PREDICTION OF FREE CHLORIDE CONTENT IN CEMENT BASED MATERIALS USING ARTIFICIAL NEURAL NETWORKS

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ABSTRAK

Korosi baja tulangan merupakan suatu fenomena degradasi yang sering ditemukan pada struktur beton bertulang. Kerusakan ini terutama disebabkan adanya kandungan khlorida bebas dalam beton yang dapat merusak selaput tipis pelindung tulangan dan berlanjut dengan korosi yang terjadi pada tulangan baja tersebut. Fenomena penetrasi khlorida ke dalam beton dipengaruhi oleh banyak faktor, salah satunya adalah jenis material yang digunakan, namun hingga saat ini belum dapat ditemukan metode analisis yang tepat untuk memprediksi hubungan antara komposisi adukan beton dengan kadar khlorida bebas di dalamnya. Dalam penelitian ini diusulkan penggunaan jaringan syaraf tiruan untuk memprediksi kandungan khlorida bebas dalam pasta semen dengan berbagai jenis bahan tambah mineral. Data yang diperlukan untuk membangun jaringan syaraf tiruan diperoleh dari hasil uji laboratorium pada 70 buah sampel pasta semen dengan mengganti sebagian semen dengan bahan GGBS (20%, 40%, 60%), silica fume (5%, 10%, 15%) dan fly ash (10%, 20%, 30%) dengan menambahkan khlorida pada saat pencampuran (*internal chloride*) dengan takaran sekitar 0,1%, 0,2%, 0,3%, 0,5%, 1,0%, 1,5%, 2,0%, 2,5% dan 3,0% berdasarkan berat semen. Selanjutnya dilakukan analisis dengan jaringan syaraf tiruan menggunakan *backpropagation algorithm* dengan empat neuron input, dua *hiden layer* masing-masing terdapat empat neuron dan tiga neuron, dan dilakukan dalam 10.000 *epochs*. Hasil pengujian menunjukkan bahwa jaringan syaraf tiruan dengan arsitektur di atas mampu memberikan prediksi kandungan khlorida bebas dalam pasta semen dalam hubungannya dengan jenis bahan dasarnya dan takaran *internal chloride* yang ditambahkan dengan hasil yang baik. Hal ini ditunjukkan dengan nilai *root mean square error* (*RMS*) sebesar 0,031, *mean absolute error* (*MAE*) sebesar 0,023, nilai koefisien determinasi regresi linear (r^2) sebesar 0,9898, dan persentase rata-rata kesalahan sebesar 9,094%.

Kata Kunci :   Jaringan syaraf tiruan, khlorida bebas, *internal chloride*, pasta semen, *mineral admixtures*.

INTRODUCTION

Performance of concrete against sulfate attack, acid attack, carbonation, alkali-aggregate reaction, freezing–thawing, abrasion, etc is named as durability. Chloride-induced corrosion is recognized as a major problem with regard to the service life of reinforced concrete. It is well known that the chlorides, no matter whether added during mixing or later transported into concrete, can be bound to the hydrated products in concrete by physisorption and chemisorption. This is called chloride binding capacity of concrete. The

1

threshold chloride level for onset of chloride-induced corrosion is generally expressed by total chloride content per weight unit cement. It is apparent that chloride binding capacity of concrete has influence on the threshold chloride level, since only unbound, or free, chloride ions in pore solution can possibly destroy the passive film on the surface of the steel bar and initiate corrosion.

Nowadays facts show that many type of mineral admixtures have been widely used in concrete production based on economically reasons (lower quantity of cement required in concrete mixture), environmental (recycling waste from industrial process and saving natural resources), and also some performance reasons. Ground granulated blast furnace slag (GGBS), fly ash (FA) and silica fume (SF) are the most common mineral admixtures that widely used as concrete admixture to increase performance of concrete. According to Ha, et al (2007), fly ash could improve the permeability characteristics, increase chloride binding capacity of concrete and delayed the initial corrosion time and decrease of corrosion rate.

The theory related with chloride binding capacity of cement based materials is still not fully developed due to the complexity of the problem and the large number of parameters controlling this behavior. The prediction of the free chloride content in a mixture of cement based materials is very important for reinforced concrete long term performance, especially in reinforcement corrosion aspect. The proposed prediction method utilizes neural networks, an AI-based technique that emulates the human ability to learn from the past experience and derive quick solutions to new situations. The developed neural network based prediction model can be used by civil engineers to predict the free chloride content that closely related with corrosion initiation in reinforced concrete members. Because durability performance of concrete is influenced by many factors, this paper has been only focused on the free chloride content in various types of cement pastes. In the cement paste mixtures, admixtures to cement ratios were chosen as 20%, 40%, 60% for ground granulated blast furnace slag (GGBS), 10%, 20%, and 30% for fly ash (FA) and 5%, 10%, and 15% of silica fume (SF). In this way, the free chloride content in the cement pastes with different admixtures can be compared. Based on that reason, this paper aimed to evaluate the free chloride content in various cement paste mixtures using artificial neural network (ANN).

LITERATURE REVIEW

Chloride in Reinforced Concrete Structures

Chloride ions when present in reinforced concrete can cause very severe corrosion of the steel reinforcement. The chloride ions will eventually reach the steel and then accumulate

to beyond a certain concentration level. The protective film around the steel is destroyed and corrosion will begin when oxygen and moisture are present in the steel-concrete interface. Chlorides can originate from two main sources as follows: Chloride added to the concrete at the time of mixing, often referred to as **Internal Chloride.** This category includes calcium chloride accelerators for rapid hardening concrete, salt contaminated aggregates and the use of sea water or other saline contaminated water. Chloride ingress into the concrete from the environment often referred to as **External Chloride. T**his category includes both de-icing salt as applied to many highway structures and marine salt, either directly from sea water in structures such as piers, or in the form of air-borne salt spray in structures adjacent to the coast. The effect of chloride salts depends to some extent on the method of addition. If the chloride is added at the time of mixing, the calcium aluminate (C3A) within the cement paste will react with the chloride to some extent, chemically binding it to form calcium chloroaluminate that usually called as **bound chloride**. In this form, the chloride is insoluble in the pore fluid and is not available to take part in damaging corrosion reactions. The ability of the cement to chemically react with the chloride is however limited and depends on the type of cement. Sulphate resisting cement, for example, has a low C3A content and is therefore less able to react with the chlorides.

Experience suggests that if the chloride exceeds about 0.4% by mass of cement, the risk of corrosion increases. This does not automatically mean that concretes with chloride levels higher than this are likely to suffer severe reinforcement corrosion: this depends on the permeability of the concrete and on the depth of carbonation in relation to the cover provided to the steel reinforcement. When the concrete carbonates, by reaction with atmospheric carbon dioxide, the bound chlorides are released. In effect this provides a higher concentration of soluble chloride immediately in front of the carbonation zone. Normal diffusion processes then cause the chloride to migrate into the concrete. This process, and normal transport of chlorides caused by water soaking into the concrete surface, is responsible for the effect sometimes observed where the chloride level is low at the surface, but increases to a peak a short distance into the concrete (usually just in front of the carbonation zone). The increase in **unbound chloride** or **free chloride** means that more is available to take part in corrosion reactions, so the combined effects of carbonation and chloride are worse than either effect alone.

The depth/concentration profile for External chloride, which has penetrated hardened concrete, will show levels decreasing further from the surface. Chlorides present in the fresh concrete will tend to be evenly distributed throughout the concrete. Passivation of the steel

3

reinforcement in concrete normally occurs due to a two component system comprising a portlandite layer and a thin pH stabilized iron oxide/hydroxide film on the metal surface. When chloride ions are present, the passivity of the system is lost by dissolution of the portlandite layer, followed by debonding of the passive film. Physical processes operating inside the passive film may also contribute to its disruption. When chlorides have ingressed from an external source, particularly in conditions of saturation and low oxygen availability, insidious pitting corrosion of the reinforcement can occur, causing massive localised loss of cross section. This can occur in the early stages without disruption of the concrete underneath.

The critical chloride content required to initiate corrosion depends on whether the chloride was present at the time of mixing, or has ingressed after hardening, as discussed above. Clearly this also depends on the temperature and humidity of the concrete and also whether the concrete has carbonated. Good quality concrete can often show a remarkable tolerance for chloride without significant damage, however, at chloride contents up to about 1% by mass of cement (usually for chloride added at the time of mixing) reinforced concrete is much less tolerant of ingressed chloride.

Artificial Neural Networks (ANN)

One type of network sees the nodes as 'artificial neurons'. These are called artificial neural networks (ANNs). An artificial neuron is a computational model inspired in the natural neurons. Natural neurons receive signals through *synapses* located on the dendrites or membrane of the neuron. When the signals received are strong enough (surpass a certain *threshold*), the neuron is *activated* and emits a signal though the *axon*. This signal might be sent to another synapse, and might activate other neurons.
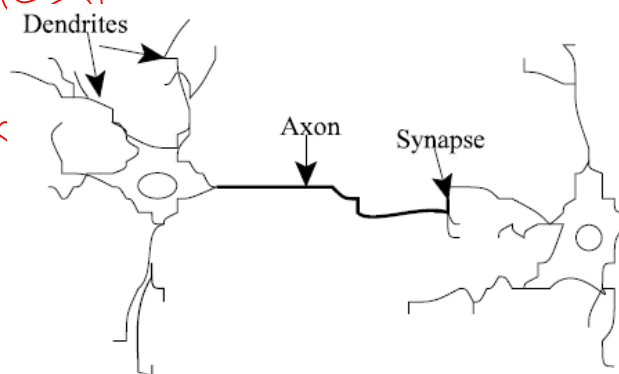

Figure 1. Biological Neural System

The complexity of real neurons is highly abstracted when modelling artificial neurons. These basically consist of *inputs* (like synapses), which are multiplied by *weights* (strength of the respective signals), and then computed by a mathematical function which determines the *activation* of the neuron. Another function (which may be the identity) computes the *output* of the artificial neuron (sometimes in dependance of a certain *threshold*). ANNs combine artificial neurons in order to process information.
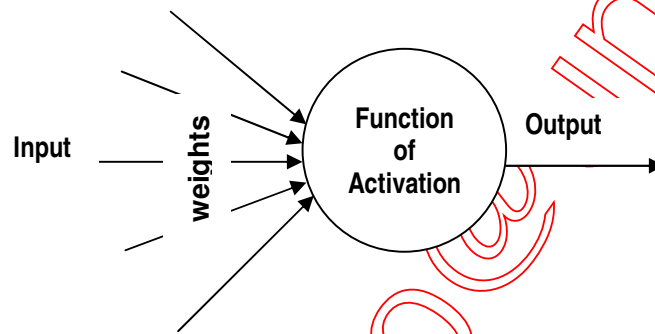

Figure 2. Working System of an Artificial Neuron

The higher a weight of an artificial neuron is, the stronger the input which is multiplied by it will be. Weights can also be negative, so we can say that the signal is *inhibited* by the negative weight. Depending on the weights, the computation of the neuron will be different. By adjusting the weights of an artificial neuron we can obtain the output we want for specific inputs. But when we have an ANN of hundreds or thousands of neurons, it would be quite complicated to find by hand all the necessary weights. But we can find algorithms which can adjust the weights of the ANN in order to obtain the desired output from the network. This process of adjusting the weights is called *learning* or *training*.

The number of types of ANN and their uses is very high. Since the first neural model by McCulloch and Pitts (1943) there have been developed hundreds of different models considered as ANN. The differences in them might be the functions, the accepted values, the topology, the learning algorithms, etc. Since the function of ANN is to process information, they are used mainly in fields related with it. There are a wide variety of ANNs that are used to model real neural networks, and study behavior and control in animals and machines, but also there are ANNs which are used for engineering purposes, such as pattern recognition, forecasting, and data compression. Applications of neural networks in civil engineering are mainly oriented toward estimating or predicting values of some particular random variable,

such as: 1) forces on structures, 2) structural damage indicators, 3) scour depth and liquefaction, and 4) concrete materials science.

In this research, ANN which learns using the backpropagation algorithm for learning the appropriate weights was used, since it is one of the most common models used in ANN, and many others are based on it.
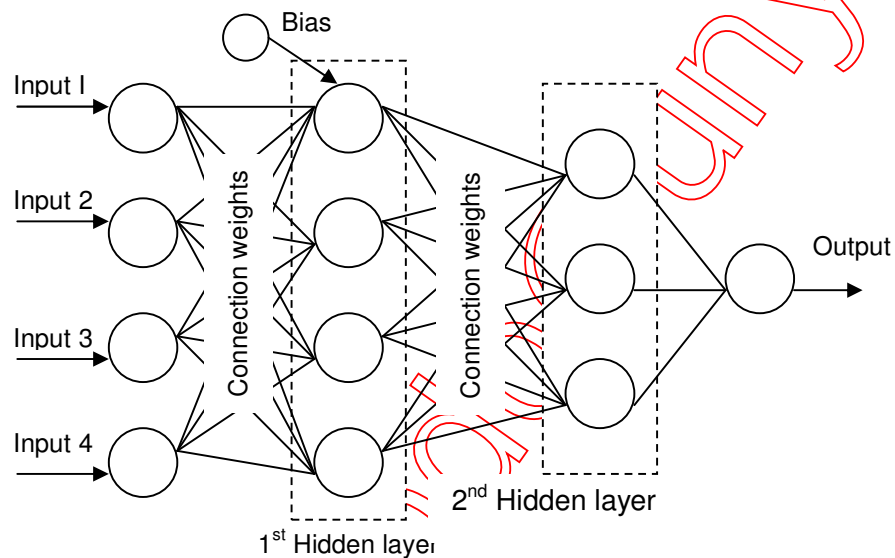

Figure 3. Framework of an ANN System

The backpropagation algorithm that proposed by Rumelhart and McClelland (1986) is used in layered feed-forward ANNs. This means that the artificial neurons are organized in layers, and send their signals "forward", and then the errors are propagated backwards. The network receives inputs by neurons in the *input layer*, and the output of the network is given by the neurons on an *output layer*. There may be one or more intermediate *hidden layers*.

The backpropagation algorithm uses supervised learning, which means that we provide the algorithm with examples of the inputs and outputs we want the network to compute, and then the error (difference between actual and expected results) is calculated. The idea of the backpropagation algorithm is to reduce this error, until the ANN *learns* the training data. The training begins with random weights, and the goal is to adjust them so that the error will be minimal.

RESEARCH METHODOLOGY

Experimental Setup

Ordinary portland cement (OPC type I), ground granulated blast furnace slag (GGBS), pulverized fly ash (PFA), silica fume (SF), tap water, and sodium chloride (NaCl) were used in this experiment. In the cement paste mixtures, addition of mineral admixtures to cement ratios were chosen as 20%, 40%, 60% for ground granulated blast furnace slag (GGBS), 10%, 20%, and 30% for fly ash (FA) and 5%, 10%, and 15% of silica fume (SF) with the value of water/binder ratio is 0.4. Internal chloride was also added in the mixtures in approximately 0.1%, 0.2%, 0.3%, 0.5%, 1.0%, 1.5%, 2.0%, 2.5%, and 3.0% by weight of the binder.

After mixing and casting process, the curing period was done for 28 days using polyethylene wrapping method. The last procedure of this experiment was measuring the free chloride content (measured in percentage by weight of the binder) using titration method according to NT Build 208 (1996). In detail, this procedure was done by crushing cement paste specimens and collecting the dust (smaller than 75 µm), stirring up to certain temperature, extracting free chloride using filter, and analyzing free chloride content in titration method.

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Building a Neural Network

To train a neural network, it is necessary to have a large number of data sets of high quality. The data that used for ANN training in the case of binder types effect on free chloride content in cement pastes, which is presented in this paper are based on the experimental result that have been done in Concrete Mechanics Materials and Engineering (CMME) Laboratory, Yonsei University, Seoul. The data have been collected from 70 specimens of cement paste, and all that data will be involved in the ANN training.

The artificial neural network (ANN) analysis was performed in backpropragation learning method by using iData Analyzer (iDA) software, which is quite simple and helpful to be used.

Trial and error method was used, in order to find a good neural networks architecture. Finally, it was found that a network architecture which was trained for 10,000 epochs (network pass) to learn the target mapping using 2 hidden layers with 4 neurons in the first hidden layer and 3 neurons for the second layer as shown in figure 4, can produce a good result.
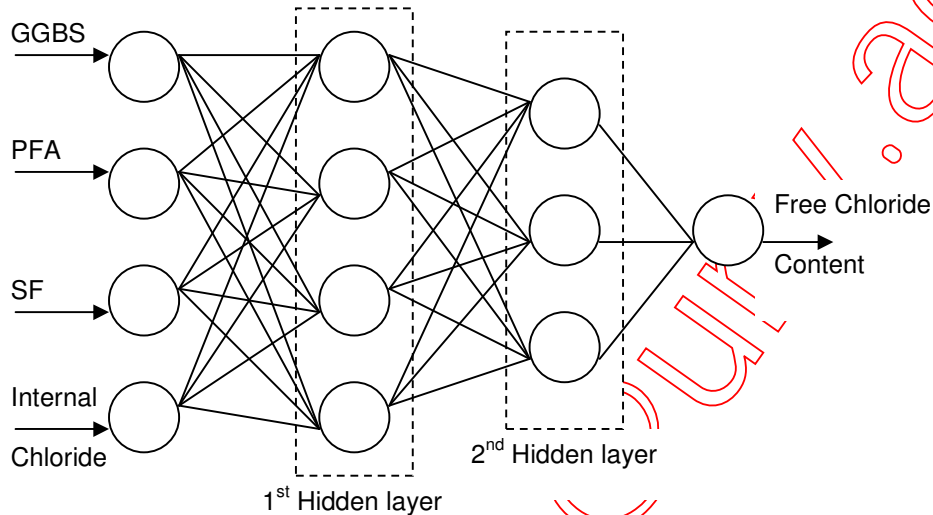
7

Fig. 4. Illustration of developed ANN model for free chloride content prediction

RESULTS AND DISCUSSION

ANN training was done using four independent variables (dosage of GGBS replacement, SF replacement, PFA replacement and addition of internal chloride) as input neurons, and one dependent variable (free chloride content) as the output neuron, and involving 70 instances. Table 1 show the comparison between experimental result and ANN prediction of the instances which are involved in the training.

TABLE 1. Comparison of experimental results and ANN Prediction

Instance	GGBS	SF	PFA	Internal Chloride	Experiment Results	ANN Prediction	Absolute Error (%)
#1	0.000	0.000	0.000	0.100	0.023	0.032	39.130
#2	0.000	0.000	0.000	1.500	0.633	0.778	22.907
#3	0.000	0.000	0.000	1.999	1.453	1.177	18.995
#4	0.000	0.000	0.000	2.500	1.705	1.672	1.935
#5	0.000	0.000	0.000	3.000	2.150	2.110	1.860
#6	0.000	0.000	0.100	0.180	0.032	0.047	46.875
#7	0.000	0.000	0.100	0.269	0.053	0.062	16.981
#8	0.000	0.000	0.100	0.899	0.500	0.394	21.200
#9	0.000	0.000	0.100	1.350	0.788	0.756	4.061
#10	0.000	0.000	0.100	1.799	1.206	1.100	8.789
#11	0.000	0.000	0.100	2.250	1.500	1.506	0.400

8

Instance	GGBS	SF	PFA	Internal Chloride	Experiment Results	ANN Prediction	Absolute Error (%)
#12	0.000	0.000	0.100	2.700	1.880	1.953	3.883
#13	0.000	0.000	0.100	3.000	2.325	2.162	7.011
#14	0.000	0.000	0.200	0.400	0.123	0.115	6.504
#15	0.000	0.000	0.200	0.799	0.396	0.357	9.848
#16	0.000	0.000	0.200	1.200	0.699	0.686	1.860
#17	0.000	0.000	0.200	1.599	1.026	0.989	3.606
#18	0.000	0.000	0.200	1.999	1.258	1.310	4.134
#19	0.000	0.000	0.200	2.500	1.743	1.801	3.328
#20	0.000	0.000	0.200	3.000	2.351	2.183	7.146
#21	0.000	0.000	0.300	0.350	0.069	0.102	47.826
#22	0.000	0.000	0.300	0.700	0.317	0.285	10.095
#23	0.000	0.000	0.300	1.050	0.586	0.566	3.413
#24	0.000	0.000	0.300	1.400	0.792	0.846	6.818
#25	0.000	0.000	0.300	1.750	1.109	1.107	0.180
#26	0.000	0.000	0.300	2.100	1.452	1.401	3.512
#27	0.000	0.000	0.300	2.500	1.824	1.798	1.425
#28	0.000	0.000	0.300	3.000	2.232	2.183	2.195
#29	0.000	0.050	0.000	0.190	0.048	0.050	4.167
#30	0.000	0.050	0.000	0.290	0.077	0.068	11.688
#31	0.000	0.050	0.000	0.950	0.493	0.451	8.519
#32	0.000	0.050	0.000	1.430	0.930	0.845	9.140
#33	0.000	0.050	0.000	1.900	1.309	1.226	6.341
#34	0.000	0.050	0.000	2.380	1.743	1.705	2.180
#35	0.000	0.050	0.000	3.000	2.266	2.198	3.001
#36	0.000	0.100	0.000	0.090	0.038	0.047	23.684
#37	0.000	0.100	0.000	0.448	0.109	0.151	38.532
#38	0.000	0.100	0.000	0.899	0.500	0.478	4.400
#39	0.000	0.100	0.000	1.350	0.878	0.855	2.620
#40	0.000	0.100	0.000	1.799	1.279	1.207	5.629
#41	0.000	0.100	0.000	2.250	1.621	1.630	0.555
#42	0.000	0.100	0.000	2.700	1.951	2.054	5.279
#43	0.000	0.100	0.000	3.000	2.284	2.223	2.671
#44	0.000	0.150	0.000	0.250	0.060	0.092	53.333
#45	0.000	0.150	0.000	0.850	0.471	0.468	0.637
#46	0.000	0.150	0.000	1.698	1.170	1.137	2.821
#47	0.000	0.150	0.000	2.120	1.555	1.485	4.502
#48	0.000	0.150	0.000	2.550	1.886	1.898	0.636
#49	0.000	0.150	0.000	3.000	2.307	2.206	4.378
#50	0.200	0.000	0.000	1.200	0.556	0.624	12.230
#51	0.200	0.000	0.000	1.599	0.860	0.910	5.814
#52	0.200	0.000	0.000	1.999	1.134	1.218	7.407
#53	0.200	0.000	0.000	2.400	1.430	1.596	11.608
#54	0.200	0.000	0.000	2.500	1.783	1.698	4.767
#55	0.200	0.000	0.000	3.000	2.116	2.119	0.142

| Instance	GGBS	SF	PFA	Internal Chloride	Experiment Results	ANN Prediction	Absolute Error (%)
#56	0.400	0.000	0.000	0.899	0.430	0.478	11.163
#57	0.400	0.000	0.000	1.200	0.617	0.692	12.156
#58	0.400	0.000	0.000	1.500	0.793	0.892	12.484
#59	0.400	0.000	0.000	1.799	0.989	1.097	10.920
#60	0.400	0.000	0.000	1.999	1.227	1.252	2.037
#61	0.400	0.000	0.000	2.500	1.670	1.718	2.874
#62	0.400	0.000	0.000	3.000	1.997	2.124	6.360
#63	0.600	0.000	0.000	0.600	0.303	0.341	12.541
#64	0.600	0.000	0.000	0.799	0.519	0.480	7.514
#65	0.600	0.000	0.000	1.000	0.633	0.619	2.212
#66	0.600	0.000	0.000	1.200	0.775	0.750	3.226
#67	0.600	0.000	0.000	1.500	0.958	0.935	2.401
#68	0.600	0.000	0.000	1.999	1.366	1.280	6.296
#69	0.600	0.000	0.000	2.500	1.749	1.733	0.915
#70	0.600	0.000	0.000	3.000	2.147	2.128	0.885
Mean of absolute error percentage							9.094

Test Data RMS = 0.031

Test Data MAE = 0.023
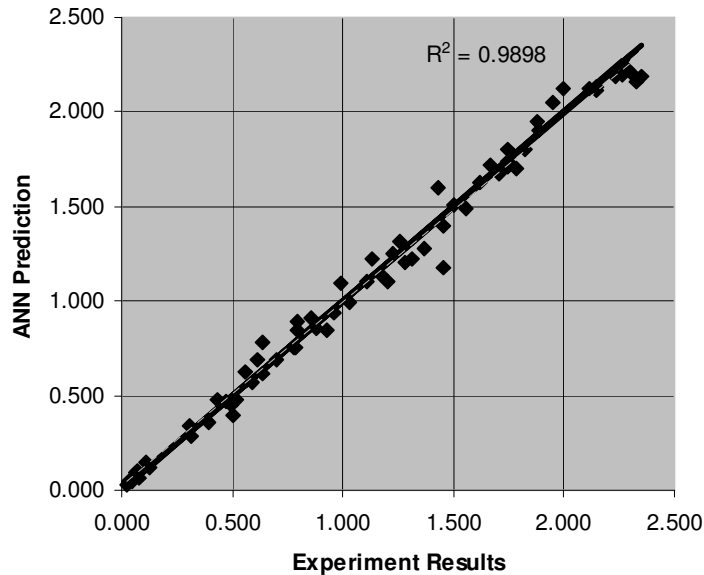
Figure. 5. Comparison of experimental results and ANN prediction

The outcomes that obtained using ANN modeling compared with the experimental results listed in Table 1, and plotted in Figure 5. ANN modeling result shows that the value of

10

root mean square error (RMS) is 0,031, mean absolute error (MAE) is 0,023, and the mean percentage of absolute error is 9,094%. According to Figure 5, it can be shown that the value of determination coefficient (R^2) between experimental results and ANN prediction in linear regression ($y=x$) is 0.9898. Considering the value of RMS, MAE, mean of absolute error percentage, and determination coefficient (R^2), it shows that the ANN modeling can predict the free chloride content close enough with the experimental results with relatively small error.

CONCLUSION

In this study, artificial neural networks (ANN) approach was employed to characterize relationship between free chloride content of cement pastes and its related parameters (ground granulated blast furnace slag (GGBS) replacement, pulverized fly ash (PFA) replacement, silica fume (SF) replacement, and added internal chloride). Actually, the ANN model exhibited relatively close performances with 0.9898 in terms of determination coefficient (R^2) value, 0,031 for RMS, 0,023 for MAE, and 9,094% for the mean percentage of absolute error values. Based on above results, it can be concluded that ANN is possible to be utilized in the purpose of concrete durability performance prediction, especially for free chloride content prediction.

Acknowledgements

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11

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