Prediction of Expansion due to Sulfate of Ground Bottom Ash Mortar by an Artificial Neural Network

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Abstract. *This paper presents the application of the artificial neural network model (ANN) to predict the expansion of ground bottom ash mortar due to sodium sulfate. Portland cement type I was replaced by ground bottom ash at ratios of 0, 10, 20, 30, 40, 50 and 60 percent by weight of binder. The expansion of mortar which immersed in 5% sodium sulfate at various ages was measured. To show the efficiency of the proposed model, the prediction results of the ANN model are compared with the multiple linear regression (MLR) and the multiple second order polynomial regression (MSPR) models through statistical values. From the prediction results, it was found that the ANN model has a very high expansion prediction accuracy and more effective than the MLR and MSPR. The ANN model has a statistical value of absolute variance higher than 0.99. Therefore, it is concluded that the ANN model has a strong prediction capability of expansion due to sulfate of ground bottom ash mortar.*

Keywords:

prediction, expansion of mortar, ground bottom ash mortar, sodium

1. Introduction

Artificial intelligence systems such as artificial neural network (ANN) models have become very popular in civil engineering applications. This is because it is an algorithm that has the outstanding ability to predict experimental results very accurately. For example, Seung-Chang Lee [1] and Lin & Wu [2] used ANN to predict the strength of concrete. The results showed that ANN can predict better than traditional methods. Tuntisukrarom & Cheerarot [3] predict the compressive strength behavior of ground bottom ash concrete by ANN. The results show that ANN can effectively predict the behavior of parameters that affecting the compressive strength. Khan et al. [4] study the use of ANN model by available Levenberg-Marquardt Backpropagation (LMBP) for training algorithm to predict the compressive strength of concrete with normal strength and high strength. The results showed that the ANN model can propose the accurately prediction of compressive strength. Vellaipandian et al. [5] used ANN to predict the concrete compressive strength of high strength concrete. The results showed that the values obtained from ANN close to the experimental value (R^2=0.95). Moreover, the ANN models have also been extended to predict concrete properties, for example, Topçu & Sarıdemir [6] predicted the mechanical properties consisting of compressive strength and split tensile strength of recycled aggregate concrete with silica fume. The results showed that the ANN model had a strong potential to predict the mechanical properties of recycled aggregate concrete containing silica fume. Yu et al. [7] predicted the compressive strength, flexural strength, and tensile strength of concrete with metakaolin (MK) and silica fume (SF) under hydrochloric acid corrosion using the ANN model. The prediction results show that the ANN model has great potential to predict the mechanical properties of concrete with MK and SF. Mohamed et al. [8] used ANN to predict chloride permeability and compressive strength of concrete. The results of the experiment showed that the ANN model have the ability to predict at an acceptable level. Sahoo & Mahapatra [9] used the ANN model to predict the compressive strength of fly ash concrete due to long-term sulfate attack. The results showed that the predicted data and the experimental data were similar. Inthata et al. [10] used the ANN model to predict the chloride penetration of concrete with pozzolanic materials. It found that the ANN model has ability to learn and practice datasets and be able to predict outcomes effectively.

Currently, pozzolanic materials are an important alternative to partially replace cement in concrete mixes. This is because pozzolanic materials can help improve the properties of fresh and hardened concrete. After the hydration reaction by mixing cement granules with water, a second stage of reaction called pozzolan reaction occurs, in which silicon dioxide and alumina trioxide react with calcium hydroxide. This produces a binder compound called calcium silicate hydrate (CSH) and calcium aluminate hydrate (CAH) which these compounds increase the compressive strength of concrete [3, 11]. The most popular pozzolan materials used in concrete are fly ash, silica fume, slag furnace, and bottom ash.

Bottom ash (BA) is a by-product of the combustion of powder coal in an electric power plant as same as fly ash (FA). At high temperatures, FA is melted and it agglomerates to form BA at low temperatures. All ashes are One of the major problems of all coal combustion power plants because they have effects on environment such as air pollution and groundwater quality problem due to leaching of metals from the ashes. Use of all ashes to replace cement result in decreasing both energy and CO_2 from the production of cement. This CO_2 is thought to be a major contributor to the greenhouse effect and the global warming of the planet [10]. Chaisakulkiet et al. [12] used BA as a fine and coarse aggregate in concrete. Experimental results showed an increase in the compressive strength and chloride resistance of concrete. Abdulmatin, A. et al. [13] studied the BA as pozzolan material. The results showed that BA at 20% replacement with appropriate fineness can be used as a pozzolanic material. González-Fonteboa et al. [14] also studied the replacement of cement by BA. It found that the use of BA had a higher compressive strength and better durability. Abdulmatin et al. [15] proposed an approach improve the quality of BA to be used as a pozzolan material, which studies the effects of particle size and optimal percent replacement of BA to the compressive strength and penetration of chlorides. The results show that the finer particle size provides the higher compressive strength and greater resistance to chloride ion infiltration compared to the control concrete.

In Thailand, Mae Moh thermal power plants use pulverized lignite coal as the fuel to produce electricity. FA and BA are by-products of this process. The study of the original BA from Mae Moh power plant [16-17] showed that the compressive strength of original BA mortar at the ages of 7 and 28 days were than 50% of the standard mortar. At the original status, the BA cannot be used as pozzolanic material to replace Portland cement in concrete mixtures. However, several studies [18-21] found that BA could be ground to develop the necessary properties as partial replacements of cement in concrete mixtures because the decrease in particle size of BA increases its pozzolanic activity and improves the mechanical and physical properties of concrete.

It is well known that sulfate compounds are harmful to concrete because they cause concrete to expand, resulting in reduced strength of concrete. The common sulfate compounds are usually dissolved in seawater, brackish water, or saline soil. The mechanism of destruction by sodium sulfate begins with the reaction between sodium sulfate (NS) and calcium hydroxide (CH). As shown in equation (1), sodium hydroxide (NH) causes the pH value of the cement paste to increase to 13.5, which is higher than the pH value of saturated calcium hydroxide (CH) solution, thus maintaining the stability of calcium silicate hydrate (CSH) and ettringite (C_6ASH_{32}) from reacting to become other products. Gypsum (CSH_2) obtained from equations (1) will react with some hydration reaction products such as calcium aluminate hydrate (C_4AH_{13}), monosulfate (C_4ASH_{12}) and/or the remaining tricalcium aluminate (C_3A). From the hydration reaction, secondary ettringite is obtained, as shown in equations (2) to (4). Nature ettringite has a much lower density than the products of other types of hydration reactions that causes expansion in concrete.

$$CH + N\bar{S} + 2H \rightarrow C\bar{S}H_2 + NH \tag{1}$$

$$C_4AH_{13} + 3C\bar{S}H_2 + 14H \rightarrow C_6A\bar{S}H_{32} + CH \tag{2}$$

$$C_4A\bar{S}H_{12} + 2C\bar{S}H_2 + 16H \rightarrow C_6A\bar{S}H_{32} \tag{3}$$

$$C_3A + 3C\bar{S}H_2 + 26H \rightarrow C_6A\bar{S}H_{32} \tag{4}$$

where C = CaO, N = Na_2O, $\bar{S}$ = SO_3, H = H_2O, CH = $Ca(OH)_2$, A = Al_2O_3

This paper aims to examine the ANN model to predict the expansion of the ground bottom ash mortar due to sodium sulfate. The predictive results of the presented model are compared with the multiple linear regression (MLR) and the multiple second order polynomial regression (MSPR) models. The statistical values were used to show the performance of the presented model

2. Research Method

A. Materials

In this study, ordinary Portland cement type I and BA from Mae Moh power plant in northern Thailand were used. BA was ground by a ball mill until the particle size retained on sieve No. 325 less than 5% by weight. The chemical compositions and physical properties of materials are shown in Table 1.

Table 1 Chemical composition and Physical properties [10]

Sample	OPC	GBA
Chemical composition (%)		
SiO_2	20.62	48.12
Al_2O_3	5.22	23.47
Fe_2O_3	3.10	10.55
CaO	65.00	11.65
MgO	0.91	3.45
K_2O	0.07	3.45
Na_2O	0.50	0.07
SO_3	2.70	1.76
LOI	1.13	3.41
$SiO_2 + Al_2O_3 + Fe_2O_3$	-	82.14
Specific gravity	3.13	2.70
Retaining on a sieve No.325 (%)	13.21	4.90
Blaine fineness (cm^2/g)	3,270	6,250
Median particle size (μm)	13.0	10.5

Note: OPC = Ordinary Portland cement, GBA = Ground bottom ash

B. Mix proportions

A ratio of binder material to sand was set at a constant of 1 to 2.75 by weight and maintained flow of mortar between 105-115 to cast mortar in accordance with ASTM C 109. Portland cement type I was replaced by GBA at the rate of 0, 10, 20, 30, 40, 50, and 60% by weight of binder material. All specimens were removed from the mold after casting 24 hours and were immersed in sodium sulfate solution at a concentration of 5.0% by weight and measure the expansion of the mortar at the age of 1, 7, 14, 60, 120, 180, 240, 300, 360, 420, 480, 540, 600, 660, 720, and 780 days.

3. Artificial Neural Network

Artificial Neural Network (ANN) is a type of computational system created from a large number of processors. This is based on mimicking the behavior of neural cell networks in the human brain. The neural network may not be the same as the entire neural cell network in the human brain, but it also has a loop in the human brain. The general architecture of the ANN model is shown in Figure 1. It consists of 3 important parts: input layer, hidden layer, and output layer.

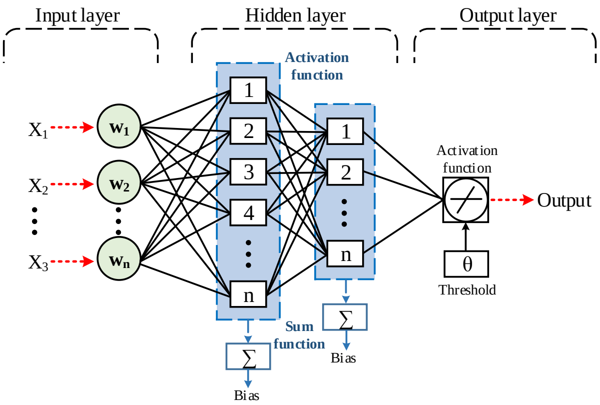


Fig. 1 The ANN architecture

A. The ANN architecture design

The synthesis of neural network models in this research uses a tool called Neural network toolbox which is available in the MATLAB program to predict the effect of expansion due to the sulfate solution of the ground bottom ash mortar, the procedure is as follows:

- For training and testing models, there are two variables of cement replacement rate and test age were used as data inputs (Input variable) in matrix form. They prepare variable data for import data and target data or experimental results (Output variable).
- The number of variables for the input data must be defined. Data output and number of hidden layers, with each hidden layer having to determine the number of neural (training cells). In this research, the synthesis structure of the neural network model to determine the optimal form of synthesis is defined as shown in Table 2 and 3. It shows that there are 120 models in total. Log-sigmoid, tan-sigmoid, and purelin linear activation functions were used to evaluate the performance against [3]. Levenberg-marquardt (LM), Resilient backpropagation (RP), and Bayesian regularisation (BR) learning algorithms were used to perform the training process for the ANN model in the MATLAB software. Meanwhile, the network performance function of the sum squared error (SSE) was measured to search the best technique based on the statistic value to minimize error between the actual output and the target output.

Table 2 The adjustment parameters used in the ANN models

Adjustment parameters	Quantity
Number of input layer (neuron)	2
Number of output layer (neuron)	1
Number of hidden layer (layer)	2
Number of neurons in the first hidden layer	4, 5, 6, 7, 8
Number of neurons in the second hidden layer	1, 2
Activation function in hidden layer	Log sigmoid, Tan sigmoid
Activation function in output layer	Purelin linear
Learning algorithm	lm, rp, br
Network's performance function	sse
Learning epochs	10000

B. Evaluation of model performance

To evaluate the performance of the ANN model, the following statistical methods are used.

- Absolute fraction of variance (R^2) determine the discrepancy between the data set used in learning and the data set used in the test, expressed in the absolute value of the decimal proportion of the total variance, which can be calculated from the equation (5).

$$R^2 = 1 - \frac{\sum_j (P_j - T_j)^2}{\sum_j (T_j)^2} \quad (5)$$

- Root mean square error (RMSE) is an assessment of the difference between data sets that are the primary variables (Experimental datasets) and dependent variables (Predictive datasets). The resulting unit is the same as the original variable, which can be calculated from the equation (6).

$$RMSE = \sqrt{\frac{1}{n}\sum_j (P_j - T_j)^2} \quad (6)$$

- Mean absolute percentage error (MAPE) is an assessment of the difference between the primary and dependent variable data sets, where the resulting units are in the form of percentages, so the difference between data sets that do not necessarily have the same units can be determined. This can be calculated from the equation (7).

$$MAPE = \frac{100}{n}\sum_j \left(\frac{T_j - P_j}{T_j}\right) \quad (7)$$

where P is the value prediction of j^{th} pattern, T is the actual value of j^{th} pattern, and n is the number of patterns.

Table 3 ANN models studied in this work

Number	Number of neurons in the 1st hidden layer	Number of neurons in the 2nd hidden layer	Activation function in 1st hidden layer	Activation function in 2nd hidden layer	Learning algorithm	ANN Model
1	4	1	log	log	lm	4-1-log-log-lm
2	4	1	log	tan	lm	4-1-log-tan-lm
3	4	1	tan	log	lm	4-1-tan-log-lm
…	…	…	…	…	…	…
119	8	2	tan	tan	rp	8-2-tan-tan-rp
120	8	2	tan	tan	br	8-2-tan-tan-br

4. Results and discussion

A. Expansion of the mortar in sulfate solution

The expansion of ground bottom ash mortar immersed in sodium sulfate solution at a concentration of 5.0% by weight is shown in figure 2. It shows the relationship between the percentage expansion of the mortar that replaced cement with at the rate of 0, 10, 20, 30, 40, 50, and 60% (PR0, PR10, PR20, PR30, PR40, PR50, and PR60), and the age of the mortar. From the figure, it can be seen that at early age, mortar without ground bottom ash (PR0) has increased slowly expansion and then expands rapidly at final age. The mortar PR0 soaked in sodium sulfate solution at the age of 780 days had an expansion about 4%.

For ground bottom ash mortars, they were found that the use of ground bottom ash gave a reduced expansion value as shown in Figure 2, because finely ground bottom ash can perform the pozzolanic reaction well. It can also reduce the amount of calcium hydroxide and C_3A by reducing the amount of cement [16]. Mortar mixed with the higher percent replacement of pozzolanic materials has lower expansion than that with the lower one. This result is similar to the other studies [16-17], which used GBA to replace Portland cement. They found that when the GBA has high fineness, at later age, the concretes with higher percent replacement of GBA produce higher compressive strength than those with lower replacement and the control concretes [13-16]. The mortar PR60 immersed in sodium sulfate solution at the age of 780 days had an expansion about 2% which less than the mortar PR0 about 2 times. The experiment shows that the percent replacement of GBA are important factors that affect the expansion of mortar. From the result, it can be concluded that ground bottom ash is a good pozzolanic material for sulfate resistant. By replacing 60%, the maximum sulfate resistance is achieved.

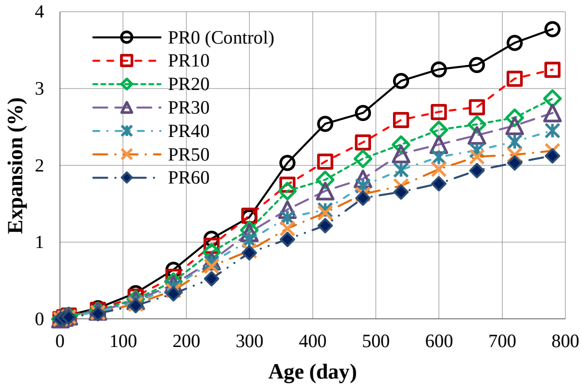
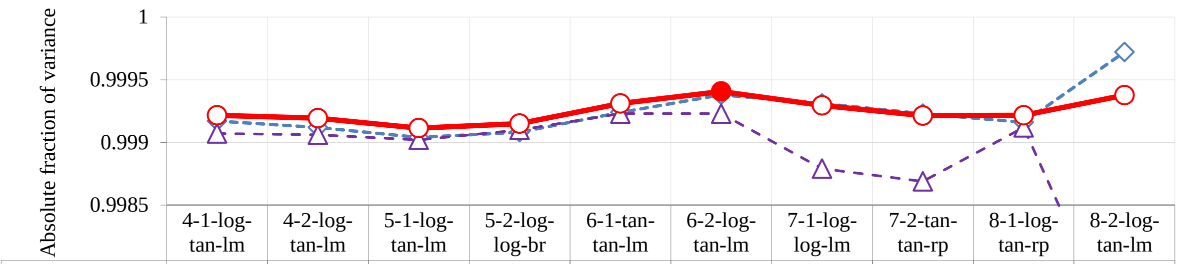


Fig. 2 Expansion of ground bottom ash mortars

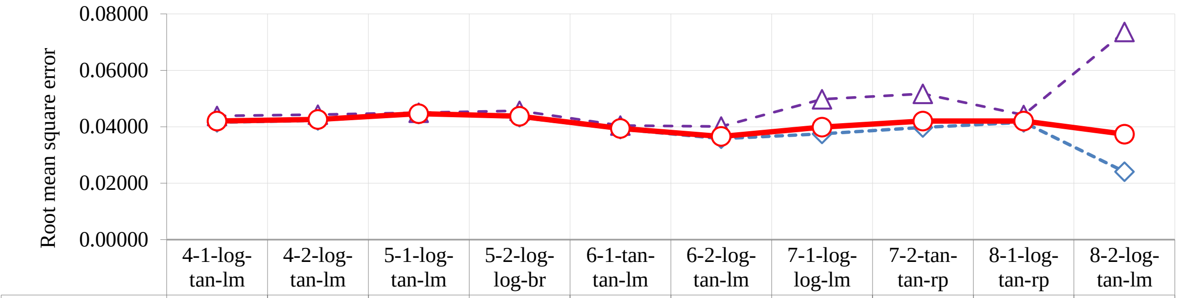
B. Synthesis of neural network models

In this study, 80% and 20% of the experimental dataset were randomly selected and used to train and test the model, respectively. The optimal ANN model is selected from the best of statistical value of the absolute fraction of variance (R^2), root mean square error (RMSE) and mean absolute percentage error (MAPE). All statistical values of the ANN models are shown in figures 3 to 5. The results indicate that the optimal ANN model is ANN-6-2-log-tan-lm model, which has two hidden layers with 6 neurons in the first hidden layer and 1 neuron in the second hidden layer, the log-sigmoid and tan-sigmoid activation functions in the first and second hidden layers, respectively. A high-accuracy predictive model with acceptable error



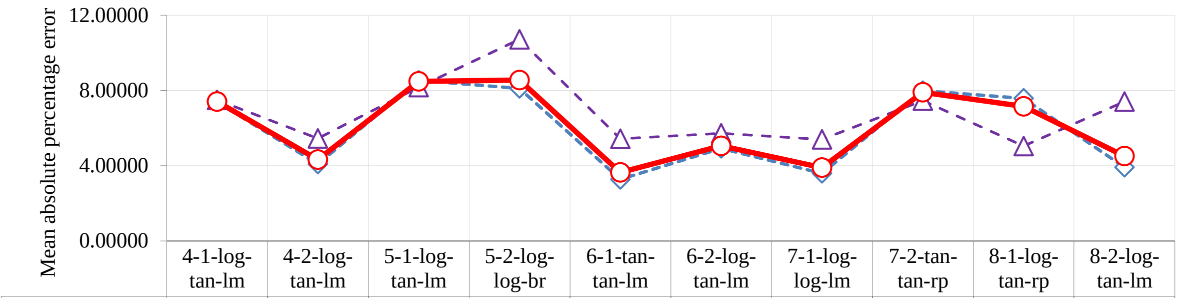
	4-1-log-tan-lm	4-2-log-tan-lm	5-1-log-tan-lm	5-2-log-log-br	6-1-tan-tan-lm	6-2-log-tan-lm	7-1-log-log-lm	7-2-tan-tan-rp	8-1-log-tan-rp	8-2-log-tan-lm
Training	0.99917	0.99912	0.99904	0.99908	0.99924	0.99938	0.99931	0.99923	0.99916	0.99972
Testing	0.99907	0.99906	0.99902	0.9991	0.99923	0.99923	0.99879	0.99869	0.99912	0.99734
Total	0.999216	0.999193	0.999114	0.999151	0.99931	0.999406	0.999294	0.999214	0.999217	0.999378

Fig. 3 The absolute fraction of variance (R^2) of the ANN models



	4-1-log-tan-lm	4-2-log-tan-lm	5-1-log-tan-lm	5-2-log-log-br	6-1-tan-tan-lm	6-2-log-tan-lm	7-1-log-log-lm	7-2-tan-tan-rp	8-1-log-tan-rp	8-2-log-tan-lm
Training	0.04162	0.04226	0.04459	0.04339	0.03922	0.03579	0.03749	0.03979	0.04158	0.02409
Testing	0.04381	0.04432	0.04494	0.04565	0.04046	0.04010	0.04976	0.05175	0.04416	0.07362
Total	0.04200	0.04261	0.04465	0.04378	0.03943	0.03656	0.03984	0.04206	0.04203	0.03744

Fig. 4 The root mean square error (RMSE) of the ANN models



	4-1-log-tan-lm	4-2-log-tan-lm	5-1-log-tan-lm	5-2-log-log-br	6-1-tan-tan-lm	6-2-log-tan-lm	7-1-log-log-lm	7-2-tan-tan-rp	8-1-log-tan-rp	8-2-log-tan-lm
Training	7.39091	4.09128	8.53569	8.10775	3.27367	4.91644	3.58580	7.98877	7.57462	3.90988
Testing	7.49092	5.44366	8.16666	10.71776	5.43051	5.71575	5.38780	7.46559	5.04494	7.40222
Total	7.40788	4.32070	8.47309	8.55052	3.63956	5.05204	3.89150	7.90001	7.14548	4.50233

Fig. 5 The mean absolute percentage error (MAPE) of the ANN models

is obtained, where the statistical values of R^2, RMSE and MAPE are 0.99938, 0.03579, 4.91644, respectively, for the training dataset and 0.99923, 0.04010, 5.71575, respectively, for the testing dataset and 0.999406, 0.03656, 5.05204, respectively, for total dataset. Equation for predicting of the optimal ANN model is shown as equation (8) to (10).

Table 4 shows the weight values and bias vectors of the optimal ANN model. At the beginning, the sum of the weights of the import variable is calculated with the bias value of the first hidden layer as in equation (8).

$$x(i_1) = (a_{11}(i_1) \times PR) + (a_{12}(i_1) \times AC) + bh_1(i_1) \quad (8)$$

where PR and AC are the replacement percentage and age of the mortar respectively, $a_{11}(i_1)$ and $a_{12}(i_1)$ is the weight of the import variable of the first hidden layer of the first hidden layer of the neuron, i_1 and $bh_1(i_1)$ is the bias value of the first hidden layer of the neuron that i_1 then calculates the log-sigmoid activation function of the first hidden layer as in equation (9).

$$x_2(i_2)=\left(a_{21}(i_2)\times\frac{1}{1+e^{x(1)}}\right)+\left(a_{22}(i_2)\times\frac{1}{1+e^{x(2)}}\right)$$
$$+\left(a_{23}(i_2)\times\frac{1}{1+e^{x(3)}}\right)+\left(a_{24}(i_2)\times\frac{1}{1+e^{x(4)}}\right)$$
$$+\left(a_{25}(i_2)\times\frac{1}{1+e^{x(5)}}\right)+\left(a_{26}(i_2)\times\frac{1}{1+e^{x(6)}}\right)+bh_2(i_2) \quad (9)$$

where $x(1),x(2),...,x(6)$ is the sum of the weight of the import variable with the bias value of each neuron in the first hidden layer, $a_{21}(i_2),a_{22}(i_2),...,a_{26}(i_2)$ is the weight value in the ^{2}nd hidden layer of i_2, and bh_2 is the bias value of the ^{2}nd hidden layer of i_2. Finally, the expansion of the mortar (Exp) can be calculated from the tan-sigmoid activation function of the second hidden layer, as in equation (10).

Table 4 Weight values and bias vectors of the optimal ANN model

1 st Hidden layer				2 nd Hidden layer								Output layer	
i1	Weight values		Bias	i2	Weight values						Bias	Weight	Bias
	a11	a12	bh1		a21	a22	a23	a24	a25	a26	bh2	y	bo
1	-0.36583	0.05518	-14.64170	1	0.95484	-0.47924	-56.24200	5.86203	0.15606	24.88946	25.42493	-0.79638	-13.6322
2	0.28808	-0.00403	1.17423	2	-0.00141	0.02006	1.34915	0.03504	-0.00332	-0.68790	-1.11726	-34.61090	
3	0.01596	-0.00170	4.31336										
4	0.00931	-0.01122	3.95133										
5	-9.72170	0.49948	28.19837										
6	1.47099	0.03275	3.30107										

$$Exp=\sum_{i_2=1}^{2}\left(y(i_2)\times\left(\frac{2}{1+e^{-2(x_2(i_2))}}-1\right)\right)+b_o \quad (10)$$

where $x_2(i_2)$ is the log-sigmoid activation function of the first hidden layer, $y(i_2)$ is weight of the output layer and b_o is the bias value of the output layer.

C. Comparison of performance

The multiple linear regression (MLR) and the multiple second order polynomial regression (MSPR) models are shown in equation (11) and (12), respectively. From the prediction results, it was found that the MLR and MSPR models give the statistical values of R^2, RMSE and MAPE of 0.973060, 0.24497, 141.04111 and 0.991748, 0.13612, 63.89480, respectively. To show the efficiency of the proposed model, the prediction results of the optimal ANN model are compared with the multiple linear regression (MLR) and the multiple second order polynomial regression (MSPR) models through statistical values. From the prediction results, it was found that the ANN model has a very high expansion prediction accuracy and more effective than the MLR and MSPR as shown in figure 6. This is consistent with past research that found ANN model to be more accurate than the regression models [22-26]. The ANN model has a statistical value of absolute variance higher than 0.99. Therefore, it is concluded that the ANN model has a strong prediction capability of expansion due to sulfate of ground bottom ash mortar.

$$Exp = 0.327294 - 0.01233(PR) + 0.003883(AC) \quad (11)$$

$$Exp = -0.06785 - 0.00755(PR) + 0.00577(AC))$$
$$+0.000139(PR^2) - 0.000001(AC^2)$$
$$-0.000038(AC)(PR) \quad (12)$$

When PR and AC is the replacement percentage and age of the mortar, respectively.

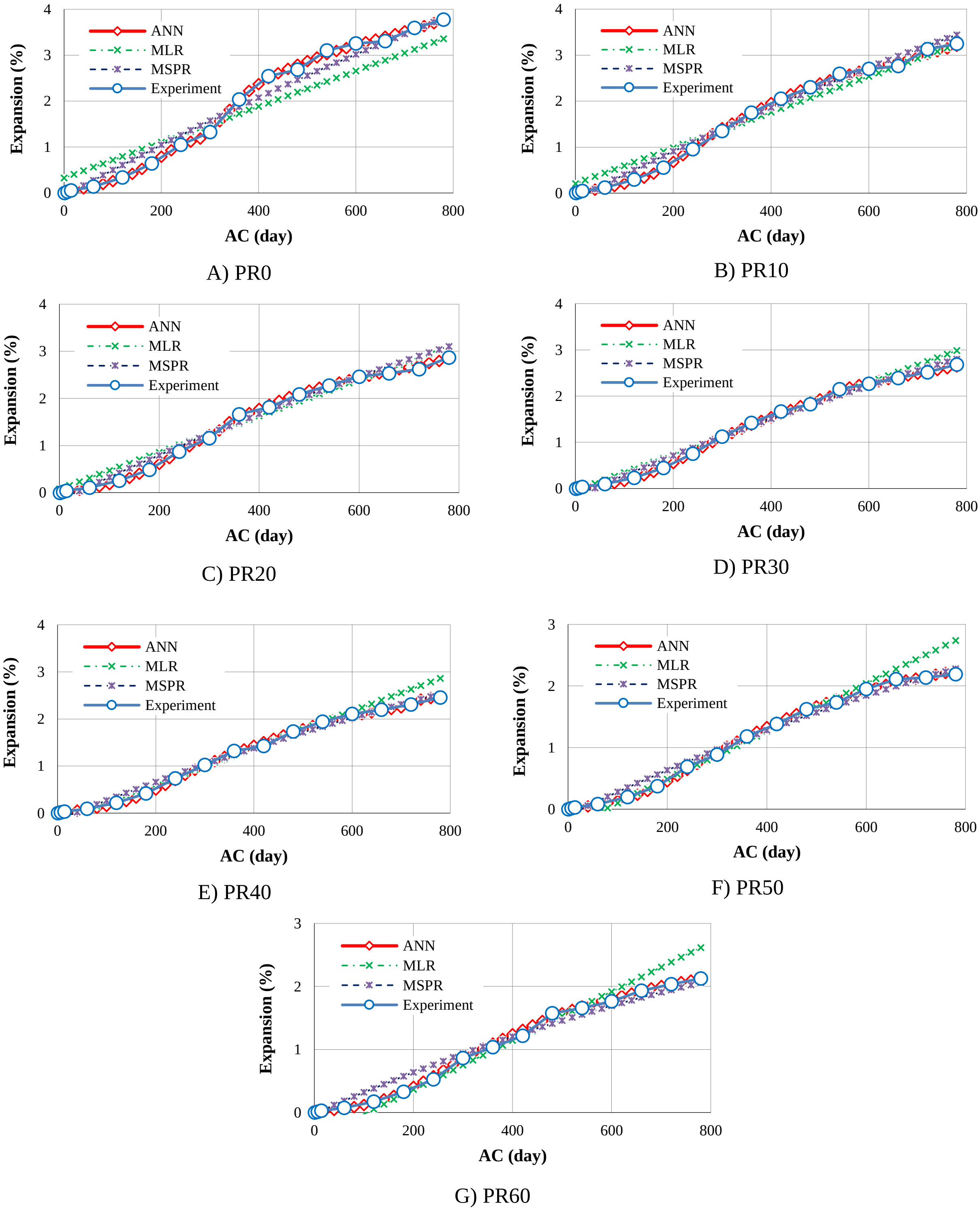


Fig. 6 Comparison among the experimental results and predictive results

5. Conclusion

From the investigation, it can be concluded that the optimal ANN model is the model architecture with two hidden layers with 6 neurons in the first hidden layer and 1 neuron in the second hidden layer which use the log-sigmoid and tan-sigmoid activation functions in the first and second hidden layers, respectively, levenberg-marquardt in the learning algorithm and sum square error in the network performance. It has a high-accuracy predictive model that the statistical values of R^2, RMSE and MAPE are 0.999406, 0.03656, 5.05204, respectively, it has a very high expansion prediction accuracy and more effective than the MLR and MSPR.

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