unknowns. Following are the corresponding equations

$$\frac{\partial E}{\partial C_k} = \sum_{i=1}^{N}\left[Z_i - \sum_{k=0}^{n} C_k \phi_k(x_i,y_i)\right] \times \phi_k(x_i,y_i) = 0 \tag{8}$$

Table 1 Values of Constants lk and mk in Eq. (1)

k	0	1	2	3	4	5	6	7	8	9	…	………………n
lk	0	1	0	2	1	0	3	2	1	0	…	n n-1 n-2…0
mk	0	0	1	0	1	2	0	1	2	3	…	0 1 2 …n

The above equation containing the orthogonal polynomials may be solved for the unknowns C_k and approximated value of Z may be obtained if these be substituted in the polynomial equation. It may be worth mentioning that due to the orthogonal system of the functions, Eq. (8) reduces to

$$\begin{bmatrix} \sum_{i=1}^{N}\phi_0^2(x_i,y_i) & 0 & 0\ 0\ 0 & 0 \\ 0 & \sum_{i=1}^{N}\phi_1^2(x_i,y_i) & 0\ 0\ 0 & 0 \\ 0 & 0 & .\ . & 0 \\ 0 & 0 & .\ .\ . & 0 \\ 0 & 0 & .\ .\ . & 0 \\ 0 & 0 & .\ .\ . & 0 \\ 0 & 0 & .\ .\ . & 0 \\ 0 & 0 & 0\ 0\ 0 & \sum_{i=1}^{N}\phi_k^2(x_i,y_i) \end{bmatrix} \cdots \begin{bmatrix} C_0 \\ C_1 \\ . \\ . \\ . \\ . \\ . \\ C_K \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{N} Z_i\phi_0^2(x_i,y_i) \\ \sum_{i=1}^{N} Z_i\phi_1^2(x_i,y_i) \\ . \\ . \\ . \\ . \\ . \\ \sum_{i=1}^{N} Z_i\phi_k^2(x_i,y_i) \end{bmatrix}$$

where the left hand side matrix is a diagonal matrix. Thus the unknowns C_k may be evaluated directly if the orthogonal system in the regression analysis is used in multi parameter problems. The efficacy of the various relationships are computed by the coefficients of determination and the same may be written as

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(Z_i - \hat{Z}_i)^2}{\sum_{i=1}^{n} Z_i^2 - \frac{\left(\sum_{i=1}^{n} Z_i\right)^2}{n}}$$

Where, Z_i = Experimental values

$\hat{Z}_i$ = Computed values

From the values of R^2 we may define the fittings as usual,

$R^2 = 0$ => Lack of fit

$R^2 \approx 1$ => Perfect Fit

$$F_{cal} = \frac{R^2/k}{(1-R^2)/[n-(k+1)]}.$$

Then the Test Statistic is written as,

The corresponding rejection region is for $F > F_{0.05}\,(k, (n-k+1))$ and if $F_{cal} > F_{0.05}\,(k, (n-k+1))$ then the model is useful and correct.

2.4. Numerical results

Twenty six different mixes depending on various percentages of fly ash, sand and cement are prepared and corresponding bricks are made and tested for their product parameters viz. compressive strength, bulk density and water absorption.

First the polynomial Eq. (1) of 1st order, 2nd order and 3rd order is taken into consideration. The experimental data sets for product parameters of flyash cement bricks are used to generate the evolved relationships. The constants C_k for 1st, 2nd or 3rd order models are found from Eq. (3). Results for the product parameters i.e. compressive strength, bulk density and water absorption are computed then by substituting the constants in Eq. (1) for various models. R^2 values for these models are shown in Table 2. Corresponding F values are also computed and entered in Table 2.

Next the proposed procedure i.e. the use of two dimensional orthogonal polynomials in the regression analysis is used to compute the results. For this the regression polynomials as mentioned above is first generated by Gram Schmidt Orthogonalization Process. It is to be noted that numerical difficulties were encountered in inverting the matrix or while solving the matrix equation when orthogonal polynomials were not used. But by using the proposed procedure, these difficulties minimized and the method gives direct solution without any inversion of matrix for two dimensional case. So, using the experimental data in Eq. (6), the orthogonal polynomials are

Table 2 Values of F and R^2

	1storder regression model	2ndorder regression model	3rdorder regression model	1storder orthogonal model	2ndorder orthogonal model
R^2	0.7948607	0.7980145	0.9460368	0.6529068	0.7993603
F-computed	44.5594700	15.8034	31.66460	21.63231	15.93624
F-value from Table	19.45	4.56	3.01	19.45	4.56
K & $N-K+1$	2,23	5,20	9,16	2,23	5,20

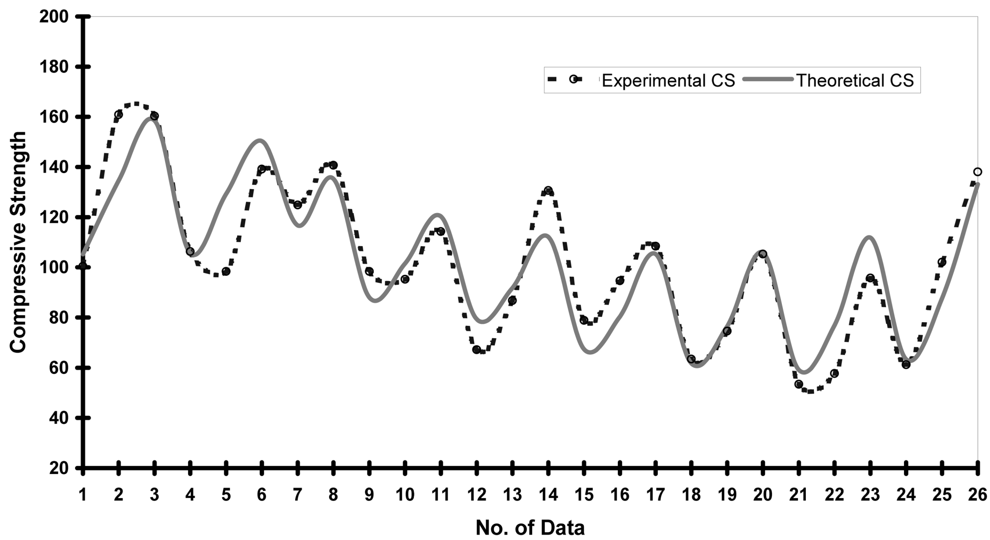

Fig. 1 Trend of theoritical Compressive Strength with Experimental Data w.r.t. No. of Samples

generated and these were tested for their orthogonality. Then the experimental data along with the above generated and tested two dimensional orthogonal polynomials are substituted in Eq. (8) to get the constants C_k. After putting these C_k values in Eq. (4) one can get direct prediction of the product parameters. Corresponding R^2 and F values are also incorporated in Table 2. It may however be seen that the R^2 values are either better or similar in comparison to the simple regression analysis and the procedure to get the results is much efficient and straight forward without the numerical difficulties.

Figs 1, 2 and 3 depicts respectively the comparison of values of compressive strength, bulk

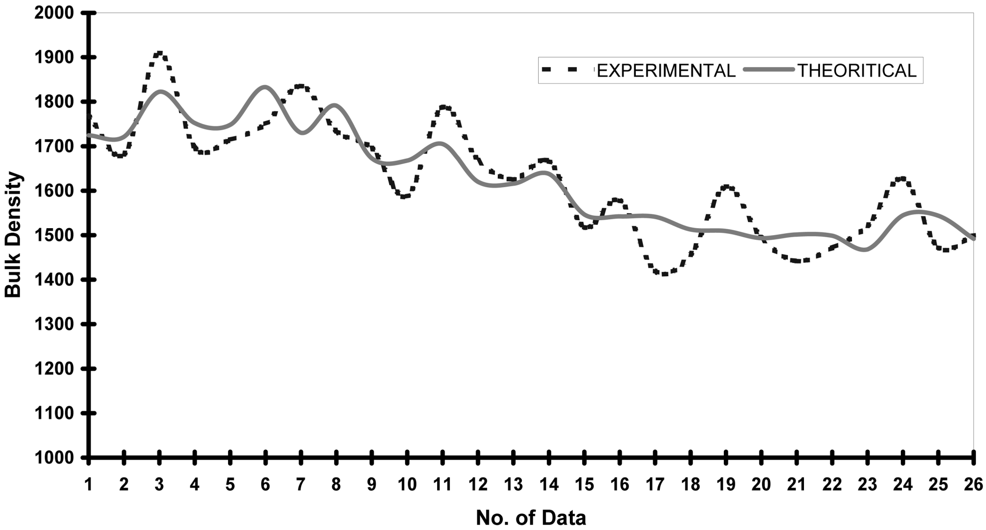

Fig. 2 Trend of Theoritical Bulk Density with Experimental Data w.r.t. No. of Samples

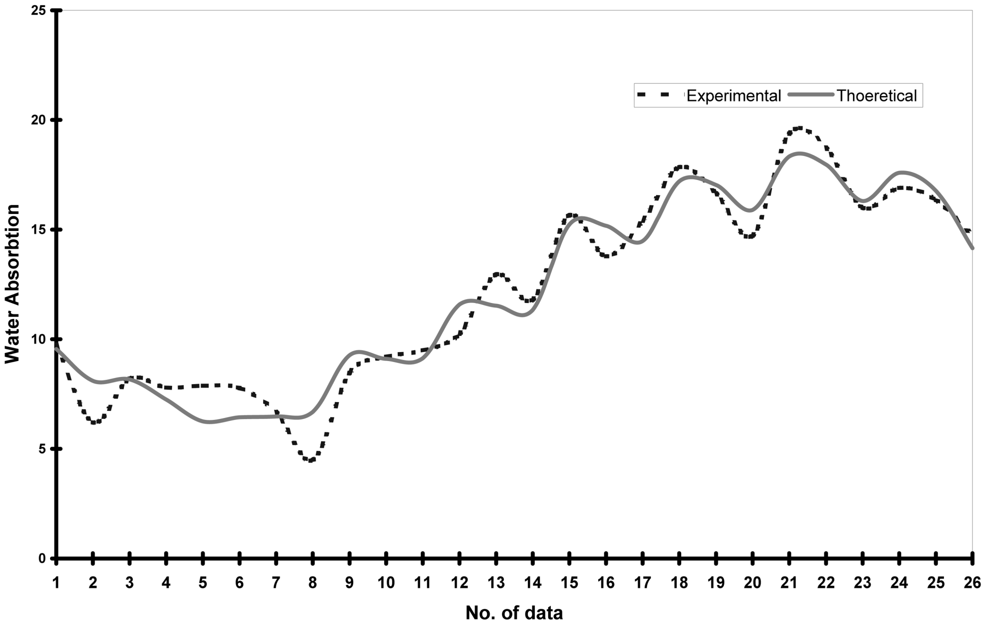

Fig. 3 Trend of Theoretical Water Absorbtion with Experimental Data w.r.t. No. of Samples

Table 3 Input parameters for fly ash cement bricks for testing the model

Fly ash (in %)	Cement (in %)	Sand (in %)
30	12	58
38	8	54
40	8	52
43	10	47
47	12	41
50	10	40

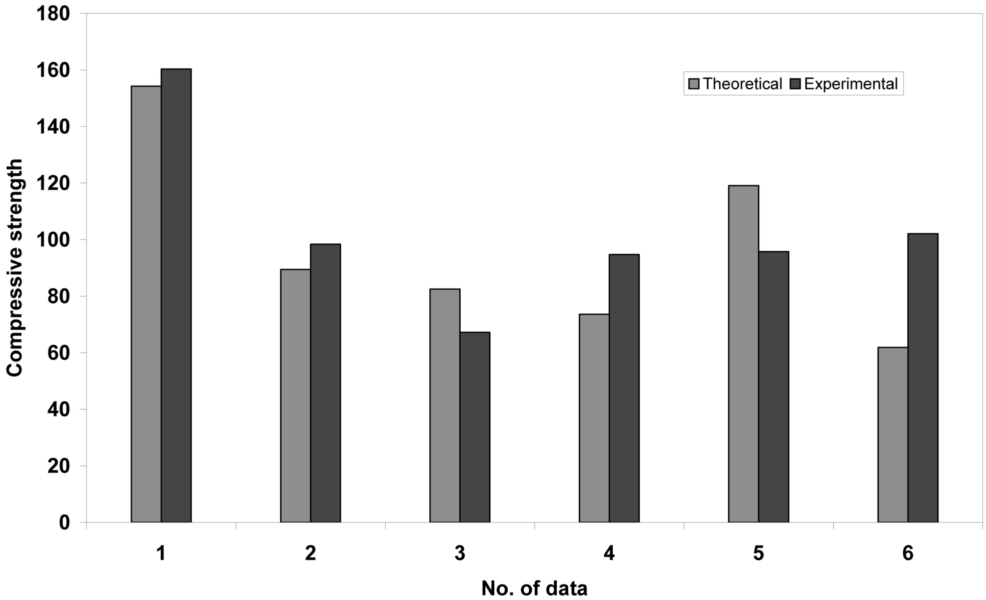

Fig. 4 Comparision between experimental and theoretical results for compressive strength

density and water absorption obtained by two dimensional orthogonal polynomial regression method with corresponding experimental values taking all twenty six samples. The results may be seen to be in good agreement. In order to see the powerfulness and validation of the proposed multi parameter model, the authors executed their analysis by inputting some other data for the process variables that were not used during the numerical modeling. For this some new data as given in Table 3 are entered into the program and theoretical product parameter results are computed. Correspondingly Figs. 4, 5 and 6 show the comparison of the theoretical values obtained from the model and the experimental values. These figures show the efficacy, reliability and accuracy of the model. User may obtain the corresponding product parameters of the flyash cement bricks by following the present model without doing repeated experiments.

3. Conclusions

Here the modeling has been done for product parameters of fly ash cement bricks where fly ash

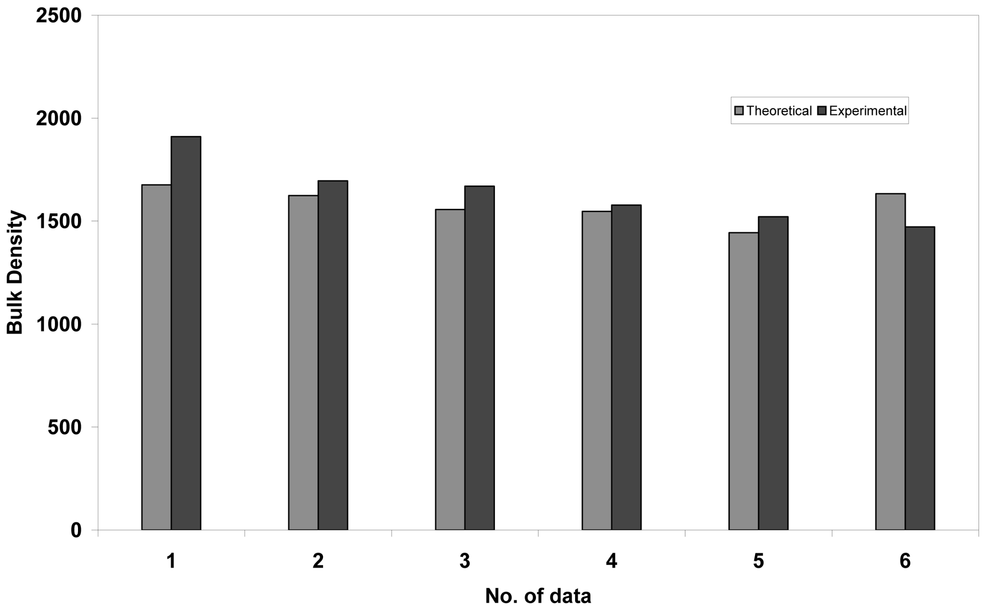

Fig. 5 Comparision between theoretical and experimental results for Bulk Density

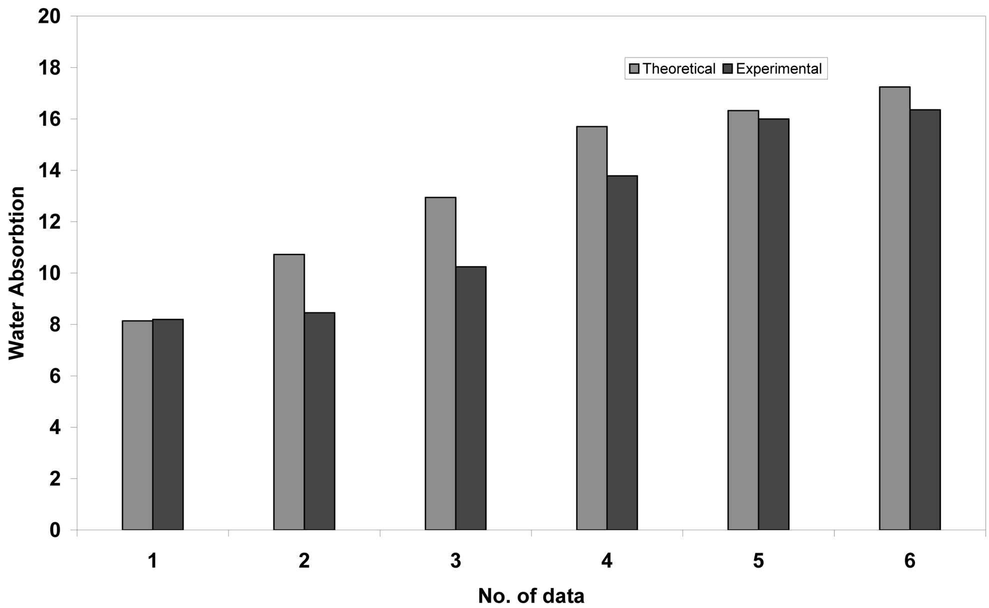

Fig. 6 Comparision between theoretical and experimental results for Water Absorption

and sand are collected from NTPC, Dadri, New Delhi and cement used is of 43 grade. The investigators did experiments with various percentages of the process parameters as mentioned above. First the usual regression model of various orders is developed. Then a computationally efficient method of generating two dimensional orthogonal polynomials is mentioned and those are used in the regression analysis. This turns the procedure to a simple and straightforward analysis as no inversion of matrix or any matrix solution methods are needed. The investigators used two dimensional orthogonal polynomials, as the process parameters considered are two variables. The one dimensional orthogonal polynomials are easy to generate and those may be used for only the one parameter problems. However if more then two variable process parameters to be used then higher dimensional orthogonal polynomials are to be used for the analysis in the similar fashion as described in this paper.

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