OPTIMIZATION OF CH CONTENT OF TERNARY CEMENTITIOUS SYSTEMS AND ITS PREDICTION USING ARTIFICIAL NEURAL NETWORKS

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Abstract
Hydration of cement constituents brings about setting and hardening of cement. It involves chemical reactions of individual components with water. This paper presents the application of artificial neural networks for the prediction of hydration of high strength concrete. The progress of hydration was monitored by measuring the amount of CH content at various ages using TGA on cement paste incorporating fly ash up to 40% and silica fume up to 15% as partial cement replacements for the preparation of various combinations of binary and ternary blended systems. The interactive effect of fly ash and silica fume on CH content is reported. Based on the experimentally obtained results, the applicability of artificial neural network for the prediction of hydration using artificial neural networks has a good correlation between the experimentally obtained values. Therefore, it is possible to predict hydration of high strength concrete using artificial neural networks.

1. INTRODUCTION
Hydration of cement constituents brings about setting and hardening of cement. It involves chemical reactions of individual components with water. When water is added to cement, each of the compounds undergoes hydration and contributes to the final concrete product. Tricalcium silicate rapidly reacts to release calcium ions, hydroxyl ions, and a large amount of heat. The reaction slowly continues producing calcium and hydroxyl ions until the system becomes saturated. The formation of the calcium hydroxide (CH) and calcium silicate hydrate gel provides "seeds" upon which more calcium silicate hydrate can form. However, CH crystals in portland cement pastes are a source of weakness because cracks can easily propagate through or within these crystals without any significant resistance [1]. In the presence of pozzolanic materials, the reduction in the content of CH leads to an increase in strength.

The use of fly ash in concrete has been widely practised, as it helps to reduce the cost, conserve energy and resources, reduce environmental impact and enhance the workability for
a given water content. Fly ash, however, results in low early-age strength development even though the concrete may have higher strength and durability in the longer term. To overcome the low-early strength when fly ash is incorporated, the inclusion of silica fume is seen as a possible solution, since it is a highly reactive pozzolan. The reaction of silica fume particles with CH may provide higher amounts of hydrates at early-ages to compensate for the reduction in hydrates due to the replacement of cement by fly ash.

The number of ingredients and the number of properties of high strength concrete, which needs to be considered in its design, are more than those for ordinary concrete. Therefore, it is difficult to predict the properties of this type of concrete using statistical empirical relationship. An alternative approach is to use an artificial neural network (ANN). The ANN approach is good for modelling non-linear systems. A neural network model is a computer model whose architecture essentially mimics the learning capability of the human brain.

2. NONLINEAR MODELING

In this investigation, a nonlinear autoregressive model with exogenous inputs (NARX) [2], which provides a concise representation for a wide class of nonlinear systems, was used. An RBF network was employed to model the input-output relationship described as follows.

2.1 Radial basis function

An RBF network can be regarded as a special two-layer network which is linear in the parameters provided all the RBF centres are prefixed. Given fixed centers i.e. no adjustable parameters the first layer or the hidden layer performs a fixed nonlinear transformation, which maps the input space onto a new space. The output layer then implements a linear combiner on this new space and the only adjustable parameters are the weights of this linear combiner. These parameters can, therefore, be determined using the linear least square method, which is an important advantage of this approach. A schematic of the RBF network with n inputs and a scalar output is shown in Figure 1. Such a network could be represented as

\[
\hat{y}(t) = w_0 + \sum_{i=1}^{n} w_i f(\|x(t) - c_i\|)
\]

where:
\(\hat{y}(t)\) : - is the network predicted output;
\(x(t)\) : - is the network’s input vector and presented as \(x(t) = [y(t-1),...y(t-n_y),u(t-1),...u(t-n_u)]^T\)
\(w_i\) : are the weights or parameters;
\(c_i\) : are known as RBF centres
\(n_r\) : is the number of centers or the hidden neurons.

The nonlinear functional form \(f(.)\) in the RBF expansion, used in this study is the Guassian function. The orthogonal least square provides an elegant method for determination of model structure as well as parameter estimation [3]. Once the functional form \(f(.)\) and the centres \(c_i\) are fixed, and the set of input \(x(t)\) and the corresponding desired output vector \((y(t)\) in this study) provided, the weights \(w_i\) can be determined using the linear least squares method.

Assuming the RBF network in Equation (2) as a special case of the linear regression model is presented as follows:
\[ y(t) = \sum_{i=1}^{M} p_i(t) \theta_i + \varepsilon(t) \]  

(2)

where:
\( y(t) \): is the desired output;
\( p_i \): are known regressors, (some nonlinear functions of lagged outputs and inputs).

A constant term \((w_0 \text{ in Figure } 1)\) can be included in Equation (2) by setting the corresponding term \( p_i(t) = 1 \). The residual \( \varepsilon(t) \) is assumed to be uncorrelated with the regressors \( p_i(t) \). Centre \( c_i \) with a given nonlinear function \( f(\cdot) \) corresponds to \( p_i(t) \) in Equation (2).

![Radial basis function network](image)

Figure 1: Radial basis function network

3. METHODS FOR MEASURING HYDRATION

Hydration progress of the pozzolanic reaction can be monitored by measuring the amount of CH content and non-evaporable water content. In this investigation, the progress of the pozzolanic reaction was monitored by measuring the amount of CH content at various ages using TGA. TGA is a technique whereby the weight of a substance, in an environment heated at a controlled rate, is recorded as a function of temperature. A weight loss vs temperature curve for hardened cement paste between temperatures of 105 and 1000°C can be separated into [4]:

a) weight loss from temperature 105°C to 420°C is associated with dehydration reactions which include, among others, most of the calcium silicate hydrate phases.

b) weight loss from temperature 420°C to 550°C is associated with dehydroxylation of the CH.

c) weight loss from temperature 550°C to 780°C is due to decarbonation of the CaCO₃.

Determination of the CH content was carried out using equation 3. In order to take into account the possibility of carbonation, knowledge of the weight loss above 550°C is essential for the determination of calcium hydroxide. Therefore, in this investigation the total amount
of Ca(OH)$_2$ has been estimated using both stages of weight losses i.e., between 420 – 550°C and above 550°C. The total amount of Ca(OH)$_2$ was estimated as follows:

$$W_{CH} = \frac{74}{18}[\Delta W_1] + \frac{74}{44}[\Delta W_2]$$

(3)

where:

$W_{CH}$ - is total amount of CH content (%)

$\Delta W_1$ - corresponds to weight loss between 420 – 550°C

$\Delta W_2$ - corresponds to weight loss between 550 – 1000°C

4. EXPERIMENTAL PROGRAM

4.1 Materials and sample preparation

Ordinary portland cement (OPC) complying with BS 12: 1991 and fly ash complying with BS 3892: Part 1: 1993 were used throughout the investigation. Fly ash up to 40% and to these blends 0, 5, 10 and 15% silica fume replacement levels were incorporated. A water / binder (w/b) of 0.27 was used throughout. Mixes were cast in plastic cups, properly consolidated and sealed to prevent evaporation of moisture. The samples were kept in the mist room and demoulded the following day and left in the mist room for curing prior to testing. At the testing ages 1, 3, 7, 28, 90 and 180 days the samples were taken out of the mist room and then placed in an oven set at 105°C. The samples were kept in an oven for drying until constant weight was achieved, usually after 12 hours. The samples were then ground to fine powder and passed through a 75 μm sieve in order to improve the uniformity of the sample. The process of grinding was done as quickly as possible (usually within 5 minutes) in order to minimize the carbonation. The powdered sample was sealed in air-tight small glass vials and immediately loaded in the thermobalance for testing.

4.2 Apparatus and test procedure

The equipment used in this investigation was thermogravimetry balance Stanton Redcroft model TG-760. The instrument consists mainly of an electronic microbalance, a furnace and an operational programmer unit. The sample size used was 20-24 mg and the test was performed in flowing nitrogen gas flowing at the rate of 15 ml/min. The samples were heated between the temperature 105°C to 1000°C. The clarity of these peaks depends on the rate of heating and different modes adopted for the test. Therefore, for the clarity of peaks, a slow rate of heating was employed (10°C/min). The furnace was cooled by water in order to achieve a fast cooling rate. The thermobalance was connected to the plotter at the chart speed of 12 cm/hr and the raw data curves were obtained. These curves were analyzed for the weight loss of sample at various stages by following a method given in the literature [4, 5].

5. RESULTS AND DISCUSSION

Calcium hydroxide content in binary paste systems and ternary paste systems containing fly ash and silica fume as cement replacements at various ages investigated are shown in Figures 2 and 3. For the sake of clarity Figure 2a and 3a have been redrawn showing the testing age between 1 and 28 days as shown in Figure 2b and 3b, respectively.
5.1 Binary paste systems

The calcium hydroxide content decreased with an increase in fly ash content (Figure 2). The mixes with 20%, 30% and 40% fly ash demonstrated calcium hydroxide contents of 11.9%, 10.7% and 9.5%, respectively at 1 day of hydration as compared to 12.3% calcium hydroxide content of plain OPC paste. The calcium hydroxide contents of all fly ash mixes increased up to 3 day and then gradually decreased after that. The decrease at 1 day in comparison to that of the plain OPC mix indicates reduced production of calcium hydroxide at early ages which is associated with lower OPC content. After 3 days, the decrease in calcium hydroxide content suggested the beginning of pozzolanic reaction. It can be seen from these results that at early ages the presence of fly ash depressed the production of calcium hydroxide. This is in agreement with the findings of other researchers [6].

The paste containing 5% silica fume exhibited 10.3% and 11.4% calcium hydroxide at 1 day and 3 days, respectively (Figure 2). It can be seen that the majority of the calcium hydroxide is produced in the first 3 days, thereafter a very slow increase was registered. This slow increase beyond 3 days indicates that there is insufficient silica fume available to further deplete the calcium hydroxide during hydration process. Therefore, the 5% silica fume may have largely reacted in the first 3 days. The paste with 10% silica fume demonstrated a similar pattern to that of paste containing 5% silica fume up to the age of 7 days but exhibited lower calcium hydroxide than that of a 5% silica fume mix. After 7 days it decreased gradually and reached 9.2% at 180 days which is about 7.5% lower than that of the OPC mix. Whilst the mix containing 15% silica fume showed 7.8% calcium hydroxide at 1 day and at 3 days it increased slightly. Beyond the 3 days a gradual decrease was registered, reaching 5.1% at 180 days (about 11.7% lower than that of plain OPC mix).

5.2 Ternary paste systems

It can be seen that all ternary paste systems investigated, demonstrated reduction in calcium hydroxide as compared to that of plain OPC control mix (Figure 3). The inclusion of silica fume content reduced the calcium hydroxide content as early as 1 day. It is evident from this figure that calcium hydroxide content decreased with an increase in both fly ash and silica fume contents. However, the rate of decrease in calcium hydroxide content is more due to silica fume as compared to fly ash. All fly ash mixes containing 5% silica fume resembled the paste mixes containing only fly ash (Figure 2b) in that calcium hydroxide content rapidly increased at 3 days, and then decreased gradually. This is associated with the dominance of fly ash in these paste systems as compared to silica fume.

The paste systems containing fly ash along with 10 and 15% silica fume contents demonstrated the significant influence of silica fume. In these systems, at first calcium hydroxide content increases up to 3 days, which resembled both binary blended systems containing silica fume and fly ash of their own. Secondly, the calcium hydroxide content is much lower in silica fume paste than in fly ash pastes, indicating the influence of silica fume. It can be seen from the results obtained in this investigation that the combination of fly ash and silica fume does not consume as much as the sum consumed by these materials acting alone. This suggests a retarded pozzolanic reaction of silica fume with the calcium hydroxide in the presence of fly ash. This retardation may be associated with the reduction in the pH value at early ages and the competition between the two pozzolans for lime which reduces the availability of lime in the vicinity of individual pozzolan particles [7].
Figure 2: CH content of binary paste systems
(a) 1, 3, 7, 28, 90 and 180 days (b) 1, 3, 7 and 28 days.
Figure 3: CH content of ternary blended paste systems
(a) 1, 3, 7, 28, 90 and 180 days
(b) 1, 3, 7 and 28 days.
6. ARTIFICIAL NEURAL NETWORK SOLUTION

In this investigation, ANN based on the radial basis function (RBF) have been used [8]. The network developed in this investigation has eight units in the input layer and two units in the output layer. The experimentally obtained data have been divided into two sets, one for the network learning called learning set, and the other for testing the network called testing set. Each set is composed of dozens of pairs of input vectors and output vectors (vectors in the input layer called input vectors, and in the output layer called output vectors). An input vector consists of 8 components which influence the output vector, CH content (Figure 4).

The predicted values obtained using ANN for the CH content been plotted against their respective experimentally obtained values as shown in Figure 5. It can be seen from this figure that there is a good correlation between experimental values and those predicted using ANN. Therefore, it is possible to predict the hydration (CH content) of cement paste systems using artificial neural networks.

7. CONCLUSIONS

In OPC-fly ash systems the CH content increased up to 3 days beyond which it gradually decreased and the reduction was greater for higher fly ash contents. This is associated with the pozzolanic reaction of fly ash.

Silica fume reduced the CH content in the paste as early as 1 day and the reduction is associated with the silica fume dosage. Most of the silica fume reacted before 7 days.

The reduction in early-age hydration as a result of fly ash incorporation in binary systems is reversed with the addition of 10% silica fume. All ternary blended paste systems investigated exhibited lower CH content in comparison to their respective blended pastes.

Based on the experimentally obtained results, ANN has been used to establish its applicability for the prediction of the hydration of paste. It was demonstrated that the hydration progress can be predicted using ANN.

\[ x_1(t) \]
\[ x_2(t) \]
\[ x_3(t) \]
\[ x_4(t) \]
\[ x_5(t) \]
\[ x_6(t) \]
\[ x_7(t) \]
\[ x_8(t) \]

\[ x_1 = \text{Cement (kg/m}^3\text{)}; \quad x_2 = \text{fly ash (kg/m}^3\text{)}; \quad x_3 = \text{silica fume (kg/m}^3\text{)}; \quad x_4 = \text{water (kg/m}^3\text{)}; \]
\[ x_5 = \text{superplasticizer (kg/m}^3\text{)}; \quad x_6 = \text{fine agg. (kg/m}^3\text{)}; \quad x_7 = \text{coarse agg. (kg/m}^3\text{)}; \quad x_8 = \text{age (days)} \]

Figure 4: Schematic diagram of ANN solution
REFERENCES


