Computers and Concrete, *Vol. 19, No. 6 (2017) 717-724*
DOI: https://doi.org/10.12989/cac.2017.19.6.717

Modelling the flexural strength of mortars containing different mineral admixtures via GEP and RA

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(Received August 25, 2016, Revised February 28, 2017, Accepted March 4, 2017)

Abstract. In this paper, four formulas are proposed via gene expression programming (GEP)-based models and regression analysis (RA) to predict the flexural strength (f_s) values of mortars containing different mineral admixtures that are ground granulated blast-furnace slag (GGBFS), silica fume (SF) and fly ash (FA) at different ages. Three formulas obtained from the GEP-I, GEP-II and GEP-III models are constituted to predict the f_s values from the age of specimen, water-binder ratio and compressive strength. Besides, one formula obtained from the RA is constituted to predict the f_s values from the compressive strength. To achieve these formulas in the GEP and RA models, 972 data of the experimental studies presented with mortar mixtures were gathered from the literatures. 734 data of the experimental studies are divided without pre-planned for these formulas achieved from the training and testing sets of GEP and RA models. Beside, these formulas are validated with 238 data of experimental studies un-employed in training and testing sets. The f_s results obtained from the training, testing and validation sets of these formulas are compared with the results obtained from the experimental studies and the formulas given in the literature for concrete. These comparisons show that the results of the formulas obtained from the GEP and RA models appear to well compatible with the experimental results and find to be very credible according to the results of other formulas.

Keywords: mineral admixtures; flexural-compressive strengths; gene expression programming

1. Introduction

Recently, GGBS, SF and FA have been employed as a highly active and effective pozzolans for the partial replacement of cement used in mortar and concrete production (Qian and Li 2001). This is because most of the physical, mechanical, durability, high toughness, long service life and impermeability properties of concrete containing different mineral admixtures are better than those of conventional concrete. Mineral admixtures are made possible by diminishing inhomogeneity, porosity and micro-cracks in concrete and the interfacial zone of aggregate particles-cement matrix. Fortunately, these mineral admixtures are by-products coming out in the industry factory and aid in decreasing the quantity of cement essential to perform concrete less expensively, less energy excessive, and more environmental friendly (Goldman and Bentur 1989, Mehta and Monteiro 1993, Shah and Ahmad 1994, Nawy 1996, Neville 1997, Shannag 2000, Tanyıldızı 2017). In addition, the lower cement demand brings about a reduction for CO_2 emerged by the manufacture of cement (Chan and Wu 2000, Roy *et al*. 2001, Ferraris *et al*. 2001, Oner and Akyuz 2007). The advantages from the employed of these mineral admixtures in mortar and concrete result partially from the pozzolanic and cementitious reactivity, and partially from their particle size dispersion characteristics (Mehta 1983, Malhotra and Mehta 1996, Oner and Akyuz 2007).

SF is an industrial by-product of ferro-silicon alloy industry and silicon metal in place of a waste product. Recently, the use of SF in mortar and concrete has grown up (Köksal *et al*. 2008, Zhang and Li 2013). Due to an important developments attained on interface zone of aggregate particles-cement matrix, SF is known to develop the strength, durability and impermeability of mortar and concrete in the early ages, and create a high-strength mortar and concrete (Köksal *et al*. 2008). In addition, SF exhibits a significant role on development of mechanical properties of mortar and concrete due to possessing a pozzolanic activity. Filling influence of SF is more dominant than pozzolanic influence of SF. The best known influence of SF on mortar and concrete is the development on interface zone aggregate particles-cement matrix that is known as the weakest interface zone on concrete (Toutanji and Bayasi 1999, Massazza 2000, Atiş *et al*. 2005, Köksal *et al*. 2008).

Blast-furnace slag (BFS) is an industrial by-product in the produce of pig iron and the quantities of iron. The use of GGBFS in mortar and concrete has a favorable influence on consuming the calcium hydroxide ($Ca(OH)_2$) that reduces the properties of mortar and concrete (Roy and Idorn 1982, Papadakis and Tsimas 2002, Oner *et al*. 2005, Oner and Akyuz 2007). This binding creates a more intensely microstructure, as the $Ca(OH)_2$ is used up and calcium silicate hydrate (C-S-H) gels are composed (Mazloom *et al*. 2004, Bentz 2006, Chidiac and Panesar 2008, Bilim *et al*. 2009). The partial replacement of GGBFS by weight of cement may reduce the strength in the early ages, but very significantly improve the strength, microstructure and durability of mortar and concrete in the later ages (Malhotra

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http://www.techno-press.org/?journal=cac&subpage=8
ISSN: 1598-8198 (Print), 1598-818X (Online)

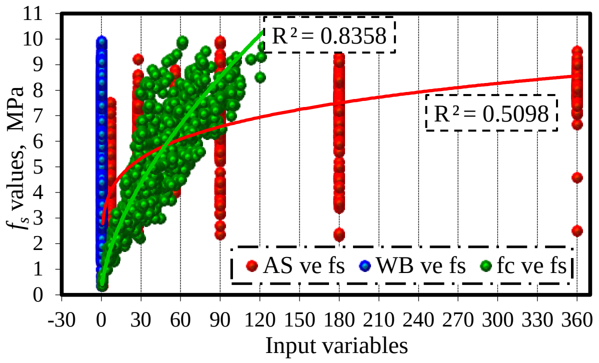


Fig. 1 Distribution of input variables and f_s used in the GEP

1987, Song and Saraswathy 2006, Bilim *et al*. 2009).

FA is an industrial by-product of coal-fired electric power stations (Papadakis 1999, Memon *et al*. 2002). The pozzolanic reactivity is that when FA is employed, $Ca(OH)_2$ is turned into new C-S-H gels, bringing about the conversion of bigger pores into smaller pores due to the pozzolanic reaction of FA. The employment of FA has a favorable influence on the properties of mortar and concrete by using up the $Ca(OH)_2$ (Memon *et al*. 2002, Papadakis and Tsimas 2002, Oner *et al*. 2005). The basic effects of partial replacement of FA by weight of cement in mortar and concrete allows improvement of micro-structure, reduction of the pore size and better workability of mortar and concrete mixture (Kondraivendhan and Bhattacharjee 2015).

In this study, three formulas obtained from the GEP-I, GEP-II and GEP-III, and one formula obtained from the regression analysis are proposed for the f_s prediction of mortars containing mineral admixtures at different ages. The age of specimen (AS), water-cement ratio (WB), compressive strength (f_c) and f_s values of mortars containing mineral admixtures employed in the training, testing and validation sets of the GEP-based models were gathered from technical literatures (Wong *et al*. 1999, Elkhadiri *et al*. 2002, Atiş *et al*. 2004, Özcan 2005, Özdemir 2006, Bilim 2006, Mercan 2007, Ulaş 2009, Li *et al*. 2015). First formulation obtained from the GEP-I model is proposed to predict the f_s values from the f_c, second formulation obtained from the GEP-II model is proposed to predict for the f_s values from the AS and f_c, and third formulation obtained from the GEP-III model is proposed to predict the f_s values from the AS, WB and f_c values. Moreover, one formula obtained from the regression analysis is proposed for to predict the f_s values from the f_c values. The results of these formulas obtained from in the training, testing and validation sets of the GEP-based models and RA were compared with the results of experimental studies and the formulas given in the literature for concrete.

2. Gene expression programming

The main purpose of gene expression programming (GEP) revealed by Ferreira (Ferreira 2001) is to obtain a formula that is appropriate an actual data set introduce to GEP model. For this formula, GEP makes the typical regression employing the most of the genetic operators that make use of the genetic algorithms like mutation, inversion, recombination, transposition and gene duplication (Ferreira 2001, Ferreira 2004, Ferreira 2006, Kayadelen *et al*. 2009, Sarıdemir 2010, Kara 2011, Severcan 2012). The process in GEP starts with the casual production of the chromosomes of beginning population. After these chromosomes are determined, the suitability of each individual is reviewed against a set of suitability status. Afterwards, the individuals are chosen in accordance with their fitness to reproduce with alteration, separating seed with new properties. The process of new individuals is iterated for a certain number of breeds, until the suitable and efficient solution has been obtained (Ferreira 2004, Ferreira 2006, Sarıdemir 2010). As a result of these process, GEP present a mathematical formula from the chromosomes of character sequences called as expression tree (Ferreira 2001).

Table 1 Parameters employed in the GEP models

Parameter Definitions	GEP-I	GEP-II	GEP-III
Function set	+, -, ×, /, 3Rt	+, -, ×, /, Ln, X2, Pow10, 3Rt, 4Rt	+, -, ×, /, Inv, Exp, Pow, 4Rt
Number of chromosomes	10	20	30
Head size	6	8	6
Number of genes	1	2	3
Constants per gene	5	5	10
Linking function	Multiplication	Multiplication	Addition
Mutation		0.00138	
Inversion		0.00546	
One and two-point recombination		0.00277	
Gene recombination		0.00277	
Gene transposition		0.00277	
Random chromosomes		0.0026	

2.1 GEP models

In this paper, the purpose of creating the models depend on the GEP is to obtain a formula to predict the f_s of mortars containing different mineral admixtures that are SF, GGBS and FA at the ages of 1, 2, 3, 7, 28, 56, 90, 180 and 360. These models called as GEP-I, GEP-II and GEP-III are suggested to predict the f_s from the f_c or WB and f_c or AS, WB and f_c. To create these models, among 972 experimental data given with mortar mixtures containing different mineral admixtures that are SF, GGBS and FA gathered from the fourteen different existing literatures (Wong *et al*. 1999, Elkhadiri *et al*. 2002, Atiş *et al*. 2004, Özcan 2005, Özdemir 2006, Bilim 2006, Mercan 2007, Ulaş 2009, Li *et al*. 2015), about 50% and 25% of the whole data (489 and 245 data) literatures (Elkhadiri *et al*. 2002, Özcan 2005, Özdemir 2006, Bilim 2006, Ulaş 2009) were employed without prior planning as training and testing sets, respectively, and 238 data (25% of the whole data) literatures (Wong *et al*. 1999, Atiş 2004, Mercan 2007, Li *et al*. 2015) un-used in training and testing sets was employed as validation set. The distributions of AS, WB and f_c used as inputs in response to the f_s values used as output in the sets of models are shown in Fig. 1. As shown in figure, the

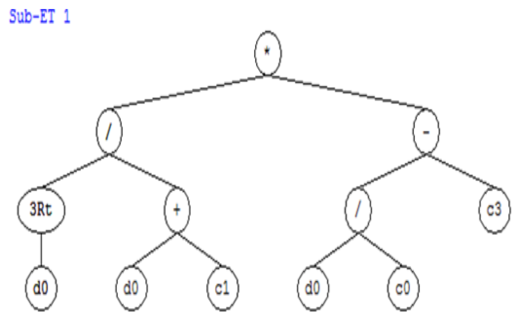


Fig. 2 Expression tree of GEP-I proposed for predicting f_s from f_c

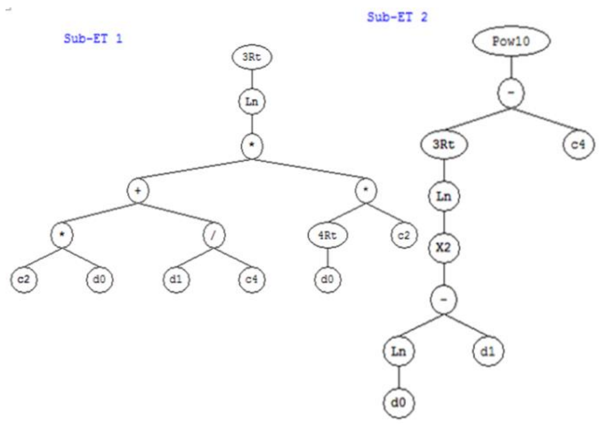


Fig. 3 Expression tree of GEP-II proposed for predicting f_s from AS and f_c

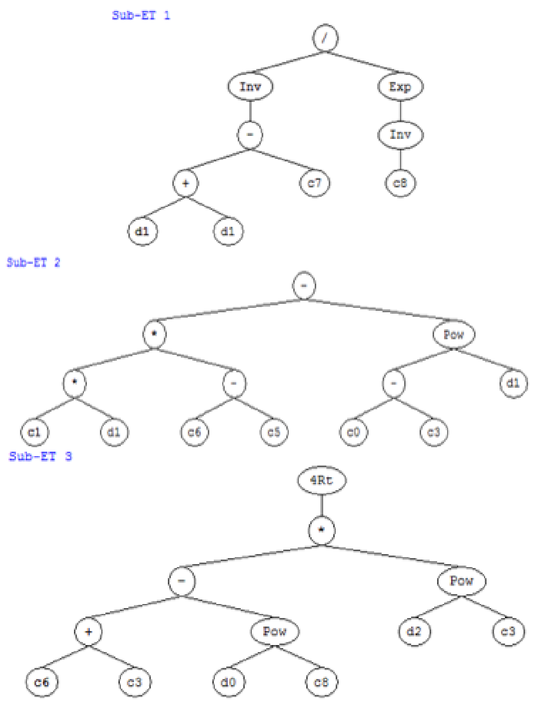


Fig. 4 Expression tree of GEP-III proposed for predicting f_s from AS, WB and f_c

chances in the input variables directly affect the output variable.

In this paper, as stated above, firstly, the terminal set f_s and the function sets AS, WB and f_c to create the chromosomes are preferred, namely, $f_{s\text{-I}}=\{f_c\}$, $f_{s\text{-II}}=\{\text{AS and } f_c\}$ and $f_{s\text{-III}}=\{\text{AS, WB and } f_c\}$. For the connection of function variables, the fundamental arithmetic operators and a few fundamental functions are determined. After trying many the numbers of genes and the head sizes, to find the best model performance in the GEP-I, GEP-II and GEP-III, the number of genes are determined as 1, 2 and 3, and the head sizes are determined as 6, 8 and 6, respectively. The genetic operators (mutation, inversion, recombination and transposition) in these models was employed as set of genetic operators. Parameters employed in the training set of the GEP-I, GEP-II and GEP-III are presented in Table 1.

For the GEP-I, GEP-II and GEP-III, the mathematical expressions obtained from the expression trees exhibited in Figs. 2-4 are given in the Eqs. (1)-(3), respectively. The real parameters (variables) and constants used in the GEP-I, GEP-II and GEP-III are given in Table 2. The mathematical expressions are 3Rt=cube root ($\sqrt[3]{}$), 4Rt=quartic root ($\sqrt[4]{}$), X2=x to the power of 2, Inv=inverse, Pow=x to the power of y, Pow10=10x and Exp=exponential seen in Figs. 2-4. Considering the above-stated variables and constants, the final mathematical formulas obtained from the expression trees depend on the GEP-I, GEP-II and GEP-III models to predict the f_s from the f_c or WB and f_c or AS, WB and f_c of mortars containing different mineral admixtures are given in the Eqs. (4)-(6), respectively.

$$f_{s-I}=\left(\left(\frac{\sqrt[3]{d0}}{d0+c1}\right)\times\left(\frac{d0}{c0}-c3\right)\right) \tag{1}$$

$$f_{s-II}=\left(\sqrt[3]{\mathrm{Ln}\left(\left(c2\times d0+\frac{d1}{c4}\right)\times\left(\sqrt[4]{d0}\times c2\right)\right)}\right)\times\left(10^{\sqrt[3]{\mathrm{Ln}((\mathrm{Ln}(d0)-d1)^2)}}-c4\right) \tag{2}$$

$$f_{s-III}=\left(\frac{1}{(2d1-c7)\times\left(e^{\frac{1}{c8}}\right)}\right)+\left(\left((c1\times d1)\times(c6-c5)\right)-\left((c0-c3)^{d1}\right)\right)+\left(\sqrt[4]{\left((c6+c3)-d0^{c8}\right)\times\left(d2^{c3}\right)}\right) \tag{3}$$

$$f_{s-I}=\left(\left(\frac{\sqrt[3]{f_c}}{f_c+14.987}\right)\times(2.10f_c+4.16)\right) \tag{4}$$

$$f_{s-II}=\left(\sqrt[3]{\mathrm{Ln}\left((5.93\times AS-0.14f_c)\times\left(\sqrt[4]{AS}\times 5.93\right)\right)}\right)\times\left(10^{\sqrt[3]{\mathrm{Ln}((\mathrm{Ln}(AS)-f_c)^2)}}-1.48\right) \tag{5}$$

$$f_{s-III}=\left(\frac{1}{(28.4WB-12.50)}\right)+\left((6.28\times WB)-\left((13.136)^{WB}\right)\right)+\left(\sqrt[4]{\left(1.362-AS^{(-0.357)}\right)\times\left(f_c^{\,1.882}\right)}\right) \tag{6}$$

3. Regression analysis

Regression analysis is a statistical tool to research of correlations between variables input and output variables for an adequate example. Commonly, the regression analysis is the method of fitting mathematical models to example data. On the principle of mathematical expressions, the regression analysis is known as a nonlinear regression and/or linear regression. As stated above, different regression formulas depend on relationship have been suggested in some national building codes and in the literature to model the f_s values from f_c of concrete. In this paper, formulas obtained from regression analysis have been proposed for the calculation of f_s values from f_c values of mortars containing different mineral admixtures.

Table 2 Variables and constants employed in the GEP models

	d0	d1	d2	c0	c1	c2	c3	c4	c5	c6	c7	c8
GEP-I	f_c											
Sub-ET 1				0.475	14.987		4.160					
GEP-II	WB	f_c										
Sub-ET 1						5.930		-7.162				
Sub-ET 2								1.480				
GEP-III	AS	WB	f_c									
Sub-ET 1				6.482	-1.989		-6.654				0.880	0.377
Sub-ET 2									4.836	1.679		
Sub-ET 3							1.882			-0.520		-0.357

Table 3 Statistical parameter results of GEP models, regression and other equations

	MAPE			RMSE			R^2		
	Training	Testing	Validation	Training	Testing	Validation	Training	Testing	Validation
GEP-I	15.465	16.652	15.815	0.979	1.004	0.964	0.773	0.794	0.738
GEP-II	14.616	15.872	16.548	0.900	0.912	0.986	0.808	0.830	0.752
GEP-III	12.133	13.662	13.234	0.760	0.784	0.876	0.863	0.876	0.777
RA	16.743	17.631	16.084	0.996	1.020	0.973	0.765	0.787	0.736
ACI318R-95	26.532	26.399	21.104	1.989	1.962	1.582	0.767	0.789	0.737
ACI363R-92	20.057	22.065	24.335	1.112	1.134	1.231	0.767	0.789	0.737
Ahmad and Shah	15.935	17.131	13.866	1.042	1.068	0.997	0.757	0.779	0.732

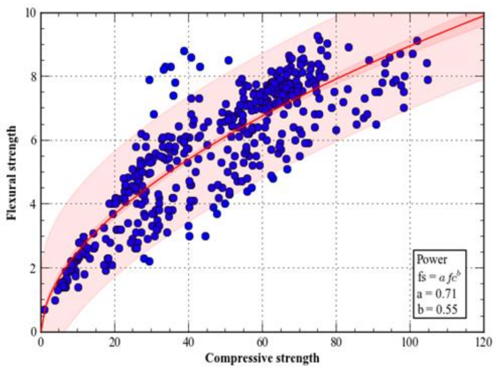


Fig. 5 The correlation between the f_s and f_c of mortars

3.1 Regression analysis model

RA model was applied by the curve fitting method named as a powder function for the calculation of f_s values from f_c values of mortars containing different mineral admixtures. The same experimental data were used for the results of the sets in the GEP and RA models compared with the results attained from the formulas given in some national building codes and in the literature for concrete. The relationship between the f_s and f_c values of mortars are evaluated with formula obtained from power expression as shown in Fig. 5. The common format of the powder regression model is expressed by Eq. (7).

$$f_s = \mathrm{a}(f_c)^{\mathrm{b}} \tag{7}$$

Where f_s and f_c are the flexural strength (MPa) and compressive strength (MPa) at the same age of mortars containing different mineral admixtures. *a* and *b* represent the constants found from the RA. Eq. (8) has been obtained for explaining a correlation between the f_s and f_c values of mortars containing different mineral admixtures.

$$f_s = 0.71(f_c)^{0.55} \tag{8}$$

4. Results and discussion of formulas

In this paper, the performances of the formulas derived from the GEP and RA were investigated to predict the f_s values of mortars containing different mineral admixtures. For these performances, the mean absolute percentage error (MAPE), root mean square error (RMSE) and R-square (R^2) expressed in Eqs. (9)-(11) were utilized as statistical correction parameters. These statistical parameters are used to evaluate the correlation between the results of the experimental studies, the results of the formulas obtained from the GEP, RA, and the results of the formulas given in the literature for concrete (ACI318R-95 1995, ACI363R-92 1992, and Ahmad and Shah 1985).

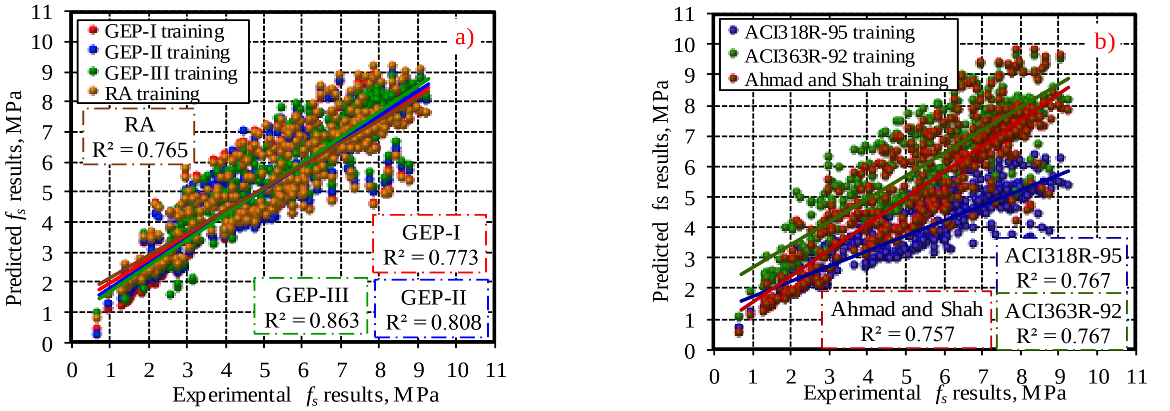
$$\mathrm{MAPE} = \frac{1}{n}\left[\frac{\sum_{i=1}^{n}|t_i - o_i|}{\sum_{i=1}^{n} t_i} \times 100\right] \tag{9}$$

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(t_i - o_i)^2} \tag{10}$$

$$R^2 = \frac{\left(n\sum_{i=1}^{n} t_i o_i - \sum_{i=1}^{n} t_i \sum_{i=1}^{n} o_i\right)^2}{\left(n\sum_{i=}^{n} t_i^2 - (\sum_{i=1}^{n} t_i)^2\right)\left(n\sum_{i=1}^{n} o_i^2 - (\sum_{i=1}^{n} o_i)^2\right)} \tag{11}$$

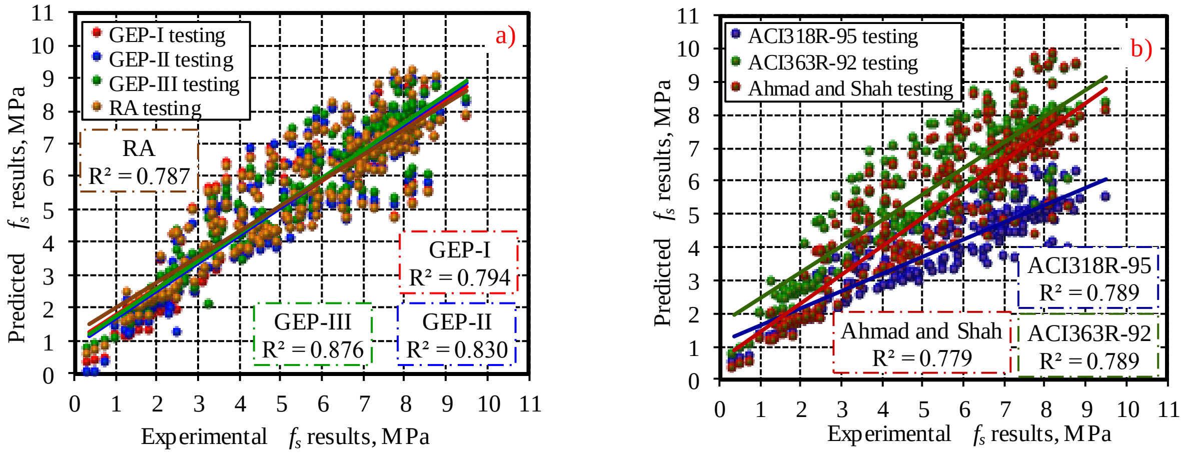
Where, *t* is the target f_s value obtained from the experimental studies, *o* is the output f_s value obtained from the formulas and *n* is sum number of experimental study data.

The statistical parameter (MAPE, RMSE and R^2) results of the training, testing, and validation sets of GEP-I, GEP-II, GEP-III, RA, ACI318R-95 1995, ACI363R-92 1992, and Ahmad and Shah 1985 formulas are given in Table 3. Considering the statistical results, the best value of R^2 and the minimum values of MAPE and RMSE are shown in the training, testing, and validation sets of GEP-III. All of the statistical parameter results given in Table 3 show that the formulas obtained from the GEP models are suitable to calculate the f_s values of mortars containing different mineral admixtures according to others formulas. The reason of obtaining better results by GEP-II and GEP-III models according to the other models is especially that the AS and/or WB parameters are added as input variables in addition to the f_c in these models. Besides, another reason of obtaining better results by GEP-II and GEP-III models is the parameters used in these models. All of MAPE, RMSE and R^2 results show that the results of the proposed GEP and RA models are applicable and can predict the f_s values



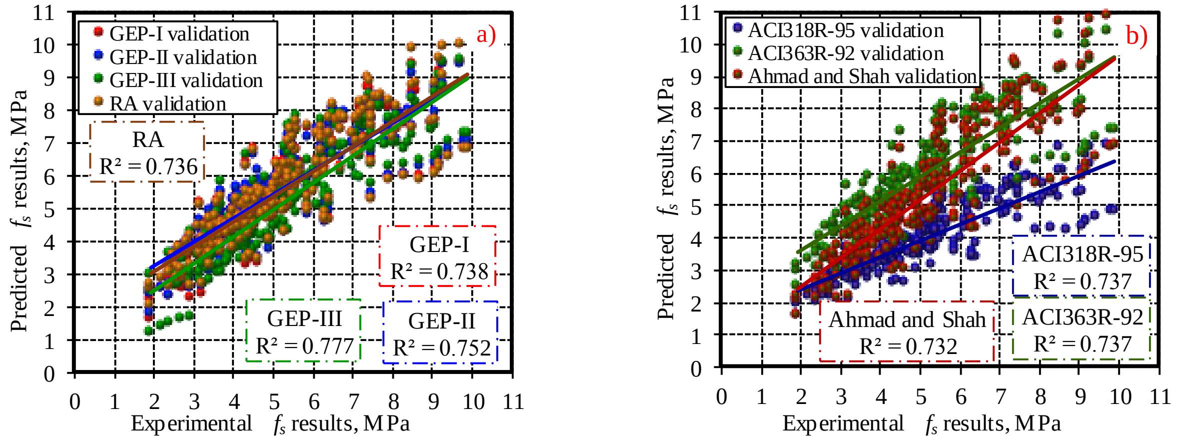
(a) f_s results of the GEP and RA models (b) f_s results of the formulas given in the literature

Fig. 6 Comparison of experimental and predicted f_s for training set



(a) f_s results of the GEP and RA models (b) f_s results of the formulas given in the literature

Fig. 7 Comparison of experimental and predicted f_s for testing set

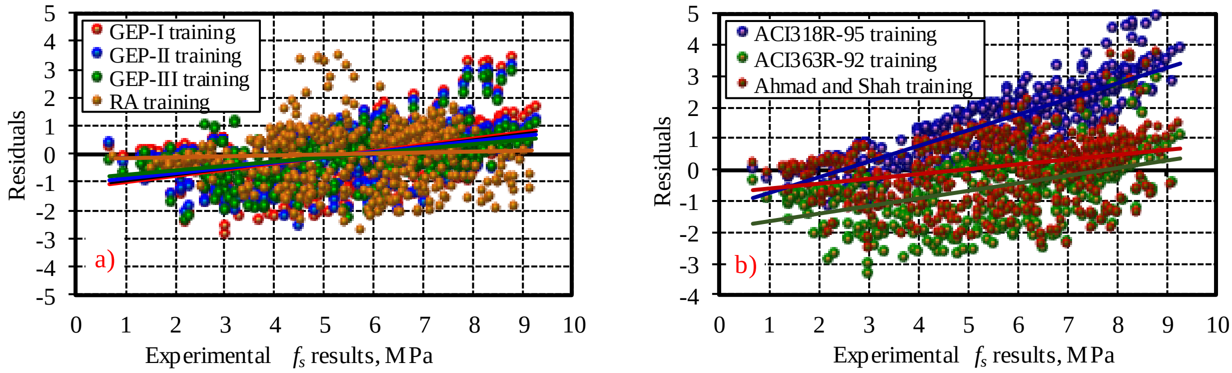


(a) f_s results of the GEP and RA models (b) f_s results of the formulas given in the literature

Fig. 8 Comparison of experimental and predicted f_s for validation set

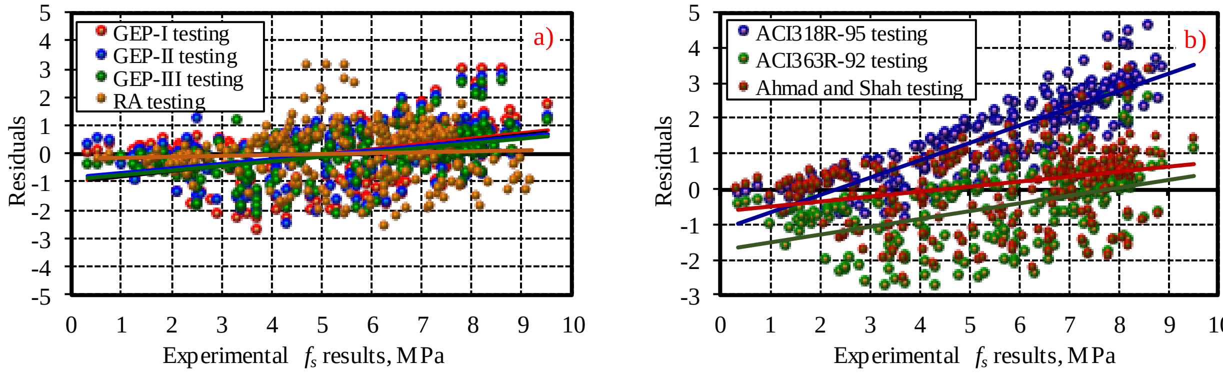
of mortars containing different mineral admixtures very close to the experimental results.

The f_s results predicted from training, testing and validation sets of GEP-I, GEP-II, GEP-III, RA, ACI318R-95 1995, ACI363R-92 1992 and Ahmad and Shah 1985 formulas versus the f_s results attained from the experimental studies are shown in Figs. 6-8, respectively. The linear least square fit line and R^2 values obtained according to results of the whole formulas were given on these figures. The results of training set (Fig. 6(a)) show that the GEP and RA formulas were successful in learning the correlation between the output and input variables. The results of testing set (Fig. 7(a)) indicate that the GEP and RA formulas were able to generalizing between the output and



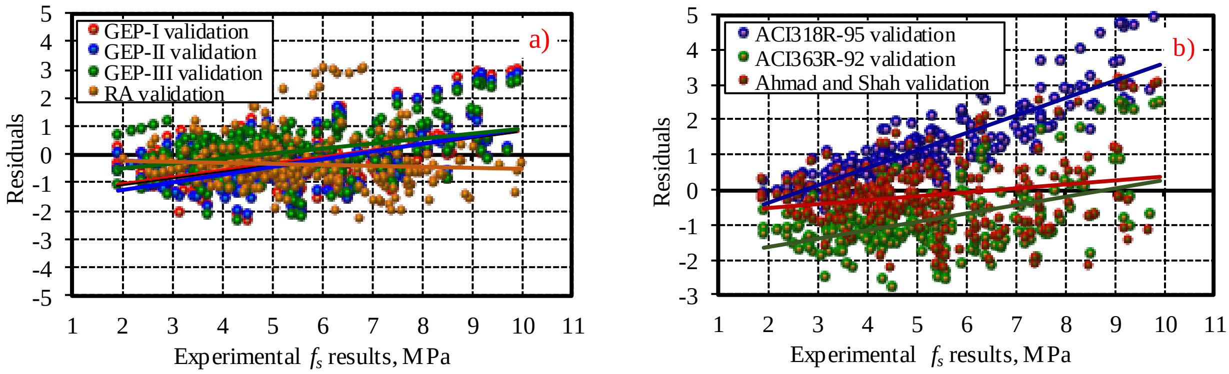
(a) residuals of the GEP and RA models (b) residuals of the formulas given in the literature

Fig. 9 Residuals of the training set within ±5% limits



(a) residuals of the GEP and RA models (a) residuals of the GEP and RA models

Fig. 10 Residuals of the testing set within ±5% limits



(a) residuals of the GEP and RA models (b) residuals of the formulas given in the literature

Fig. 11 Residuals of the validation set within ±5% limits

input variables, and eventually, the results of validation set (Fig. 8(a)) prove that the proposed formulas had good potential to predict the f_s of mortars containing different mineral admixtures. Figs. 6(b)-8(b) show that the f_s results calculated from training, testing and validation sets of formulas given in the literature to compare the results of experimental studies. Besides, the residuals of f_s results predicted from training, testing and validation sets within ±5% limits of the whole formulas are given in Figs. 9-11, respectively. As it is visible from the comparisons in these figures, the results obtained from the training, testing and validation sets of GEP and RA formulas according to the results of formulas given in the literature are very closer to the results of the experimental studies. That is, it can be seen from these figures that the GEP formulas performed better than the other formulas in predicting the f_s of mortars containing mineral admixtures.

4. Conclusions

In this study, new and efficient four mathematical formulas obtained from the models depend on the GEP-I, GEP-II, GEP-III and RA were presented to predict the f_s from the f_c or WB and f_c or AS, WB and f_c of mortars containing different mineral admixtures. The f_s results of these formulas depend on the GEP and RA are compared with the results of the experimental studies and the formulas given in the literature for concrete. All of the f_s results obtained from these formulas depend on the GEP and RA are shown to be very close to the results of experimental studies considering the results of formulas given in the literature for concrete. The comparisons between the f_s results obtained from these formulas and the f_s results of experimental studies in terms of MAPE, RMSE and R^2 values have proven this condition. The presented mathematical formulas are so easy that they can be employed by someone not completely familiar with GEP. Consequently, GEP can be employed as an efficient model and it can approach a new area to resolve the civil engineering problems.

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