Soft Computing Based Modelling of Sorptivity of Concretes Incorporating Mineral Admixtures

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Abstract— **In this paper, mathematical models derived from gene expression programming (GEP) and artificial neural network (NN) were used for prediction of sorptivity of concretes. For this, 151 data samples were collected from the previous studies. The common prediction parameters were selected as water-to-binder ratio (w/B), total binder content (B), compressive strength of 150 mm cube specimen at 28 days ($f_{cube, 28}$), aggregate-to-binder ratio (Agg./B) and age of concrete (A). Both of the proposed models were proved to be effective enough for prediction of sorptivity of concretes. However, NN model was more accurate than GEP model. Moreover, validation study also indicated that the proposed mathematical models can be utilized as reliable prediction tools for estimation of sorptivity of concretes.**

Keywords- Sorptivity of concrete, Mineral admixtures, Artificial Neural Network, Gene Expression Programming

I. INTRODUCTION

Being an index of moisture transport into unsaturated cement based materials; sorptivity has been recognized as an important indication of concrete durability. The value of sorptivity illustrates the water mass uptake by concrete from the bottom surface based on water flowing into the concrete through large connected pores. The test method used generally reflects the way how water penetrates into concrete transporting harmful agents. Specifically, it is a good measure of the quality of near surface concrete, which governs durability of reinforced concrete in relation to reinforcement corrosion. The sorptivity coefficient is essential to predict the service life of concrete as a long lasting structural material. It is a property associated with capillary effects.

Soft Computing (SC) stands for system solutions based on artificial intelligence. It represents the combination of emerging problem solving technologies such as fuzzy logic (FL) probabilistic reasoning (PR), neural networks (NNs) and genetic algorithms (GA). Each of these technologies provides complementary reasoning and searching methods for solving complex, real-world problems [1]. SC is aimed to provide rapid execution of important and timely results for the sophisticated problems consisting of many variables. It covers the following research areas: Evolutionary algorithms (e.g. genetic programming) neural science and neural net systems, fuzzy set theory and fuzzy systems, chaos theory and chaotic systems etc.

The most popular soft computing methods inherited from the philosophy of genetic algorithms and artificial neural networks are gene expression programming (GEP) and Levenberg-Marquardt back propagation algorithm based neuro computing (NN), respectively. GEP is a procedure that mimics biological evolution to create a computer program to model some physical phenomena. GEP can be used to create many different types of models including decision trees to provide best fit. On the other hand, NN is used to map between a data set of numeric inputs and a set of numeric targets to derive am model.

A number of researchers utilized soft computing in their researches [2-12]. For example, Nazari and Azimzadegan [2] utilized two models based on artificial neural networks (ANN) and gene expression programming (GEP) for predicting splitting tensile strength and water absorption of concretes containing ZnO_2 nanoparticles at different ages of curing. To develop these models, training and testing data bases containing 144 data samples obtained from 16 different concrete mixtures were used. The data in the multilayer feed forward neural networks models and input variables of genetic programming models are arranged in a format of eight input parameters that cover the cement content (C), nanoparticle content (N), aggregate type (AG), water content (W), the amount of super plasticizer (S), the type of curing medium (CM), age of curing (AC) and number of testing try (NT). According to these input parameters, in the neural networks

TABLE 1.   DATABASE USED FOR TRAINING AND TESTING THE PROPOSED PREDICTION MODEL

Source of the data	No. of data samples	I1	I2	I3	I4	I5	Y
		w/b ratio	Total binder, B (kg)	Agg/B	fc @28 days (MPa)	Age, A (days)	Sorptivity (mm/min$^{1/2}$)
Nath and Sarker [13]	12	0.29-0.41	355-518	3.37-5.42	77.6-99.2	28,180	0.078-0.135
Bai et al. [14]	110	0.5	390	4.69-4.8	40.3-64.4	28-540	0.1-0.32
Karahan and Atış [15]	15	0.35	400	3.51-4.73	60.7-81	28	0.016-0.057
Atış and Karahan [16]	12	0.35	400	4.63-4.73	53-81.1	28	0.016-0.043

and genetic programming models, the splitting tensile strength and water absorption values of concretes containing ZnO$_2$ nanoparticles were predicted. The training and testing results in these two models have shown the strong potential of the models for predicting the splitting tensile strength and water absorption values of concretes containing ZnO$_2$ nanoparticles. Although neural networks have predicted better results, genetic programming was able to predict reasonable values with a simpler method rather than neural networks.

Mermerdaş et al. [12] developed a GEP model for prediction of the strength of concretes incorporated with metakaolin and different types of calcined kaolins. Their study investigated the effects of metakaolin (MK) and calcined kaolins (CKs) on the compressive strength development of the concrete. For this, non-purified ground kaolins obtained from different sources were thermally treated at specified conditions. They used seven input parameters which are SiO2, Al2O3, kaolinite, and alunite contents, and fineness of mineral admixture, age of concrete, and replacement level. The prediction model derived from GEP illustrated almost perfect fit with the experimental values. They concluded that prediction model containing those seven parameters was compared with the experimental results and proved to be a handful tool for estimating compressive strength of concrete incorporated with commercial MK and calcined kaolins.

In this study, sorptivity prediction models obtained from GEP and NN were developed using experimental results which have been reported in the previous studies. These prediction models were explicitly formulated. The main objective of the proposed models is to provide a simple way of estimation of the capillary water absorption of concretes incorporated with binary and ternary blends of mineral admixtures.

II   EXPERIMENTAL DATABASE USED FOR MODELLING

In order to develop a prediction model from GEP and NN, a set of experimental data available in the technical literature has been utilized [13-16]. In these studies, similar sorptivity testing methods were utilized to monitor the effects of different mineral admixtures at various replacement levels and with different combinations of blends on the sorptivity of concrete. The summary of the data set including thoroughly selected 149 data samples were shown in Table 1. The database was

arbitrarily separated into two parts, namely training and sub-databases. The percentages of the sub-databases are 75% and 25% for training and testing respectively. Training database was utilized for the development of the prediction models while the test database was employed to observe the repeatability and robustness of the proposed models. To be more specific, the main role of training dataset is to adjust weights, while prevention of overfitting and confirmation of the actual predictive power of the model are functions of testing sets.

The input variables cover some mix design parameters, age of concrete at testing, and 28-day compressive strength of concrete. There is not any non-numeric input. The properties and range of the input parameters are also given in Table 1

Inputs,

I1: Water to binder ratio; w/B,

I2: Total binder content in kg/m3; B,

I3: Aggregate to binder ratio; Agg/B,

I4: Compressive strength of concrete at the age of 28 days in MPa; fc,

I5: Age of concrete for sorptivity testing in days; A

III   PROPOSED MODELS

A   NN model

In the NN architecture, there are 5 nodes in the input layer, corresponding to 5 prediction parameters, 7 nodes in the hidden layer, and one in the output layer corresponding to sorptivity index (S). Therefore, a 5-7-1 NN architecture, as shown in Figure 1, was obtained to construct the NN based model. The NN model used in this study can simply be expressed by Eq. 1. The details of input and/or layer weights, activation function (hyperbolic tangent), and biases are given in Eqs. 2-3. It should be emphasized that all numeric variables must be normalized to a range of [-1, 1] before being introduced to the NN. Therefore, one must enter the normalized values in the mathematical operations given in Eq. 2. It should also be taken into consideration that the final result obtained from Eq. 1 is in the normalized form which needs to be de-normalized according to Eq. 4 and normalization coefficients given in Eqs. 5-6.
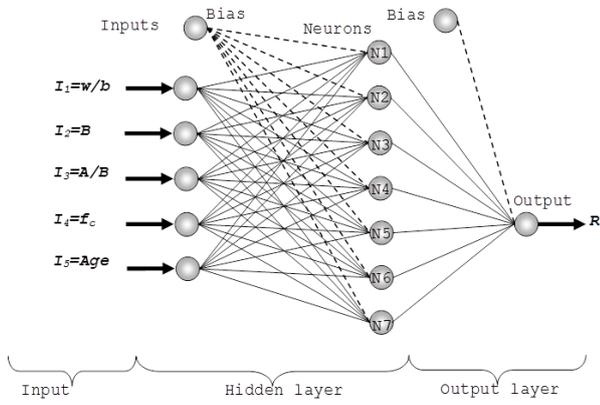
Figure 1. The architecture of NN model

$$Sorptivity = 0.12258 + \begin{bmatrix} -6.5693 \\ -1.2603 \\ 7.4333 \\ -0.2364 \\ 1.4499 \\ 1.1476 \\ 1.868 \end{bmatrix}^T \times \begin{bmatrix} f(U_1) \\ f(U_2) \\ f(U_3) \\ f(U_4) \\ f(U_5) \\ f(U_6) \\ f(U_7) \end{bmatrix}_{7 \times 1} \tag{1}$$

Where U_i values are numerical values of the nodes calculated according to the matrix operation given in Eq. 2, f(x) is activation function (hyperbolic tangent) expressed by Eq. 3.

$$\begin{bmatrix} 10.4461 & 3.996 & -12.5309 & -2.9381 & 0.0015 \\ -1.1441 & 1.4423 & 0.1448 & 0.4625 & 1.6408 \\ 6.1523 & 0.5357 & -7.2361 & -3.1199 & -0.0026 \\ -1.3587 & -2.7063 & 5.3446 & -1.9433 & 1.1693 \\ 0.1089 & -0.3923 & 0.9729 & -0.2607 & 1.2346 \\ -1.2823 & 1.2266 & -1.2457 & -0.0542 & -0.8298 \\ 1.6099 & -0.5328 & -1.1618 & 0.1492 & -0.8784 \end{bmatrix}_{7 \times 5} \times \begin{bmatrix} w/b \\ b \\ Agg/b \\ f_c \\ Age \end{bmatrix}_{5 \times 1} + \begin{bmatrix} -7.4168 \\ 4.3993 \\ -6.9137 \\ 0.0523 \\ 1.4033 \\ -1.9773 \\ 1.1699 \end{bmatrix}_{7 \times 1} = \begin{bmatrix} U_1 \\ U_2 \\ U_3 \\ U_4 \\ U_5 \\ U_6 \\ U_7 \end{bmatrix}_{7 \times 1} \tag{2}$$

$$\tanh(x) = \frac{2}{1 - e^{-2x}} - 1 \tag{3}$$

$$\beta_{normalized} = a\beta + b \tag{4}$$

Where β is the actual input parameter or output value. $\beta_{normalized}$ is the normalized value of input parameters or outputs ranging between [-1,1]. a and b are normalization coefficients given in the following equations (Eqs. 5-6).

$$a = \frac{2}{\beta_{max} - \beta_{min}} \tag{5}$$

$$b = -\frac{\beta_{max} + \beta_{min}}{\beta_{max} - \beta_{min}} \tag{6}$$

B GEP model

The prediction model derived from GEP is presented in Eq. 7. The GEP parameters used for derivation of the mathematical models are given in Table 1. As it can be seen from Table 1, in order to provide an accurate model, various mathematical operations were used.

$$\text{Sorptivity } S = S_1 \times S_2 \times S_3 \times S_4 \tag{7}$$

Where S_1, S_2, S_3 And S_4 are sub expressions

$$S_1 = \sinh\left(\tanh\left[\arctan\left(\sqrt[4]{e^{\frac{d_2}{c_1}}} \right) \right] \right) \times d_0 \tag{7a}$$

$$S_2 = \sinh\left(\sqrt[6]{d_1} \right) - \sqrt[5]{2(7.864777) + (4.222015) + d_4} \tag{7b}$$

$$S_3 = d_0 \times \left(\frac{[\tanh(4.981659)]^3}{\arctan(d_2 - 2.192108)} \right)^2 \tag{7c}$$

$$S_4 = \cos\left(\cos\left(\cos(8.963227) - \log(d_3) - \sin(d_2^2) \right) \right) \tag{7d}$$

IV COMPARISON OF NN AND GEP MODEL

In order to compare the effectiveness of the proposed model with those presented by the experimental database, Figure 2 was plotted. In the figure, the scatter of the predicted versus experimental data about bisector line (y=x) was observed. For the perfect estimation a point stands on the bisector ($S_{predicted} = S_{experimental}$). Observing Figure 2, it seems that there is a good trend in the variation of the data between predicted and experimental data. Correlation coefficients (R^2) equal to 0.98074 and 0.90081 for NN and GEP model, respectively. Thus, it was indicated that both models have strong correlation between actual and predicted values. Moreover, close values of the correlation coefficients may be considered as an evidence for the consistency and good fitness of the proposed model.
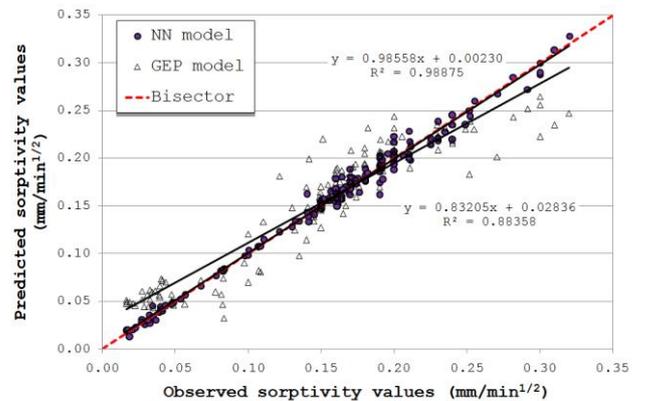

Figure 2. The performances of the proposed models

In Figure 3, comparison of the predicted results and the experimental values observed in the previous studies which were used for training and testing was shown. For all of the values NN model yielded almost perfect estimation capability. However, the results obtained from GEP model were underestimated in Figure 3a while overestimated results are observed in Figure 3c and 6d. Moreover, since the majority of the data obtained from the study of Bai et al. [14], the GEP model as well as NN model tends to be closer to the experimental results.
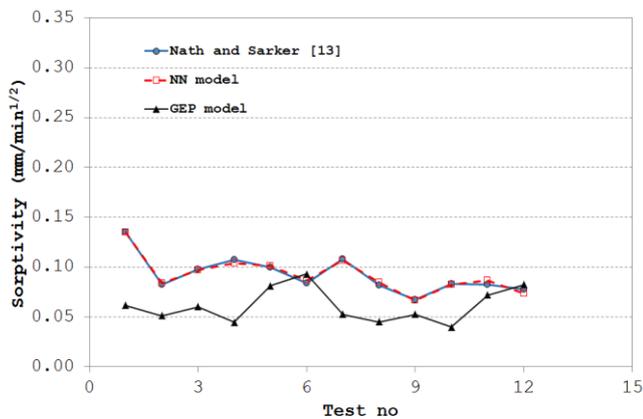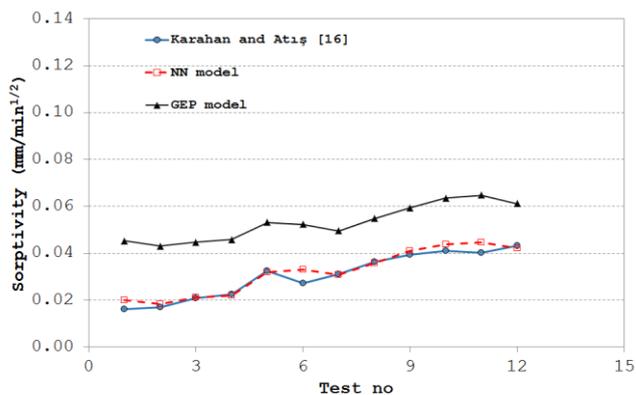

a)
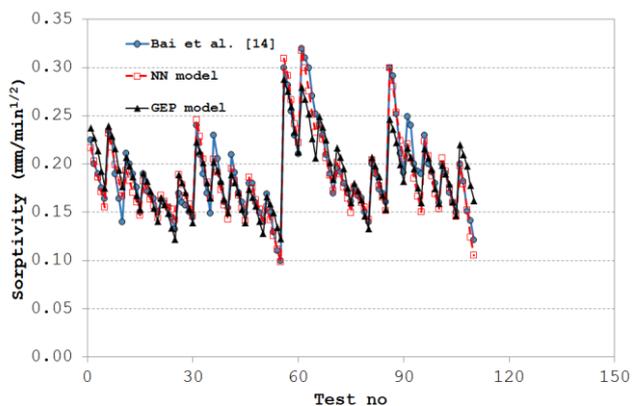
b)
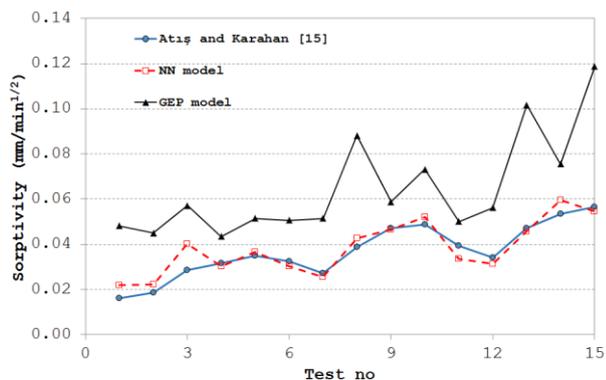
c)

d)

Figure 3. Comparison of the predicted results and the experimental values observed in the studies of a)Nath and Sarker [13], b) Bai et al. [14], c) Atış and Karahan [15], and d) Karahan and Atış [16]

Figure 4 demonstrated the analysis of the average error between observed sorptivity and prediction results with respect to various intervals of sorptivity values. For the experimental sorptivity interval of 0.10-0.25 the highest errors were observed. Nonetheless, the lowest error for GEP and NN models was observed for the sorptivity intervals of 0.2-0.25 mm/min$^{1/2}$ and 0.05-0.10 mm/min$^{1/2}$, respectively. Majority of the data were accumulated between 0.15-0.20 mm/min$^{1/2}$. When compared to other intervals, the error values at this range were seemed to be reasonably low for both of the proposed models.
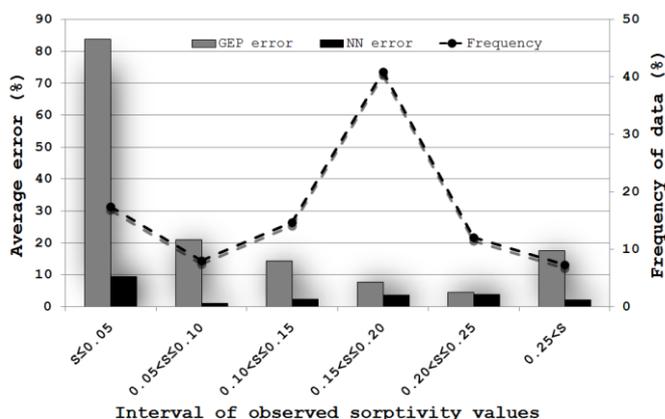

Figure 4. Error analysis of the proposed models

V CONCLUSION

In this study, explicit formulations of sorptivity of concretes incorporating mineral admixtures were presented. Based on the modelling and experimental studies the following conclusions can be drawn:

• Explicit formulation of sorptivity of concretes containing mineral admixtures was achieved. The correlation and accuracy of the proposed models are found to be good enough to be utilized for prediction purposes. This finding can be attributed to the reasonably low levels of prediction errors presented in Figure 4.

• The results of the experimental study agreed well with the prediction values obtained from the proposed models. Especially NN model had closer trend to the actual values while GEP model revealed higher fluctuations.

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