Artificial Neural Network for forecasting the Initial Setting Time of Cement Pastes

M. A. Abubakar*, A.S. Maihula¹, M.B. Jibril², A. Bashir³

*Department of Civil Engineering, Ministry of Works, Housing & Transport, Kano State, Nigeria ¹Department of Civil Engineering, Kano University of Science and Technology, Wudil, Kano. Nigeria ³Department of Civil Engineering, Sharda University G. Noida, India

Abstract

The most crucial element in cement and concrete behavior is the setting time of the cement paste; it states essential information in producing the final concrete products. In this study, Neural Network (N.N.) was applied to predict the initial setting time of the cement paste. 206 cases were collected from 14 published works of literature. The inputs selected are based on their significant effect on the setting time. The inputs are cementitious materials (slag, fly ash, and silica fume), cement's oxide (CaO, Al₂O₃, SiO₂& $Fe_2O_3),$ water-to-cement ratio, environmental fineness condition (Temperature), of cement, superplasticizer, and cement content. The performances of the model were assessed from R^2 and RMSE, and the results show a higher accuracy of 0.8949 (%).

Keywords – *NN*, cement paste setting, *R*²,*RMSE*

I. INTRODUCTION

The essential factors in cement and concrete studies that describe the performance and the stages of cement paste from the earliest starting point of mixing to the beginning stage of hardening are setting time and hydration reaction, which occur concurrently[1]. The setting is described as the solidification of the cement paste[2]. It indicates a change from a fluid to a solid-state with rising or fall in Temperature, thus having a thick paste. Setting mainly occurred through selective hydration of C₃A and C₃S accompanied by a high exothermic reaction in the cement paste. Hydration is described as the reaction that happens instantly after the cement powder comes in contact with water with the development of heat [3]. There are two forms of setting time in cement paste and concrete: the initial and final setting time. Initial setting time is the period between the time of cement mixing furthermore, time at which 1 mm square area needle cannot pierce or make an impression on the paste, placed in the Vicat's mold 5 mm to 7 mm from the base of the mold, or the

period the cement can no longer be adequately mixed. 45 minutes is the minimum time of initial set as prescribed by BS EN 197-1 for cement of strength classes 52.5 N and 62.5 N, whereas 60 minutes applies to strength classes of 32.5 N & R and 42.5 N & R [4]. The final setting time is when the time of blending and when a 1 mm needle establishes an impression on the mortar yet does not establish any impression or the time the cement starts to sustain some loads. 10 hours is the maximum time for a final setting time as prescribed by British standards, which is the same as that of the American Standards [1], [5].

The inability of the linear methods to withstand the interactions and processes in cement paste that is taking place. Alternatively, a nonlinear Artificial Neural Network is paramount and performs a vital role in imitating complex and indirect procedures [6]. Consequently, for sparing time, material, and labor, Artificial Neural Networks (ANN) is taken to generate models, with the aim that the information taken from these neural system models can be used to predict any cement mix. ANN has been considered as an effective system for establishing and predicting dynamic designing frameworks in civil engineerings, such as structural, water demand prediction, prediction of the strength of concrete.[7]. [5]evaluated the effects of using cementitious materials of Portland cement by considering blends of binary, ternary, and quaternary binders on the initial and final setting time of Selfcompacting concrete (SCC). Fly ash (F.A.), Silica fume (S.F.), Metakaoline (M.K.), Ground granulated blast furnace slag (GGBS) were the blended cementitious materials used. Backpropagation neural network (BPNN) was trained from 65 experimental cases, using Levenberg Marquart and conjugate gradient as the learning algorithm. The network was trained on 77:23 train/test ratio without validation correlation coefficient (R), and mean square error (MSE) was used to validate the network performance. 0.9999 is the R-value for both the initial & final

setting times, while 0.000212 and 0.000454 are the MSE values obtained for initial and final sets respectively. The conclusion for the reliability of the network was based on the high correlation coefficient and lower mean square error values recorded. [8] uses 250 datasets to predict the initial setting time of selfcompacting concrete using an Artificial neural network (ANN) considering 6 input parameters. Several neurons in the hidden layer, the coefficient for learning rate were considered, and the outcomes were validated using a free validation set. The outcome of the present study showed that ANN has substantial potential as a possible apparatus for predicting the setting time of cement. This is to employ the various input variable in predicting the initial setting time of cement paste.

II. MATERIALS AND METHODS

A. Data Selection and Use

In this study, a total data of 206 instances obtained from 13 different respected published

experimental works[9]–[24] were collected and used in the study. The data set for each sample case is analyzed. As a result, 12 input parameters (Cao, Al_2O_3 , Fe_2O_3 , SiO_2 , cement content, w/c, Temperature, superplasticizer, cementitious material content, slag, fly ash, silica fume) are selected due to their influence on setting time of cement paste. These data set were normalized between the range of 0 and 1.

B. Statistical and Correlation Analysis of the Data

For this study, some essential descriptive statistic was employed to analyze the general data used in this work. Table 2.1 shows the statistical analysis of data. On the other hand, correlation analysis was also performed to determine the linear relationship between the parameters. The effect of correlation is to reduce the range of uncertainty. The prediction based on correlation analysis is likely to be more variable and near to reality. Table 2.2 shows the Pearson correlation between the input and output parameters.

Parameters	Mean	Mode	Standard Deviation	Minimum	Maximum
CaO	61.02947	62.58	5.11821	45.03	66.71
Al ₂ O ₃	5.686893	5.31	1.252617	4.47	9.83
Fe ₂ O ₃	3.10	4.04	1.078413	0	4.04
SiO ₂	21.77	20.25	3.643145	16.85	33.06

Table 2.2. Correlation Analysis between the parameters						
W/C (%)	0.392454	0.32	0.165153	0.21	1	
C C (kg/m ³)	463.28	400	443.5658	70	2380	
C F (cm ² /g)	1447.71	326	1670.71	0	4963	
Temp. (°c)	29.65	22	17.55143	20	120	
SP (%)	2.59	0	3.426134	0	12	
Slag (%)	28.26019	0	62.41858	0	330	
Fly ash (%)	41.43883	0	116.1514	0	1015	
SF (%)	9.687379	0	20.68489	0	82.5	
C M F (cm ² /g)	3748.607	0	7788.954	0	21785	
IST (mins)	295.6432	300	180.9466	25	1105	

C. Model Input Combination and Selections

One of the significant challenges in nonlinear modeling systems is selecting the essential input variables from all possible input variables [25]. From a modeling perspective, incorporating only the essential variables into a model provides a more straightforward, more useful, and more reliable model; the model will also be more practical to apply because fewer variables need to be measured. From a control perspective, understanding the relative importance of variables allows the process control engineers to focus their efforts on the variables that matter, eliminating the time and cost involved in controlling and finding good set-points for unimportant variables [25]. Even when a good criterion exists for model selection, there is no guarantee that a model based on a given set of variables is optimal unless all possible combinations of variables have been explored. For this research work, 12 model input combinations were considered for the ANN model to predict the setting time of cement paste. Table 2.2 justify the reasons of combining and selecting different models base on the high strength and degree of correlation coefficient between the variables. Table 2.3 present the different input combinations used in this study.

Tuble Lief Model input combination	
Input combination	Output
	-
CaO, Al ₂ O ₃	IST-1
CaO, Al ₂ O ₃ , Fe ₂ O ₃	IST-2
CaO, Al ₂ O ₃ , Fe ₂ O ₃ , SiO ₂	IST-3
CaO, Al ₂ O ₃ , Fe ₂ O ₃ , SiO ₂ , w/c	IST-4
CaO, Al ₂ O ₃ , Fe ₂ O ₃ , SiO ₂ , w/c, cement content	IST-5
CaO, Al ₂ O ₃ , Fe ₂ O ₃ , SiO ₂ , w/c, cement content, cement fineness	IST-6
CaO, Al ₂ O ₃ , Fe ₂ O ₃ , SiO ₂ , w/c, cement content, cement fineness, Temperature	IST-7
CaO, Al ₂ O ₃ , Fe ₂ O ₃ , SiO ₂ , w/c, cement content, cement fineness, Temperature, superplasticizer	IST-8
CaO, Al ₂ O ₃ , Fe ₂ O ₃ , SiO ₂ , w/c, cement content, cement fineness, Temperature, superplasticizer,	IST-9
slag	
CaO, Al ₂ O ₃ , Fe ₂ O ₃ , SiO ₂ , w/c, cement content, cement fineness, Temperature, superplasticizer,	IST-10
slag, fly ash	
CaO, Al ₂ O ₃ , Fe ₂ O ₃ , SiO ₂ , w/c, cement content, cement fineness, Temperature, superplasticizer,	IST-11
slag, fly ash, silica fume	
CaO, Al ₂ O ₃ , Fe ₂ O ₃ , SiO ₂ , w/c, cement content, cement fineness, Temperature, superplasticizer,	IST-12
slag, fly ash, silica fume, cementitious material fineness	
	Input combination CaO, Al ₂ O ₃ CaO, Al ₂ O ₃ , Fe ₂ O ₃ CaO, Al ₂ O ₃ , Fe ₂ O ₃ , SiO ₂ CaO, Al ₂ O ₃ , Fe ₂ O ₃ , SiO ₂ , w/c CaO, Al ₂ O ₃ , Fe ₂ O ₃ , SiO ₂ , w/c CaO, Al ₂ O ₃ , Fe ₂ O ₃ , SiO ₂ , w/c, cement content CaO, Al ₂ O ₃ , Fe ₂ O ₃ , SiO ₂ , w/c, cement content, cement fineness CaO, Al ₂ O ₃ , Fe ₂ O ₃ , SiO ₂ , w/c, cement content, cement fineness, Temperature CaO, Al ₂ O ₃ , Fe ₂ O ₃ , SiO ₂ , w/c, cement content, cement fineness, Temperature, superplasticizer CaO, Al ₂ O ₃ , Fe ₂ O ₃ , SiO ₂ , w/c, cement content, cement fineness, Temperature, superplasticizer, slag CaO, Al ₂ O ₃ , Fe ₂ O ₃ , SiO ₂ , w/c, cement content, cement fineness, Temperature, superplasticizer, slag, fly ash CaO, Al ₂ O ₃ , Fe ₂ O ₃ , SiO ₂ , w/c, cement content, cement fineness, Temperature, superplasticizer, slag, fly ash, silica fume CaO, Al ₂ O ₃ , Fe ₂ O ₃ , SiO ₂ , w/c, cement content, cement fineness, Temperature, superplasticizer, slag, fly ash, silica fume

Table 2.3. Model input combination

D. Neural Network Training

For a neural network to produce the desired output as approximately as the target output, training needs to undergo [26]. Network training is a process by which the connection weights and biases of the ANN are adapted through a continuous process of simulation by the environment in which the network is embedded. The primary goal of training is to minimize an error function by searching for a set of connection strengths and biases that causes the ANN to produce equal or close to targets [25]. However, each layer comprises neurons interconnected with others by weights; an activation function is introduced in each neuron to convert the linear function to non-linear function, which is a mathematical function. This function is applied to process neurons and defined how that neuron is activated, defined in equation (1), which is a continuing nonlinear exponential function that switches between 0 and 1 gradually [27], [28].

$$f(x) = \frac{1}{1 + e^{-x}}$$
 (1)

In this study, the multilayer perceptron model is trained by the algorithms Lavenberg-Marquardt

techniques due to its outstanding performance in other literature on cement and concrete [26]. To employ ANN model for estimating the initial setting time of cement paste, the FFNN method and Back Propagation error algorithm were used in which the training and testing were categorized into seventy percent (70%) and thirty percent (30%), respectively. Fig 1 shows the diagram of the backpropagation neural network.



Fig. 1: Structure of ANN with backpropagation
[6]

E. Performance Criteria of the Model

The criteria used to determine the efficiency and performance of the model development depend on the specific problems, the statistical performance evaluation used are Determination coefficient (D.C. or R^2) and the root means square error (RMSE) [29]. The RMSE and R^2 show the differences between the measured and computed values; for the best network, both the D.C. and RMSE value should be high in training and validation; the higher D.C., the lower the RMSE under normal condition. The following equations (2) and (3) are used in determining the parameters [29], [30], [31], [32].

$$R^{2} = DC = 1 - \frac{\sum_{i=1}^{N} (s_{i} - \hat{s}_{i})^{2}}{\sum_{i=1}^{N} (s_{i} - \bar{s})^{2}}$$
(2)

RMSE =
$$\sqrt{\frac{\sum_{i=1}^{N} (S_i - \hat{S}_i)^2}{N}}$$
 (3)

Where; N = number of data used

<u></u> S , =		average observed data		
Ŝ _i ,	=	model computed value		
S _i	=	observed value		

III. RESULTS AND DISCUSSIONS

In this study, total data of 206 instances obtained from 13 different respected published experimental works were used. 12 input parameters (Cao, Al₂O₃, Fe₂O₃, SiO₂, cement content, cement fineness, w/c, Temperature, superplasticizer, cementitious material fineness, slag, fly ash, silica fume) are selected due to their effect on setting time of cement paste.

The artificial Neural Network (ANN) model was adopted to predict the initial setting time of cement pastes as the target value. In the ANN model, the data were divided into two subsets of training and test, and the initial setting time of the cement paste was predicted based on these two subsets.

The ANN was performed in the MATLAB software environment. After that, the performance of the ANN model in predicting the initial setting time of the cement paste was evaluated. The performance criteria for the results are chosen as the coefficient of determination (R^2) and Root Mean Square Error (RMSE).

Subsequently, the correlation and statistical analysis were carried out, as indicated in Table 2.1 and 2.2. From the correlation table, the bold marked

the less correlation between the parameters, which are very few in the table.

The table also indicated that S.P. (%) has a high correlation with IST, followed by $CC(kg/m^3)$, Al_2O_3 , SiO_2 , CaO, Fe_2O_3 , Slag, CMF, Fly ash, w/c, and Temperature.

Table 3.1	. Perfor	mance	Efficiency	of	ANN	70/30

Model						
Model	Training R ²	RMSE	Testing R ²	RMSE		
M-1	0.7202	0.1463	0.6063	0.2170		
M-2	0.7440	0.1399	0.2733	0.2123		
M-3	0.8148	0.1190	0.7240	0.2131		
M-4	0.8161	0.1186	0.7536	0.2103		
M-5	0.7804	0.1296	0.7162	0.2148		
M-6	0.8035	0.1226	0.7505	0.2174		
M-7	0.8831	0.0945	0.8079	0.1725		
M-8	0.8937	0.0902	0.7104	0.1662		
M-9	0.8949	0.0897	0.8406	0.1573		
M-10	0.8872	0.0929	0.7189	0.1637		
M-11	0.8416	0.1101	0.6994	0.1693		
M-12	0.8434	0.1094	0.7130	0.1655		



Fig. 5.7: Bar chart for the coefficient of D.C. and RMSE for both testing and verification

IV. CONCLUSION AND RECOMMENDATION

The objective of this study was to apply data-driven models, i.e., an artificial neural network model for prediction of initial setting time of cement paste. The modeling was carried out for the data from the published experimental works using ANN. Results demonstrated that an Artificial neural network showed good performance in the training and testing steps. Hence, it can be concluded that the ANN model is a suitable model for predicting the initial setting time for cement paste. Therefore, using the ANN model, the initial setting time of cement paste can be predicted accurately and efficiently. Therefore, it is recommended that the ANN model should be combining with other soft computing tools or algorithms to increase the efficiency performances in the prediction of setting time of cement paste.

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