Analysis of Strength of Concrete Using Design of Experiments and Neural Networks

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Abstract: This paper investigates the potential of using design of experiments and neural networks to determine the effect of fly ash replacements, from 0 to 50%, on early and late compressive strength, from 3 to 56 days, of low- and high-strength concrete, at water-cementitious material ratios in the range of 0.3–0.7. The research reported in this paper shows the following conclusions: (1) using a simplex-centroid mixture experiment design, a much smaller number of experiments need to be performed to obtain meaningful data; (2) high correlations between the compressive strength and the component composition of concrete can be developed using the generalization capabilities of the neural networks; (3) analyses of variance to test the effects of the variables and their interactions on concrete strength can be performed; (4) the strength ratio, i.e., the percentage of strength of concrete containing fly ash to strength of concrete without fly ash (pure-cement concrete) based on the same w/b and the same age, is significantly reduced as the fly ash replacement increases, is somewhat reduced as the water-binder ratio decreases, and is highly significantly reduced as the age decreases; and (5) the higher fly ash content mixes yielded lower strength ratios throughout, the difference being greater at early age and low water-binder ratio.

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Introduction

Fly ash is the primary waste material from coal-burning power plants. Production of the supplementary cementitious materials will increase as its relevant industries continue to develop. In most cases, there is an economic benefit in the price differential between cement and fly ash. At the present, there are a few specific mix proportioning methods designed for fly ash concrete. The material is used as a direct replacement of cement by weight, at proportions of 10–25% by mass of the total cementitious content, and then current proportioning techniques for concrete made with Portland cement are followed. Generally, the compressive strength of concrete containing fly ash is lower than that of a control concrete without fly ash, particularly at an early age and at replacement levels of 25% and above. At low water-to-binder (w/b) ratios of about 0.35, 28-day cube compressive strengths of 35–50 MPa have been obtained for such cements without much difficulty (Swamy and Bouikni 1990).

Over the last few decades, a considerable volume of research has been directed toward generating the strength-w/b relations for concrete in compression, the importance of which needs no elaboration. In plain Portland cement concrete, it is usually assumed that, as long as the Portland cement itself is satisfactory, the quality of the cement paste produced is primarily an inverse function of the water-cement ratio (w/c). In other words, the strength of the concrete is a function of the total void content of the material (Aitcin and Neville 1993). The addition of fly ash to the mix introduces a variable that influences paste quality and, consequently, the overall quality of the concrete. Many studies have shown that, when the water-binder ratio (w/b) (water-cementitious material ratio) is used instead of the water-cement ratio as the basis for mix designing, strength prediction becomes more accurate. However, the quality of the resulting fly ash Portland cement paste may vary with the level of replacement. Thus, it is practically known that concretes with the same w/b value may have different compressive strengths. Therefore, experimental determination of the relations has become more difficult because the composition of concrete has become more diverse (Wee et al. 1996).

This paper aims to present the experimental results of the effect of fly ash replacements on the early and late compressive strength of low- and high-strength concrete. One traditional experimental program methodology of studying the effects of various components is to vary one component at a time and keep all others constant. Response readings are then taken for different levels of this component. This process is repeated by varying other components one by one until all the components have been treated. This approach may not be satisfactory because of interactions between components. Therefore, the methodology does not seem appropriate to build the model of concrete strength, because the interactions between factors of strength are usually very large. To overcome this difficulty, recourse is made to design of experiments (DOE).

Industrial researchers typically turn to two-level factorials as their first attempt at DOE. These designs consist of all combinations of each factor at its high and low levels. With large numbers of factors, only a fraction of the runs need to be completed to produce estimates of the main effects and simple interactions. However, when the response depends upon proportions of ingre-

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Table 1. Two-Level Factorial Design of Two Controllable Factors

Run number	Cement (kg)	Water (kg)	Compressive strength (MPa)
1	360	180	34
2	360	220	28
3	440	180	45
4	440	220	34

Table 2. Simplex-Centroid Design of Three Components

Run number	Component $1x_1$	Component $2x_1$	Component $3x_1$
1	1	0	0
2	0	1	0
3	0	0	1
4	1/2	1/2	0
5	1/2	0	1/2
6	0	1/2	1/2
7	1/3	1/3	1/3

dients, such as in chemical or material formulations, factorial designs may not make sense.

For example, for a normal concrete consisting of cement, water, fine aggregate, and coarse aggregate, assume that the cement and water are controllable factors with two levels, 360 and 440, and 180 and 220 kg, respectively; and fine aggregates and coarse aggregate are uncontrollable factors with a fixed level of 800 and 1,000 kg; then, the two-level factorials are as shown in Table 1. Run 1 (both factors low) and run 4 (both factors high) have the same strength. However, it makes more sense to look at strength as a function of the proportion of water to cement, not the amount.

There are many industrial problems where the response variables of interest in the product are a function of the proportions of the different ingredients used in its formulation. This is a special type of response surface problem called a mixture problem. Design of experiments for a mixture accounts for the dependence of the response on proportionality of ingredients (Myers and Montgomery 1995).

Using polynomial regressions, the DOE approach permits calculation of the response surfaces for the parameters under study over the experimental domain. However, because of the high complexity of the relation between the compressive strength and component composition of concrete, conventional regression analysis could be insufficient to build an accurate model. Artificial neural networks (ANN) are essentially information modeling systems that mimic the biologic system of the brain. The neural network modeling approach is simpler and more direct in comparison with traditional statistical methods, particularly when modeling nonlinear multivariate interrelationships. Some recent applications of neural networks in civil engineering materials include Ghaboussi et al. (1991), Oh et al. (1999), Basma et al. (1999), Yeh (1998a,b, 1999), Yeh et al. (2002), Haj-Ali et al. (2001), Nehdi et al. (2001a,b); Peng et al. (2002), El-Chabib et al. (2003), Kim et al. (2004), and Stegemann and Buenfeld (2004). However, little research has been done on modeling the strength of concrete containing a large amount of fly ash and superplasticizer using neural networks associated with DOE.

This paper investigates the potential of using DOE and neural networks to determine the effects of fly ash replacements, from 0 to 50%, on the early and late compressive strength, from 3 to 56 days, of low- and high-strength concrete, at water-cementitious material ratios in the range of 0.3–0.7.

Introduction of Design of Experiments for Mixture

In general, suppose that the mixture consists of q ingredients or components, and let x_i represent the proportion of the ith ingredient in the mixture. In light of the preceding discussion, the mixture problem becomes

$$x_i \geq 0, \quad i = 1,2,\ldots,q \tag{1}$$

and

$$\sum_{1=1}^{q} x_i = x_i + x_2 + \ldots + x_q = 1 \tag{2}$$

The constraint in Eq. (2) makes the levels of the components x_i dependent, and this makes mixture experiments different from factorial experiments. The primary differences between a factorial experiment and a mixture experiment are that: (1) a special type of design must be used; and (2) the form of the mixture polynomial is slightly different from the standard polynomials used in factorial design (Myers and Montgomery 1995).

In this study, a mixture design called simplex-centroid design was adopted. A q-component simplex-centroid design consists of $2^q - 1$ distinct design points. These design points are the q permutations of $(1,0,0,\ldots,0)$ or single-component blends, the $\binom{q}{2}$ permutations of (1/2, 1/2, 0,…, 0) or all binary mixtures, the $\binom{q}{3}$ permutations of (1/3, 1/3, 1/3, 0,…, 0), and so forth, and the overall centroid $(1/q, 1/q,\ldots, 1/q)$. Because the mixture space is a simplex, all design points must be at the vertices, on the edges or faces, or in the interior of a simplex.

To illustrate how to apply mixture design, a simplex-centroid mixture design that involves three components is listed in Table 2. The design keeps the total of the components at one unit. Fig. 1 shows the location of the points of the design in the mixture space. In this triangular layout, the apexes represent the use of only a single, specific component. Binary blends, which provide estimates of second-order effects, occur at the midpoints of the

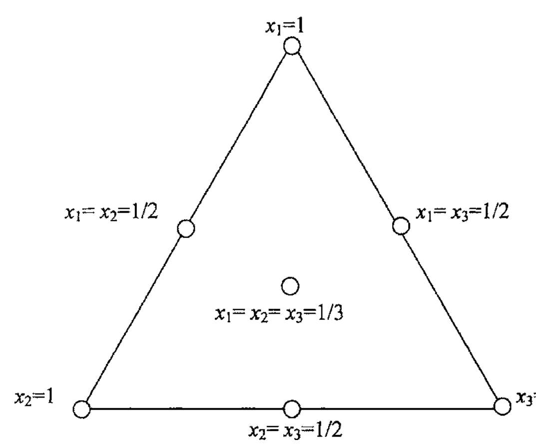

Fig. 1. Simplex-centroid mixture design that involves three components

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Table 3. Lower and Upper Bound of Each Component

Component	Lower bound (kg/m^3)	Upper bound (kg/m^3)
Cement	150	350
Fly ash	0	200
Slag	0	260
Water	125	240
SPgate	3.5	12
Coarse aggregate	850	1,160
Fine aggregate	675	980

sides on the triangle. The points in the interior represent three-part blends. The centroid point contains equal amounts of all three ingredients. The individual proportions go from zero to one from base to apex in each of the three axes (Myers and Montgomery 1995).

Constraints on individual components may be introduced. The constrained mixture problem becomes Eq. (3)

$$L_i \le x_i \le U_i, \quad i = 1,2, \ldots ,q \tag{3}$$

(where L_i and U_i=lower bound and upper bound of the ith component) and Eq. (2). However, this adds complications that go beyond the scope of this article. Myers and Montgomery (1995) is an excellent and very complete reference on the subject.

The design points in the simplex-centroid design will support the qth-order mixture polynomial

$$E(y) = \sum_{i=1}^{q} \beta_i x_i + \sum_{i<} \sum_{j}^{q} \beta_{ij} x_i x_j + \sum_{i<} \sum_{j<} \sum_{k}^{q} \beta_{ijk} x_i x_j x_k + \ldots + \beta_{12\ldots q} x_1 x_2 \ldots x_q \tag{4}$$

where x_i=proportion of the ith ingredient in the mixture; and β_i, β_{ij}, $\beta_{ijk}, \ldots, \beta_{12\ldots q}$=regression coefficients.

For $q=3$ components, this model is

$$E(y) = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{123} x_1 x_2 x_3 \tag{5}$$

which is the special cubic polynomial from Eq. (4). For $q=4$ components, the model is

$$E(y) = \sum_{i=1}^{4} \beta_i x_i + \sum_{i<} \sum_{j}^{4} \beta_{ij} x_i x_j + \sum_{i<} \sum_{j<} \sum_{k}^{4} \beta_{ijk} x_i x_j x_k + \beta_{1234} x_1 x_2 x_3 x_4 \tag{6}$$

or the special cubic model with an additional quartic term. Because of the relatively efficient designs for fitting the special cubic model, simplex-centroid designs are often used when the experimenter thinks that some cubic terms may be necessary in the final model (Myers and Montgomery 1995).

Design of Experiments for Concrete Mixture

The lower and upper bound of each component is listed in Table 3. In a mixture experiment, the response is observed at all mixture design points and the effects of component and interactions between components are investigated simultaneously.

However, in concrete mixture design, certain mixture design points are not possible and must be omitted. Such a deliberate omission of some design points creates some experimental and

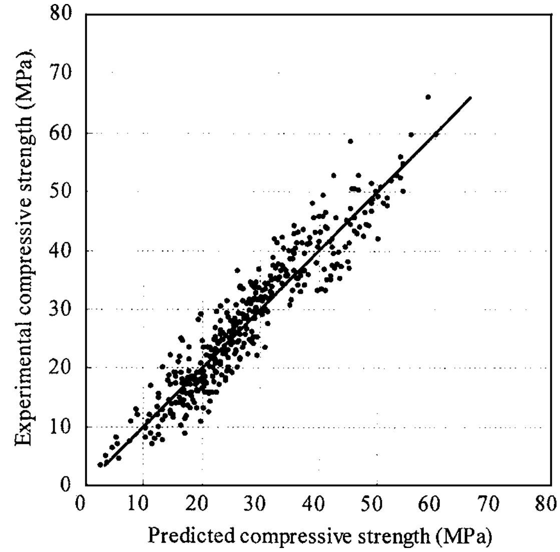

Fig. 2. Measured and predicted compressive strength of regression for training data

analysis problems, both theoretical and numerical. Therefore, a flattened simplex-centroid mixture experiment design was adopted. Thus, instead of using a total of $2^q-1=2^7-1=127$ mixture design points, 78 design points that covered a whole range of values likely to be encountered in practice were selected. The sequence in which the mixture design points were investigated was randomized to avoid any statistical significance of a blocking effect.

All compressive strengths were measured on 150 mm cylinders. These were fully compacted on a vibrating table, moist-cured for 24 h, demolded, and then cured in water at 20°C until testing at 3, 7, 14, 28, and 56 days. Therefore, there were $78\times5=390$ training data. Each quoted strength value is the average of the strengths from three cylinders.

Also, to evaluate the accuracy of the model built with the mixture design, 10 concrete mixtures and their test results at 3, 14, 28, 56, and 90 days collected from the literature (Yeh 1999) were used. Therefore, there were $10\times5=50$ testing data. Although there were only 10 mixtures used from the literature, they covered five different levels of strength, about 25, 32.5, 40, 47.5, and 55 MPa, and five different levels of workability, about 5, 10, 15, 20, and 25 cm in slump. It may be certain that these will form a fairly representative group covering all the ranges of practical use for concrete mixtures and will present the rather complete and independent information required for such an evaluation.

The results of the compressive strength tests were subjected to polynomial regression using a computer program. Various polynomials were tried to represent the measured compressive strength data for seven component contents at a specific age. The best fit for the compressive strength was obtained with a root-mean-square (RMS) error of 3.96 MPa ($R^2=0.890$) and 8.82 MPa ($R^2=0.791$) for the training data and testing data, respectively. Predictions of the strength of concrete using regressions for the training data and testing data are shown in Figs. 2 and 3, respectively. It can be seen that, although the RMS error for the training data is rather low, the RMS error for the testing data is so high as to provide inaccurate predictions. In other words, the model is lacking in generalization.

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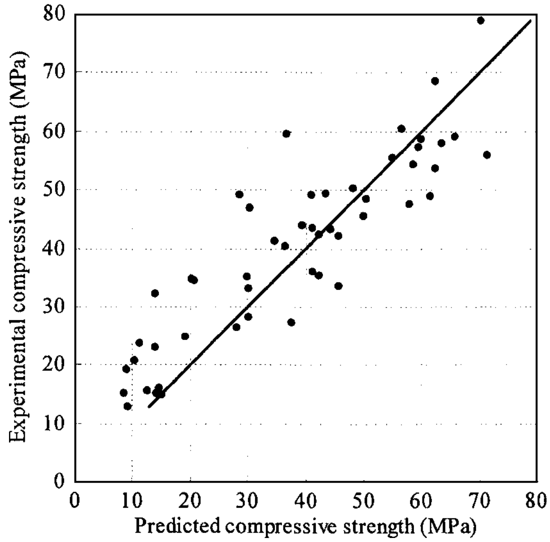

Fig. 3. Measured and predicted compressive strength of regression for testing data

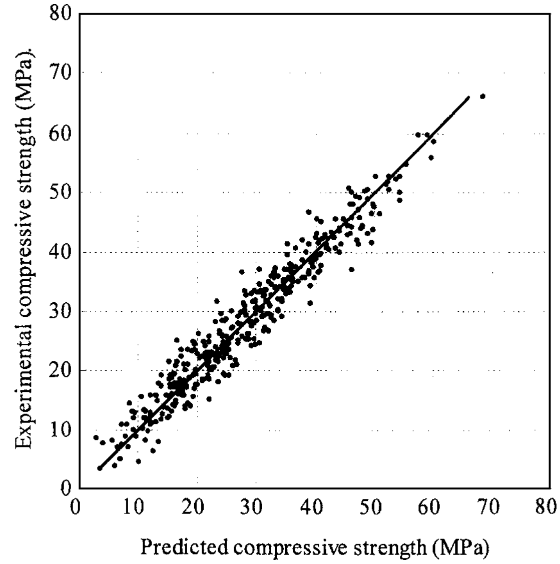

Fig. 4. Measured and predicted compressive strength of ANN for training data

Introduction of Neural Networks

A neural network is a computer model whose architecture essentially mimics the knowledge acquisition of the human brain. It consists of a number of interconnected processing elements, commonly referred to as neurons. The neurons are logically arranged into two or more layers and interact with each other via weighted connections. These scalar weights determine the nature and strength of the influence between the interconnected neurons. Each neuron is connected to all the neurons in the next layer. There is an input layer where data are presented to the neural network and an output layer that holds the response of the network to the input. It is the intermediate layers, also known as the hidden layers, which enable these networks to represent and compute complicated associations between patterns (Goh 1995). Each hidden and output neuron processes its inputs by multiplying each input by its weight, summing the product, and then passing the sum through a nonlinear transfer function to produce a result. The S-shaped sigmoid curve is commonly used as a transfer function.

The neural network "learns" by modifying the weights of the neurons in response to the errors between the actual output values and the target output values. The neural network paradigm adopted in this study utilizes the back-propagation learning algorithm. In back-propagation neural networks, the mathematical relationships between the various variables are not specified. Instead, they learn from the examples fed to them. In addition, they can generalize correct responses that only broadly resemble the data in the learning phase (Goh 1995). The details of the algorithm will not be discussed here; it has been thoroughly described by Lippmann (1987). Numerous implementations of back propagation are commercially available. In short, for the first cycle of training, random weights were assigned to the connections between the units. Training was carried out until the average sum squared error over all the training patterns was minimized. During training, the network performance is monitored by RMS error to achieve a better understanding of the network performance.

Once trained, the values for the input parameters for the project are presented to the network. Then the network calculates the node outputs using the existing weight values and thresholds developed in the training process. The neural network will produce almost instantaneous results of the output for the practical inputs provided. Such a trained neural network not only would be able to reproduce the experiment results it was trained on, but through its generalization capability should be able to approximate the results of other experiments. The degree of accuracy in this generalization depends on how comprehensive the training set is (Ghaboussi et al. 1991). The predictions should be reliable, provided the input values are within the range used in the training set (Goh 1995).

Neural Networks for Modeling Strength Behavior

To efficiently generate response surfaces of the compressive strength of concrete, instead of commercially available neural network software, the program adopted in this study was written in C language and essentially followed the formulations of Lippmann (1987).

The neural network developed in the investigation had eight units—represented as cement, fly ash, slag, water, SP, coarse aggregate, fine aggregate, and age—in the input layer and one unit represented as compressive strength in the output layer. After a number of trials, the best network architecture and parameters that minimize the RMS error of the testing data were selected as follows:

- Number of hidden layers = 1;
- Number of hidden units = 4;
- Learning rate = 1.0; and
- Learning cycle = 3,000.

Training time on a personal computer was less than 30 s. The RMS error was 3.01 MPa ($R^2 = 0.940$) and 4.32 MPa ($R^2 = 0.929$) for training data and testing data, respectively. Predictions of the strength of concrete using the network for training data and testing data are shown in Figs. 4 and 5, respectively. Comparing Figs. 5 and 3 , it may be seen that the model obtained by neural networks more accurately predicts the experimental results for the testing data in the range of concrete strength in this study.

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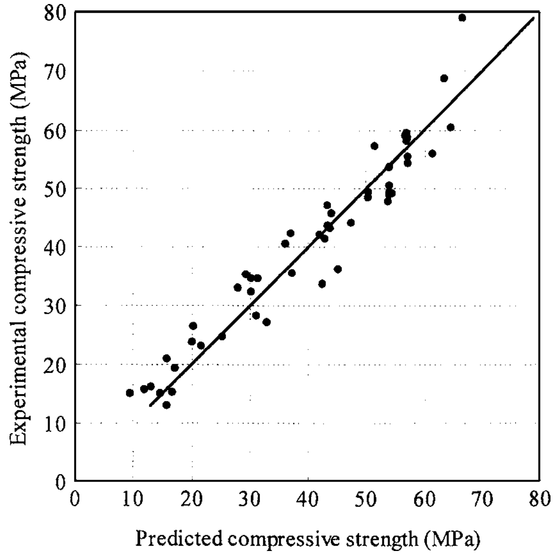

Fig. 5. Measured and predicted compressive strength of ANN for testing data

Response Surfaces of Compressive Strength

When the neural network model for compressive strength has been built, the predicted compressive strength can be regarded as a function of all the input variables. Although there are eight input variables in the model, it is more meaningful to investigate the response surface and relations between the compressive strength and age and the two ratios of components, the water-binder ratio and fly ash-binder ratio. The binder means cementitious material, that is, cement plus fly ash and slag. The range of each variable is listed as follows:

1. The water-binder ratio (w/b) was varied at 0.3, 0.4, 0.5, 0.6, and 0.7.
2. The fly ash-binder ratio (fa/b), the amount of fly ash by weight of binder, was varied at 0, 10, 20, 30, 40, and 50%.
3. The age of concrete was varied at 3, 7, 14, 28, and 56 days.

All other components or their ratios were kept constant: the slag, water, and SP contents were kept constant at 0, 175, and 5 kg/m^3, respectively; the coarse aggregate to fine aggregate was kept a constant 1.0; and the total volume of concrete was 1.000 m^3.

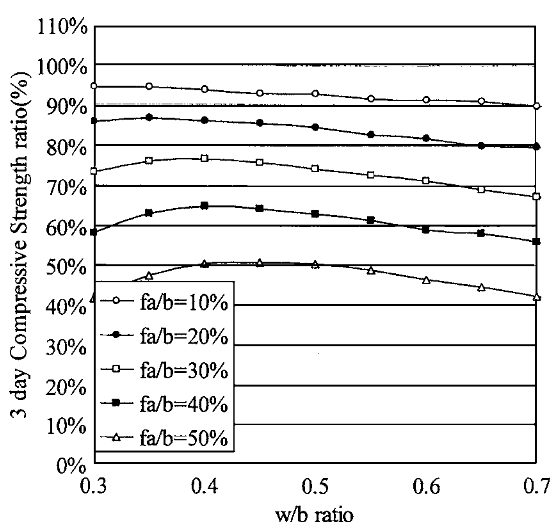

Fig. 6. w/b-strength ratio curves at 3 days

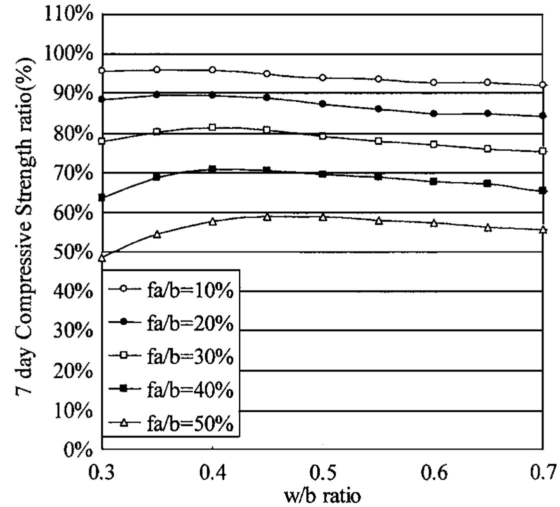

Fig. 7. w/b-strength ratio curves at 7 days

From the w/b-strength ratio curves generated using the trained neural network developed in this study with the preceding combinations, five sets of curves are shown in Figs. 6–10 to explore the effects of fa/b and w/b at 3, 7, 14, 28, and 56 days. The strength ratio means the percentage of strength of concrete containing fly ash to strength of concrete without fly ash (pure-cement concrete) based on the same w/b and the same age. In addition, five response surfaces have been shown in Figs. 11–15 to explore the interactions between fa/b and w/b at 3, 7, 14, 28, and 56 days. Some conclusions may be summarized as follows.

Effects of fa/b

At the same age and w/b, the reduction in strength ratio with fly ash content in the cement paste is proportional. For example, at an age of 28 days, as can be seen in Fig. 9, w/b=0.5, the effect of relatively small replacements (10%) is a slight decrease (2%) in strength ratio; however, the effect of relatively large replacements (50%) is a significant decrease (18%) in strength ratio.

Effects of w/b

At high fly ash replacement, the greatest proportional strength ratio decreases are at the low water-cementitious material ratios. For instance, at 28 days of age, the strength of concrete containing 50% of fly ash at w/b=0.3 and 0.7 is 72 and 82% of that of concrete without fly ash. However, at low fly ash replacement, the reduction of strength ratio produced by replacing cement with fly ash in concrete mixes prepared at a lower w/b was about the same as those prepared at a higher w/b. This phenomenon is illustrated in Figs. 6, 8, and 10 for concrete at 3, 14, and 56 days, respectively. At 3 days, the 30% fly ash mix at w/b=0.3 and 0.7 achieved 73 and 67% of the compressive strength of the reference pure cement mix; at 14 days, it was 83 and 83%, and at 56 days, it was 95 and 95%.

Effects of Age

Higher volumes of fly ash replacement result in a significantly lower strength ratio at the early ages, while resulting in a slightly

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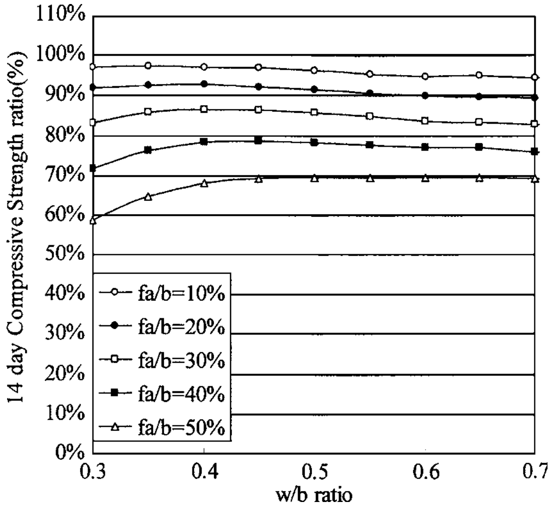

Fig. 8. w/b-strength ratio curves at 14 days

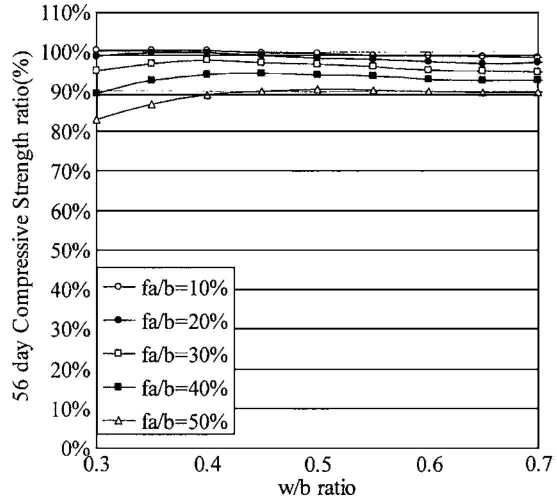

Fig. 10. w/b-strength ratio curves at 56 days

lower strength ratio at the late ages. For example, at $w/b=0.5$, the strengths of concrete containing 50% fly ash at 3 days, (Fig. 6) and 56 days (Fig. 10) are 51 and 91% of that of concrete without fly ash.

Interactions of *fa/b* and *w/b*

1. A lower volume of fly ash replacement results in about the same reduction of strength ratio at low w/b and at high w/b. For example, at 28 days of age, as can be seen in Figs. 9 and 14, the strengths of concrete containing 10% fly ash at $w/b=0.3$ and 0.7 are 99 and 97% of that of concrete without fly ash, respectively.
2. A higher volume of fly ash replacement results in a significantly lower strength ratio at low w/b, while resulting in a slightly lower strength ratio at high w/b. For example, at 28 days of age, the strengths of concrete containing 50% fly ash at $w/b=0.3$ and 0.7 are 72 and 82% of that of concrete without fly ash, respectively.

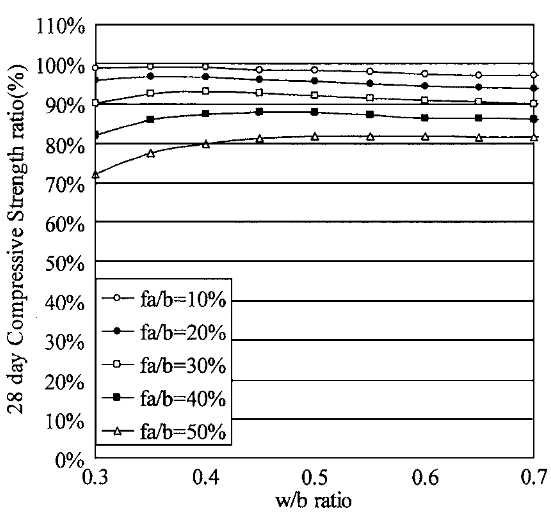

Fig. 9. w/b-strength ratio curves at 28 days

Interactions of *fa/b* and Age

1. At the early ages, fly ash contributes little to strength. For example, at 3 days, as shown in Figs. 6 and 11, at a water-binder ratio of 0.5, as compared to the concrete without fly ashes, the strength ratio is reduced by 7% for a 10% fly ash replacement, and by 49% for a 50% fly ash replacement.
2. At medium ages, fly ash contributes some to strength. For instance, at 28 days, as can be seen in Figs. 9 and 14, at a water-binder ratio of 0.5, the strength of the 10% fly ash mixes is only slightly lower (2%) than that of the pure cement mixes, although 50% fly ash replacement still results in an 18% reduction of strength ratio.
3. At the later ages, the contribution of fly ash to compressive strength is greater. For example, at 56 days, as can be seen in Figs. 10 and 15, at a water-binder ratio of 0.5, the strength of

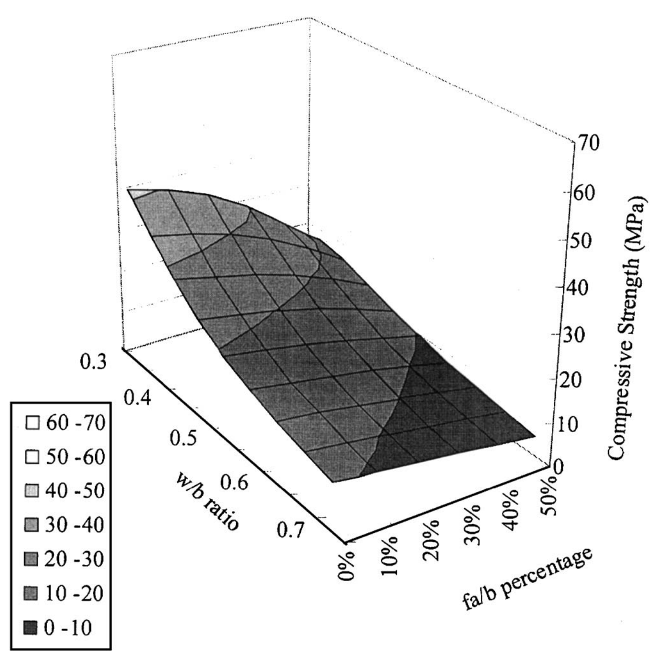

Fig. 11. Response surface of compressive strength at 3 days

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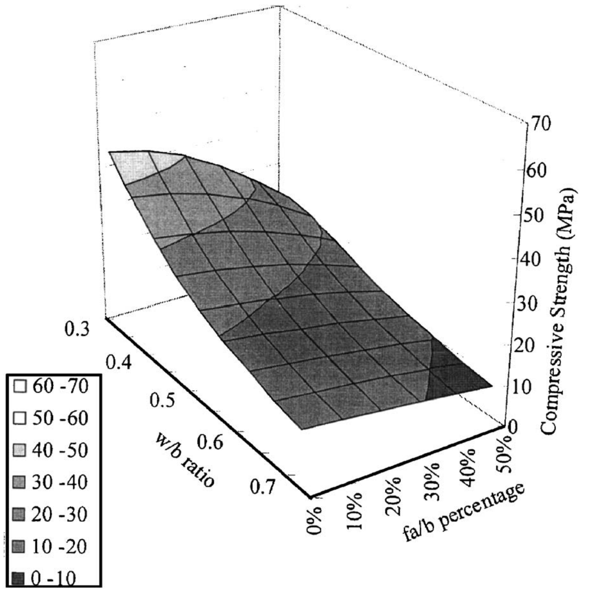

Fig. 12. Response surface of compressive strength at 7 days

the 10% fly ash mixes is the same as that of the pure cement mixes, and 50% fly ash replacement only results in a 9% reduction in strength ratio.

Interactions of w/b and Age

1. At the early ages, there is an optimum w/b for minimizing the reduction in strength ratio. For example, at 3 days, as shown in Fig. 6, the strength ratios of concrete containing 50% fly ash at $w/b=0.3$ and 0.7 are 41 and 42%, respectively; however, that at $w/b=0.45$ is 51%, a significantly greater percentage.
2. At the later ages, the higher the w/b, the higher the strength ratio. For example, at 56 days, as shown in Fig. 10,

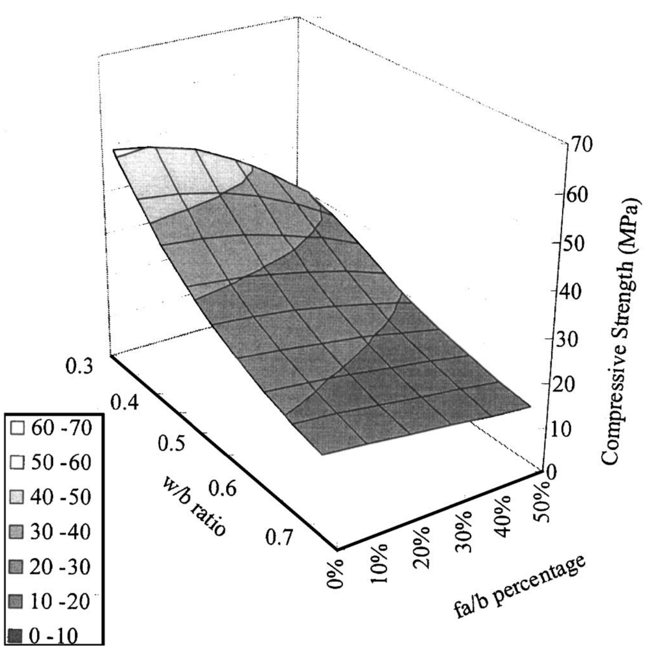

Fig. 13. Response surface of compressive strength at 14 days

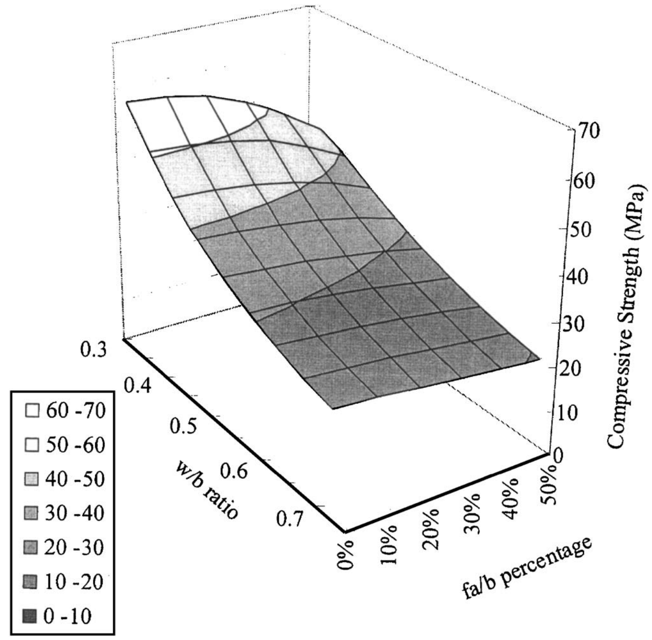

Fig. 14. Response surface of compressive strength at 28 days

the strength ratios of concrete containing 50% fly ash at $w/b=0.3$, 0.5, and 0.7 are 83, 90, and 90%, respectively.

Conclusions

The research reported in this paper shows the following conclusions:

1. For concrete compressive strength, using a simplex-centroid mixture experiment design, a much smaller number of experiments need be performed to obtain meaningful data. Such data can be satisfactorily used for building a neural network model. A q-component simplex-centroid design consists of 2^q-1 distinct design points. Therefore, because there are seven components in this study, there are $2^7-1=127$

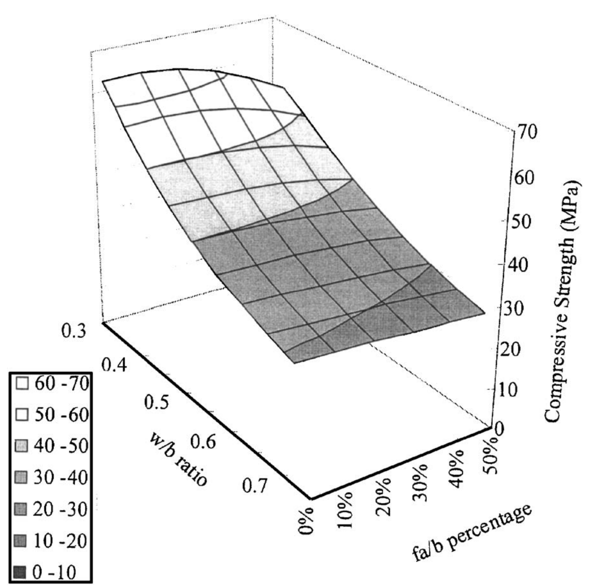

Fig. 15. Response surface of compressive strength at 56 days

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mixtures. Thus, if there are five levels for each component, the complete combinations are $5^7=78,125$ mixtures. Therefore, the simplex-centroid mixture experiment design is much more economical.

2. Based on the data obtained from the DOE for mixture, high correlations between the compressive strength and the component composition of concrete can be developed using the generalization capabilities of the neural networks. Such a model can be efficiently used for simulating the compressive strength behavior.
3. Based on simulating compressive strength with the model built using neural networks, analyses of variance to test the effects of the variables and their interactions on concrete strength can be performed. Such information can be employed to induce some interesting discoveries of effects and interactions of factors.
4. The strength ratio, which means the percentage of strength of concrete containing fly ash to strength of concrete without fly ash (pure-cement concrete), based on the same w/b and the same age, is significantly reduced as the fly ash replacement increases, is somewhat reduced as the water-binder ratio decreases, and is very significantly reduced as the age decreases.
5. The higher fly ash content mixes yielded lower strength ratios throughout, the reduction being greater at an early age and low water-binder ratio.
6. At high fly ash replacement, the strength ratio is somewhat reduced as the water-binder ratio decreases; however, at low fly ash replacement, the reduction of strength ratio produced by replacing cement with fly ash in concrete mixes prepared at a lower w/b is about the same as those prepared at a higher w/b.
7. The strength ratio is highly significantly reduced as the age decreases, the reduction being greater at high fly ash replacement and low water-binder ratio.

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