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Predicting compressive strength of concrete with fly ash, metakaolin and silica fume by using machine learning techniques

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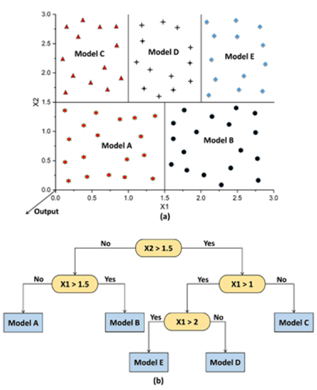
Abstract

The compressive strength (CS) is the most important parameter in the design codes of reinforced concrete structures. The development of simple mathematical equations for the prediction of CS of concrete can have many practical advantages such as it save cost and time in experiments needed for suitable design data. Due to environmental concerns with the production of cement, different supplementary cementitious materials are often used as partial replacements for cement such as fly ash (FA), metakaolin (MK), and silica fume (SF). However, little work has been done for developing simple mathematical equations for the prediction of CS with FA, MK and SF by using the M5P algorithm. Moreover, the M5P algorithm is not compared with other modelling techniques such as linear regression analysis, gene expression programming (GEP) and response surface methodology. It is established that, for concrete with FA and SF, M5P showed superior prediction capability as compared with other modelling techniques, however, GEP gave the best performance for concrete with MK: CS decrease by increasing FA content, while it increases by increasing MK and SF content.

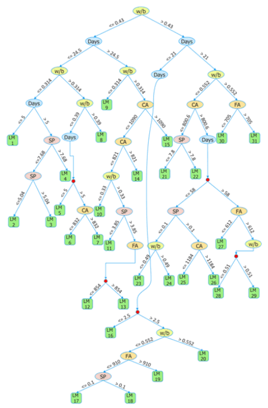
Keywords

Sustainable concrete, compressive strength, M5P model tree algorithm, machine learning

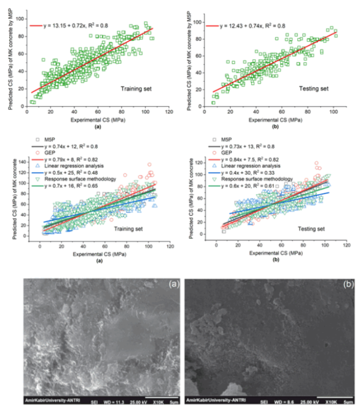
Graphical Abstract



M5 algorithm



Model tree structure of M5P



Correlation of the model and experimental results

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1 INTRODUCTION

In the world, the sustainability of human society is in danger due to the critical issue of climate change. There are many sectors responsible for climate change including the construction industry. For instance, cement production is responsible for about 7% of the total carbon dioxide emission to the atmosphere (Metz, Davidson, De Coninck, Loos, & Meyer, 2005). During cement production, the calcination process, in which CaO forms by extracting CO_2 from $CaCO_3$, is responsible for about 50% of CO_2 production while the remaining 50% CO_2 is produced by energy use (Yang, Song, & Song, 2013). The demand for cement is increasing and it was predicted that the annual usage of Portland cement would hit 6000 million tons by the year 2060 (Taylor, Tam, & Gielen, 2006). One of the solutions to lower cement consumption is to reduce its consumption by partially replacing it with supplementary cementitious materials such as fly ash (FA), metakaolin (MK), silica fume (SF), etc.

A large quantity of FA is produced every year in the world. It is beneficial when used in concrete mainly in three ways such as its pozzolanic effect, morphologic effect, and micro aggregate effect. Out of these, the pozzolanic effect has the main benefit in the enhancement of concrete mechanical strength. In the pozzolanic effect, SiO_2 and Al_2O_3 react with $Ca(OH)_2$ which is a product of cement hydration and produce calcium silicate hydrate (C-S-H) and calcium aluminate hydrate. These secondary hydration products enhance the concrete density by filling the capillary pores and improving the concrete strength (Cao, Sun, & Qin, 2000). In addition to this, FA can be used in concrete to reduce its cost (Shah, Yuan, & Photwichai, 2022). However, care should be taken while using FA in air-entrained concrete because it may deteriorate the air-void parameters (Shah, Yuan, & Zuo, 2021b).

The inclusion of MK as cement replacement in concrete can lower CO_2 emissions by up to 127 kg/ton of cement produced (Lenka & Panda, 2017). MK ($Al_2Si_2O_7$) is a high reactive pozzolanic material, which is more reactive than fly ash and silica fume (Asbridge, Walters, & Jones, 1994). It is formed by the dihydroxylation of kaolin in the temperature range of 500-800 ^oC. MK reacts with $Ca(OH)_2$ to form calcium silicate hydrate (C-S-H) and alumina containing phases, including C_3AH_6, C_2ASH_8, and C_4AH_{13}(He, Osbaeck, & Makovicky, 1995; M. Zhang & Malhotra, 1995). The incorporation of MK into concrete has many advantages: it helps to reduce CO_2 emission; increases flexural and compressive strength; increases durability and resistance to chemical attack; makes concrete denser and reduces permeability; enhances workability; enhances finishing of concrete, appearance and color; reduce the efflorescence; reduce shrinkage (Siddique & Klaus, 2009). Incorporation of MK in concrete as cement replacement or as an addition decreases the pore size distribution and enhances mechanical properties of concrete including CS, splitting tensile strength, and flexural strength (Siddique & Klaus, 2009). The addition of MK in cement paste refined the pore structure and increased the proportion of pores with radii < 20 μm (Khatib & Wild, 1996). The total porosity of paste was observed to decrease with the addition of MK by up to 20% (Bredy, Chabannet, & Pera, 1988). Poon et al. (C-S Poon, Lam, Kou, Wong, & Wong, 2001) noted that cement paste with 5-20% MK had a higher value of f'_c at all ages from 3-90 days as compared with control mix.

In the manufacturing of ferrosilicon and silicon alloys, SF is produced as a by-product. It is ultrafine particles and this fineness makes SF excellent pozzolanic material that reacts rapidly with the hydration product of cement and enhances concrete density due to the micro-filling effect(Sarıdemir, 2013). After an extensive literature survey, it was found that the SF content has been used up to 50% of cement replacement, however, more beneficial effects were observed in the dosage range of 5-20%. The higher dosage of SF maybe not be economical due to its high cost. During the cement hydration, one of the products formed is $Ca(OH)_2$ which does not contribute significantly to strength enhancement. The SiO_2 content in SF reacts with $Ca(OH)_2$ and produced an additional amount of C-S-H gel which improves the concrete mechanical strength, make the microstructure denser and results in durable concrete(Mehta & Monteiro, 2017). The high mechanical properties of concrete are desirable in many applications such as in buildings that are prone to earthquakes. High strength concrete can help to increase the resistance to seismic-induced damage in reinforced-concrete buildings (Danesh et al., 2021). It was observed that a significant amount of $Ca(OH)_2$ decreased with the addition of SF at 3 days. Moreover, it was reported that all the $Ca(OH)_2$ was consumed when 16% SF was used as cement replacement, irrespective of the water-to-binder (w/b) ratio (M.-H. Zhang & Gjørv, 1991).

In order to attain sustainability in the construction industry, there is an increasing trend of using alkali-activated materials and SCMs. The mix design of concrete, the optimum dosage of different constituents, and estimation of mechanical strength such as CS is a complex problem because of the non-homogenous nature of concrete and the non-linear relationship between mixture proportions and strength. Yet, there is a need to develop robust and reliable models for the estimation of CS of sustainable concrete with FA, MK, and SF with adequate accuracy. This will help to know the CS of sustainable concrete with mix design without time-consuming and costly experimental tests and laboratory trial batches.

For many years, researchers have been using machine learning (ML) techniques for the prediction of different properties of cement-based materials due to their superior accuracy and robustness (Chaabene, Flah, & Nehdi, 2020; Shah, Rehman, Javed, & Iftikhar). Ayaz et al. (Ayaz, Kocamaz, & Karakoç, 2015) incorporated a high volume of mineral admixtures (fly ash + slag) and predicted the CS of concrete at 3, 7, 28, and 120 days by using M5P. They observed 97% prediction accuracy of M5P. Behnood, Behnood, Gharehveran, & Alyamac (2017) had gathered 1912 data points from published literature and modelled the CS of normal and high-performance concretes by M5P. The input parameters were cement, fly ash, blast furnace slag, water, SP, fine aggregate (F.agg), coarse aggregate (C.agg), and days. They obtained a value of R^2 equal to 0.91 and 0.9 for the training and testing sets, respectively. M5P has two main advantages: it gives a simple mathematical equation and it is convenient to develop and implement an M5P model (Behnood et al., 2017). Recently, Shah, Rehman, Javed, & Iftikhar (2021a) developed a GEP model for predicting CS of FA concrete and it was compared with linear and nonlinear regression analysis and RSM. The developed model has adequate accuracy, however, complex nonlinear equations generated by GEP may be difficult to use for practical purposes. Similarly, Akin et al. (Akin, Ocholi, Abejide, & Obari, 2020) also employed GEP for the estimation of CS of concrete with MK. In addition to construction materials, machine learning techniques have been in other civil engineering sub-field such as they were used for seismic vulnerability assessment of existing reinforced concrete buildings (Kumari et al., 2022). Nonetheless, a dearth of research has been conducted to explore the CS of sustainable concrete and to generate simple mathematical equations for practical use by using the M5P model tree algorithm. The main reason for employing M5P is that it predict different properties of concrete with high accuracy and give simple mathematical equations that can be used for practical purposes. Other methods such as linear regression analysis and response surface methodology also give simple mathematical equations for prediction of different properties of concrete but their accury is inferior to M5P algorithm. In accordance with our best knowledge, little research has been done to estimate the CS of concrete with FA, MK and SF by using M5P algorithm.

To fill this research gap, M5P models have been developed for the estimation of CS of FA, MK, and SF concrete and these models were compared with gene expression programming (GEP), linear regression analysis and RSM. For this purpose, a large database was gathered from peer-reviewed published articles. Different statistical indicators such as coefficient of determination (R^2), root mean squared error (RMSE), mean absolute error (MAE), and relative squared error(RSE) were used to evaluate the performance of developed models. In addition, in order to find out the relative contribution of independent variables on dependent variables, sensitivity analysis was performed. Moreover, to explore the influence of FA, MK, and SF on the CS of concrete, parametric analysis was performed. The procedure of both sensitivity and parametric analysis can be found in Shah et al., (2022). The flow of this research article is as follows:

1) Data collection from existing literature on CS of concrete with FA, MK and SF.
2) Applying M5P algorithm for prediction of CS of concrete with FA, MK and SF.
3) Comparing M5P models with other modelling techniques such as GEP, linear regression analysis and RSM.
4) For each type of concrete (i.e. concrete with FA, MK and SF), the best model was chosen for doing sensitivity and parametric analysis.

1.1 Data collection

The database of FA concrete was collected from Shah et al. (2021b) while the databases of MK concrete were gathered from different research papers (Akin et al., 2020; Dinakar, Sahoo, & Sriram, 2013; R. Ferreira, Castro-Gomes, Costa, & Malheiro, 2016; Güneyisi, Gesoğlu, & Mermerdaş, 2008; Joshaghani, Moeini, & Balapour, 2017; Khatib, 2008; Lenka & Panda, 2017; Madandoust & Mousavi, 2012; Meddah, Ismail, El-Gamal, & Fitriani, 2018; Chi-Sun Poon, Kou, & Lam, 2006; Ramezanianpour & Jovein, 2012) and shown in Table 1 in the supplementary document. The database for SF concrete was collected from (Afroughsabet & Ozbakkaloglu, 2015; Ajileye, 2012; Altun & Oltulu, 2020; Benaicha, Roguiez, Jalbaud, Burtschell, & Alaoui, 2015; Dilbas, Şimşek, & Çakır, 2014; Elsayed, 2011; Elyamany, Abd Elmoaty, & Mohamed, 2014; Fallah & Nematzadeh, 2017; Güneyisi, Gesoğlu, & Özturan, 2004; Hanumesh, Varun, & Harish, 2015; Huchante, Chandupalle, Ghorpode, & TC, 2014; Johari, Brooks, Kabir, & Rivard, 2011; Köksal, Altun, Yiğit, & Şahin, 2008; Lam, Wong, & Poon, 1998; Luo, Si, & Gu, 2019; Mazloom, Ramezanianpour, & Brooks, 2004; Meddah et al., 2018; Meleka, Bashandy, & Arab, 2013; Mohamed, 2011; Naik & Vyawahare, 2013; Nili & Afroughsabet, 2010; Nili & Salehi, 2010; Chi-Sun Poon et al., 2006; Pradhan & Dutta, 2013; Ramadoss, 2014; Salam, 2015; Sarıdemir, 2013; Siddique et al., 2017; Sobolev, 2004; Türkmen, 2003; Uygar & Aydin, 2005; Q. L. Wang & Bao, 2012; Wong & Razak, 2005; Wongkeo, Thongsanitgarn, Ngamjarurojana, & Chaipanich, 2014; Zaw, 2019) and shown in Table 1. All the databases are for cubic specimens. The data was divided into two parts. 67% data was used for the training set and 33% data was used for the testing set as recommended by (Shah et al., 2021a). The input parameters were cement, FA/MK/SF, F.agg, C.agg, superplasticizer (SP), and age of a specimen in days and the output parameter was CS. The descriptive statistics of the database are given in Table 1 while histograms are shown in Fig. 1.

Table 1 Descriptive statistics of the database used in the training set

Statistical indicator	C (kg/m³)	FA/MK/SF (kg/m³)	w/b ratio	F.agg (kg/m³)	C.agg (kg/m³)	SP (kg/m³)	Days	CS (MPa)
				FA concrete database				
Minimum	112	0	0.19	279	0	0	1	0.8
Maximum	702	544	0.94	1293	1242	35	365	123.6
Mean	313	110	0.44	769	926	3.81	61.52	40.3
Standard error	4.8	4.94	0.0058	9.5	12.4	0.26	3.65	1.05
Standard deviation	108	110	0.13	212	277	5.78	81.64	23.4
Kurtosis	0.63	4.33	0.91	-0.133	1.54	11.8	5.3	1.22
Skewness	0.51	1.86	0.69	0.197	-1.34	3.02	2.27	1.14
				MK concrete database				
Minimum	176	0	0.21	272	175	0	1	3.84
Maximum	681	256	0.79	1007	1513	12.4	180	106
Mean	397	43.4	0.42	748	993	3.05	30.77	47
Standard error	3.25	1.54	0.005	6.82	10.4	0.12	1.51	0.94
Standard deviation	78.9	37.34	0.12	165	252.4	2.87	37	22.9
Kurtosis	0.61	5.6	0.68	-0.27	1.34	0.035	4	-0.54
Skewness	0.06	1.5	0.75	-0.28	-0.79	0.84	1.92	0.38
				SF concrete database				
Minimum	188	0	0.2	469	0	0	1	11
Maximum	1000	215	0.79	2750	1225	43	365	129
Mean	410	36	0.42	768	1045	8.4	67	60
Standard error	5.2	1.42	0.006	12.8	9.9	0.445	4.4	1.1
Standard deviation	116	32	0.14	288	222	9.95	98.2	24.4
Kurtosis	5.6	5.45	0.29	33.6	7.12	5.5	3.55	-0.34
Skewness	1.32	1.53	1.02	5.34	-2.4	2.31	2.1	0.45

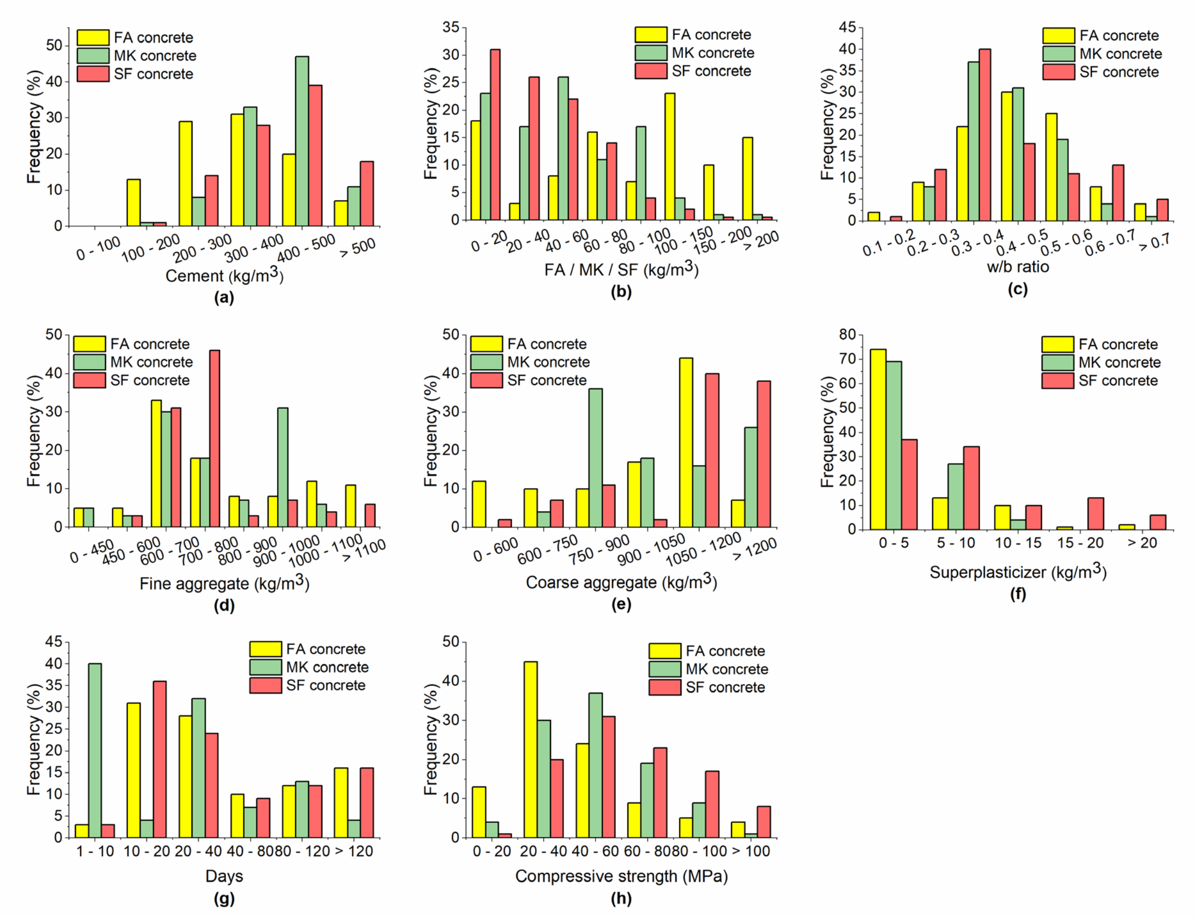

Figure 1: Histogram of (a) cement; (b) SCMs; (c) w/b ratio; (d) F.agg; (e) C.agg; (f) SP; (g) days; (h) CS

2 METHODOLOGY

2.1 M5P model tree algorithm

The M5P algorithm is the extended form of the M5 algorithm which was originally developed by Quinlan (Quinlan, 1992). Fig. 2 presents the illustration of M5. The input data is split into different groups (called sub-spaces) which include data with shared features as shown in Fig. 2a. Linear regression models are used in sub-spaces in order to reduce the variation in data. The information from sub-spaces is used for the creation of several nodes on which the splitting process is performed` based on a given attribute (Fig. 2b).

M5P is a genetic algorithm first proposed by a study(Y. Wang & Witten, 1996) and it is employed for a regression problem. In this algorithm, linear regression is adopted on the terminal node and sets to different sublocation of linear models with the help of the classification of data into various spaces. On each node, information about the error is presented and it is measured by the default value of the variance of the class that enters the node. The evaluation of any function of that node is carried out by an attribute that reduces expected error. Error calculation per node helps to give information on the dividing criteria of the M5P model tree. At the node, the standard deviation of the class values gives information about the M5P error. The node division is chosen based on the feature that reduces the expected error. Because of the branching method, smaller nodes (child nodes) have less value of standard deviation as compared with greater nodes (parent nodes). Reviewing all possible structures of the system helps to select the system that has maximum potential for the reduction of error. This division may lead to overfitting which ispruned and trimmed trees are replaced by linear functions. More information about the M5P model tree algorithm can be found in (Y. Wang & Witten, 1996).

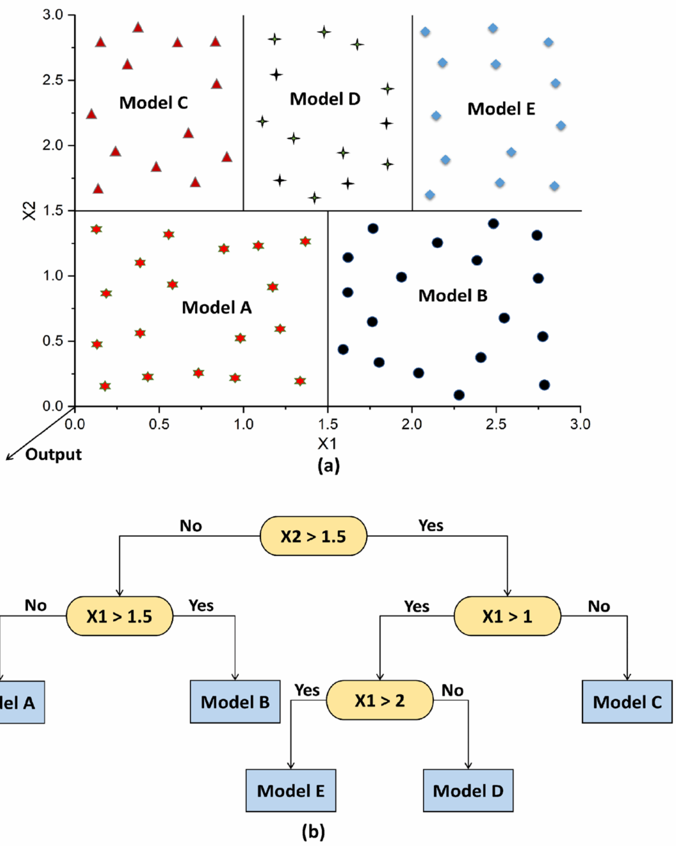

Figure 2: Illustration of M5 algorithm: (a) splitting of input space; (b) building of tree

2.2 Gene expression programming

GEP is the branch of genetic programming (GP) and it was developed by Ferreira (C. Ferreira, 2001). GP is a problem-solving approach that is independent of the domain. It solves problems on the basis of the principle of reproduction proposed by Darwinian and the survival of the fittest. GP uses a parse tree structure in order to get a solution that can alter in length during a run. GEP has five different components which are function set, terminal set, fitness function, control parameters, and terminal condition. The search space of the algorithm is regulated by the former three components, while the speed and quality of search are dealt with by the latter two components. In the GEP algorithm, the solution is obtained by using a character string of fixed length. The solution is then presented in the form of parse trees of different shapes and sizes. These trees are known as expression trees (ETs). GEP has only two main players: one is chromosomes and the other is ET. Due to a genetic mechanism at the chromosome level, it is simple to create the genetic variety in GEP. The multi-genic nature of GEP helps in the generation of complex and nonlinear programs comprised of several subprograms. More information about GEP can be found in (Ferreira, 2001). Linear regression analysis

In the linear regression analysis, a linear connection is developed between input parameters and output. The general form of the linear regression analysis is given as:

Output parameter = constant + (coefficients)*(input parameters)

2.3 RSM

It is the statistical way for the development of the relationship between input parameters and output. The quadratic model was used for the estimation of response by using the input parameter which is shown in equation 1.

$$O = \beta + \sum_{i=1}^{K} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} \beta_{ij} x_i x_j \quad (1)$$

Where O is the response (output), β, β_i, β_{ii}, and β_{ij} are the constant, linear, quadratic, and interaction coefficient, respectively. In addition, x_i $(i = 1,2, \ldots \ldots k)$ represent the input parameters.

2.4 Model development and evaluation criteria

Three M5P models were developed for the prediction of CS of FA, MK, and SF concrete. WEKA software was used for this purpose. Different parameters were tested in order to get a model with superior accuracy and it was observed that the default setting of the software results in a highly accurate model. The general form of the equation can be written as:

$$CS = \mathrm{a} + (\mathrm{b} \times \mathrm{C}) + (\mathrm{c} \times \mathrm{SCMs}) + (\mathrm{d} \times w/b) + (\mathrm{e} \times \mathrm{FA}) + (\mathrm{f} \times \mathrm{CA}) + (\mathrm{g} \times \mathrm{SP}) + (\mathrm{h} \times \mathrm{days}) \quad (2)$$

In order to compare M5P models with GEP, three GEP models were developed for the estimation of CS of FA, MK, and SF concrete. For the GEP models, different parameters were tested in order to get a model that gives a highly accurate prediction on an unseen database of the testing set. After several trials, optimum parameters of GEP models are listed in Table 2. All other parameters of the GEP models were kept default in GeneXproTools 5.0 software.

Table 2 Parameters of developed GEP models

Parameters	GEP model for FA concrete	GEP model for MK concrete	GEP model for SF concrete
Head size	8	12	8
Chromosome	150	50	100
Genes	3	4	4
Linking function	Addition	Addition	Addition
Number of generations	100, 000	100, 000	100, 000

Different statistical indicators were used to assess the performance of developed models such as RSE, RMSE, MAE, and R^2. The mathematical equations of these indicators are given in Eqs. 3-6.

$$\mathrm{RSE} = \frac{\sum_{i=1}^{n}(e_i - a_i)^2}{\sum_{i=1}^{n}(\bar{a} - a_i)^2} \quad (3)$$

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(a_i - e_i)^2} \quad (4)$$

$$\mathrm{MAE} = \frac{\sum_{i=1}^{n}|a_i - e_i|}{n} \quad (5)$$

$$\mathrm{R}^2 = 1 - \left(\frac{\sum_{i=1}^{n}(a_i - e_i)^2}{\sum_{i=1}^{n}(e_i)^2}\right) \quad (6)$$

Where, a_i and e_i are the actual/experimental and estimated values, respectively, $\bar{a}$ is the average actual/experimental value, and n represent the total number of samples. A model with a high value of R^2 and low values of RSE, RMSE, and MAE for both training and testing sets indicates that the model trained well on known data in the training set and predicted CS with high accuracy on an unseen database of the testing set.

3 RESULTS and DISCUSSION

3.1 Fly ash concrete

3.1.1 M5P developed model

Fig. 3 shows the developed model trees generated based on Eq. 2. There are 19 linear models developed and their corresponding coefficients are given in Table 3. The comparison of actual CS and estimated CS by M5P for both training and testing sets for FA concrete is shown in Fig. 4 (a and b). In the training set, the value of R^2 is 0.89 which is close to 1 and shows that the developed M5P model trained well. The accuracy of the model in the training set can be observed by the value of slope (0.86) which is close to 1. In the case of the testing set, the value of R^2 = 0.86 indicates that the developed model predicted CS with adequate accuracy based on an unseen database of the testing set. This indicates that the proposed M5P model can predict CS of concrete with FA with high accuracy which will help to obtain mix design for desired strength and schedule formwork removal. Normally, in order to obtain a mix design for desired CS, several experiments and trials need to be done in a laboratory which is a time-consuming and costly process. This developed model will save time and cost by giving a mix design for required strength by using simple mathematical linear equations.

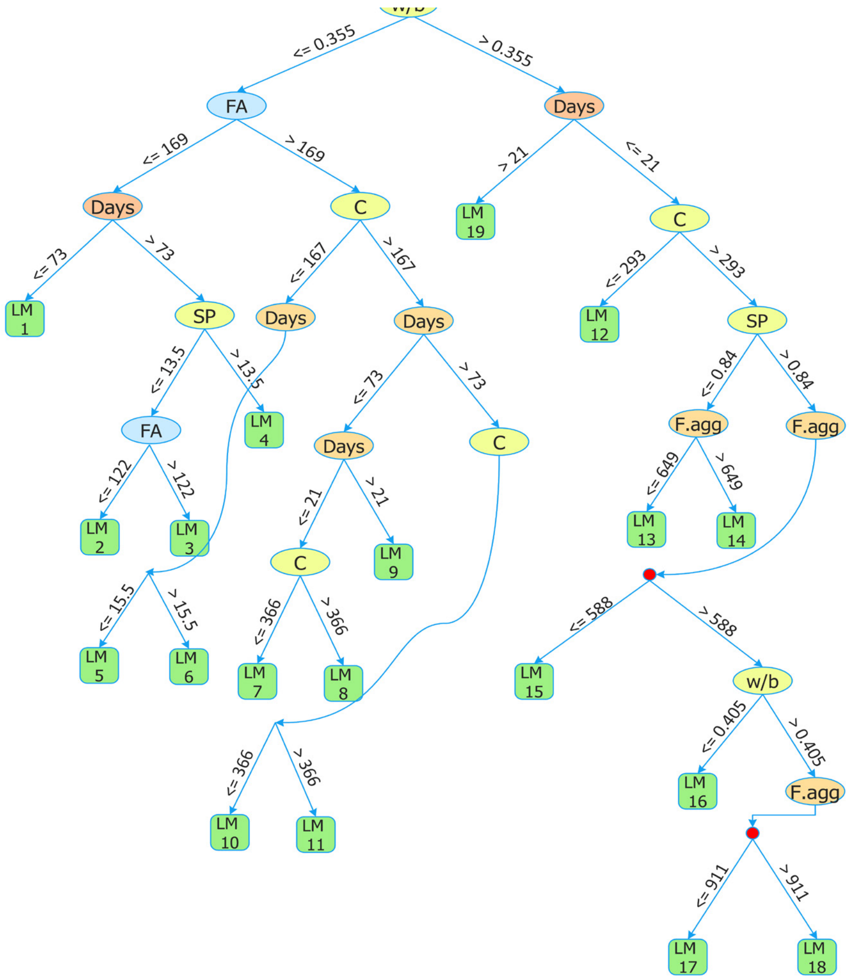

Figure 3: Model tree structure of M5P for FA concrete

Table 3 Coefficients of linear models generated by M5P model for FA concrete

Linear model	Coefficients							
	a	b	c	d	e	f	g	h
LM 1	96	0.0025	-0.061	-247	0.044	0.0017	0.154	0.446
LM2	122	0.0078	-0.04	-214	0.017	0.0017	0.266	0.104
LM 3	114	0.0078	-0.045	-190	0.017	0.0017	0.266	0.101
LM 4	99	0.0078	-0.027	143	0.017	0.0017	0.47	0.1
LM 5	54	0.069	-0.07	-62	0.01	0.0017	0.2024	0.1057
LM 6	43.6	0.123	-0.068	-62	0.0133	0.0017	0.2024	0.1088
LM 7	69	-0.0198	-0.065	-62.24	0.0133	0.0017	0.2024	0.1098
LM 8	70	-0.024	-0.065	-62.24	0.0133	0.0017	0.2024	0.1098
LM 9	69.9	-0.024	-0.06	-62.24	0.0133	0.0017	0.2024	0.116
LM 10	77.7	-0.0227	-0.07	-62.24	0.0133	0.0017	0.2024	0.089
LM 11	78.7	-0.0306	-0.07	-62.24	0.0133	0.0017	0.2024	0.0899
LM 12	-5.17	0.04	-0.008	-5.56	0.0117	0.0001	0.57	1.21
LM 13	24	0.0046	-0.018	-5.5	-0.003	0.0001	0.68	0.4264
LM 14	19	0.0046	-0.019	-5.56	-0.0009	0.0001	0.68	0.6
LM 15	28	0.004	-0.026	-22.2	0.006	0.0001	0.71	0.218
LM 16	28	-0.0027	-0.049	-15.8	0.0049	0.0001	1.04	0.46
LM 17	25	0.002	-0.045	-16	0.006	0.0001	0.94	0.54
LM 18	25	-0.0006	-0.045	-15.83	0.006	0.0001	1.11	0.56
LM 19	37	0.03	-0.05	-41.04	0.0116	0.0008	0.84	0.045

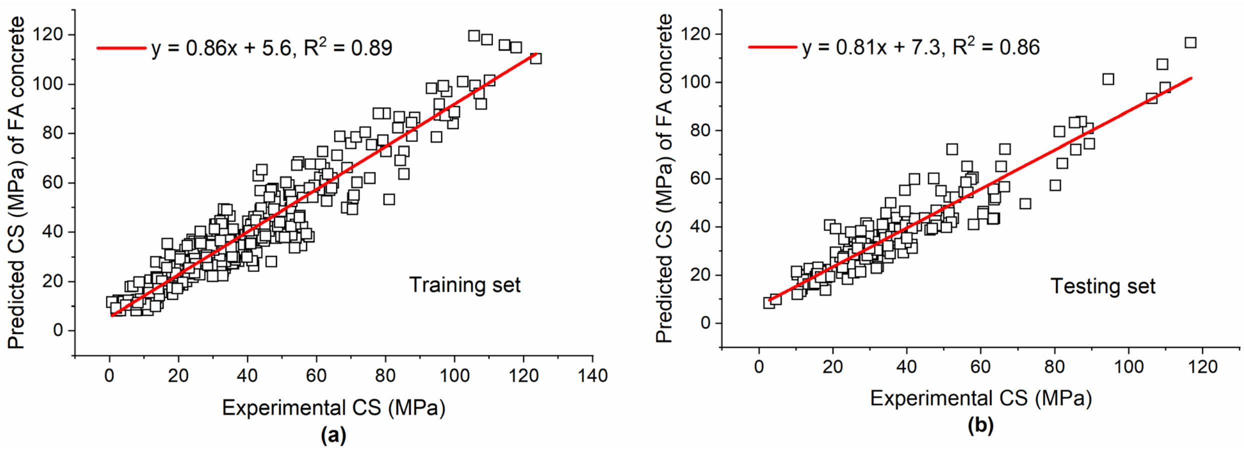

Figure 4: Experimental vs predicted values of CS of FA concrete by using M5P for (a) training set and (b) testing set

3.1.2 Comparison of M5P with other modelling techniques

Fig. 5(a) is the depiction of the comparison of M5P with GEP, linear regression analysis and RSM for the training set. The value of R^2 indicates that M5P possesses superior accuracy with R^2 = 0.89. The value of R^2 for both GEP and RSM was the same (R^2 = 0.88) and it is slightly lower as compared with M5P. The least accurate modelling method was found to be linear regression analysis. Similar to the training set, the M5P model showed higher accuracy in terms of the value of R^2 for the testing set followed by GEP, RSM, and linear regression analysis. One of the advantages of M5P over GEP and RSM is that M5P generates simple linear mathematical equations as compared with complex nonlinear equations by GEP and RSM. Similar to M5P, linear regression analysis gives a linear equation. However, the accuracy of M5P is much higher as compared with linear regression analysis because of the classification of data into various spaces. Other statistical indicators in Table 4 also confirm that the M5P model is superior compared tothe other modelling techniques for the prediction of CS of concrete with FA. Table 4 show that the values of RSE, RMSE, and MAE for M5P are lower as compared with GEP, RSM, and linear regression analysis for both training and testing sets.

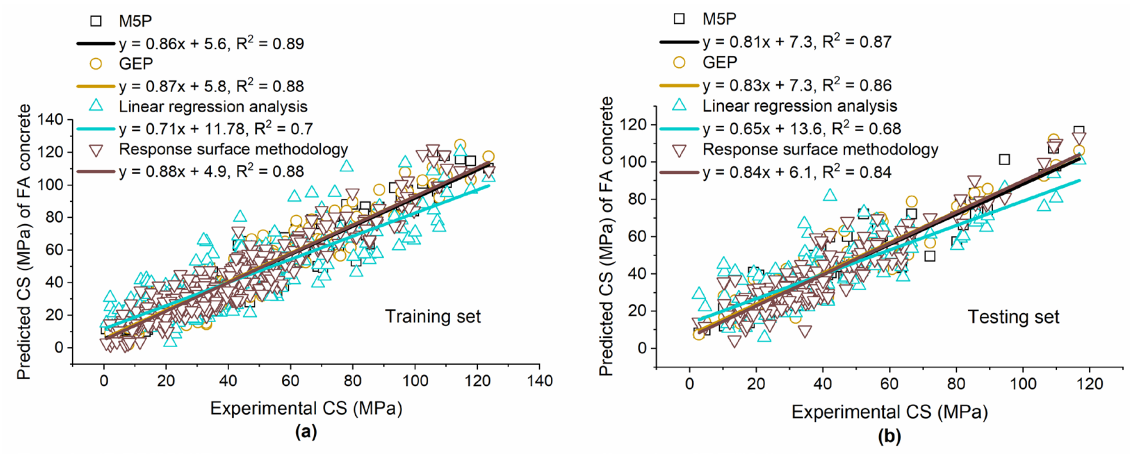

Figure 5: Comparison of M5P, GEP, linear regression analysis, and RSM for predicting CS of FA concrete for (a) training set and (b) testing set

Table 4 Statistical indicators of different models developed for predicting CS of FA concrete

Models for CS of MK concrete	Training set			Testing set		
	RMSE	RSE	MAE	RMSE	RSE	MAE
M5P	8	0.11	6.2	8.2	0.12	6.4
GEP	8.2	0.12	6.5	8.4	0.13	6.5
Linear regression analysis	13.35	0.3	10.4	13.8	0.32	10.6
RSM	8.1	0.12	6.6	8.7	0.14	6.6

3.1.3 Sensitivity and Parametric analysis

Fig. 6 presents the results of sensitivity analysis of concrete with FA. It is shown that the most contributing input parameter in CS are the w/b ratio which has a contribution of 27%. The second input contribution variable is a number of days followed by SP content. In the fourth number, cement contributes to CS followed by FA content with only 8% contribution. A lower contribution by FA is due to fact that it has slow pozzolanic activities at an early age and contributes to CS mainly due to filling effects. As expected, minor contributions were observed by both fine and coarse aggregate as they are only fillers.

Fig. 7 shows that by increasing FA content, the CS decreased linearly. This decrease in CS with FA content can be attributed to low pozzolanic activities of FA at early ages. The histogram in Fig. 1 (g) shows that most of the database of FA concrete was tested for < 40 days. It was observed that 15% FA resulted in a 16% CS reduction at the age of 3 days and at the age of 28 days, this reduction reduced to 4% (Lam et al., 1998). The decrease in CS with FA content was also reported in the study of Shah et al., 2021b). However, it was observed that the CS of concrete increased as compared to the control mix at a later age (90 d) due to pozzolanic and filler effects (Herath et al., 2020). Therefore, it is important to use the optimum content of FA as cement replacement. If FA is used at a high amount that decrease CS, then more cement will be required to increase the CS and this will increase CO_2 content in the atmosphere.

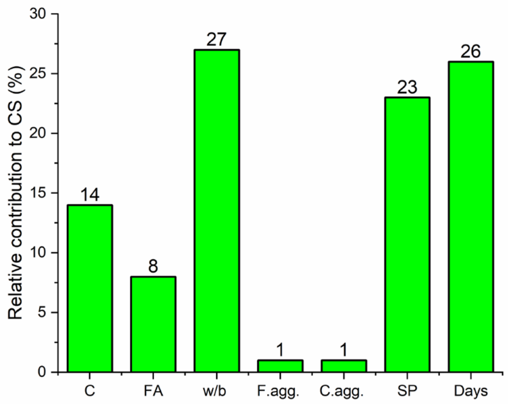

Figure 6: Relative contribution of input parameters on CS with FA

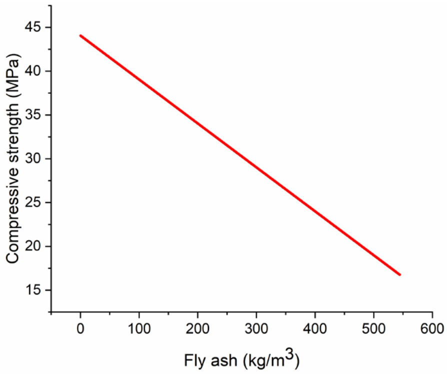

Figure 7: Variation of CS of concrete with FA

3.2 Metakaolin concrete

3.2.1 M5P developed model

The developed model tree structures generated on the basis of Eq. 2 are shown in Fig. 8 and coefficients of developed linear models are shown in Table 5. Due to the large database, the number of linear models produced is 31. The relationship between actual and estimated CS by M5P is given in Fig. 9. The value of R2 forboth training and testing sets is 0.8 and it is lower as compared with the M5P model developed for FA concrete and SF concrete. Moreover, the slope of the regression line for the training set (0.72) and testing set (0.74) is notclose to 1, showing that there is a difference between actual and estimated results.

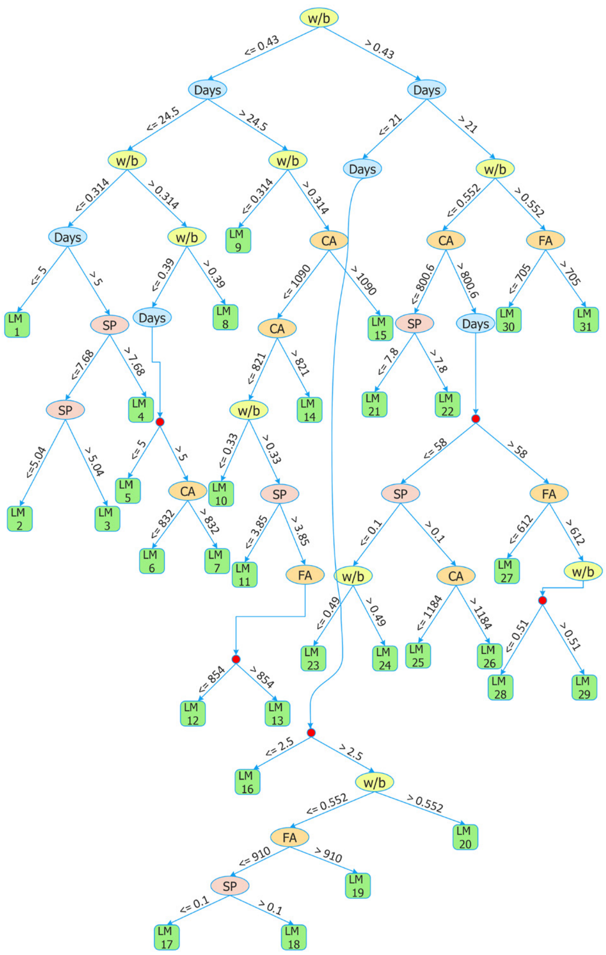

Figure 8: Model tree structure of M5P developed for predicting CS of MK concrete

Table 5 Coefficients of linear models developed for estimating CS of MK concrete by using M5P

Linear model	Coefficients							
	a	b	c	d	e	f	g	h
LM 1	63.8	-0.0008	-0.003	-16.9	-0.0034	0	-2.047	0.77
LM2	69.78	-0.0008	-0.003	-16.9	-0.0034	0	-0.152	0.61
LM 3	65.27	-0.0008	-0.003	-16.9	-0.0034	0	-0.024	0.61
LM 4	70.04	-0.0008	-0.003	-16.9	-0.0034	0	0.545	0.61
LM 5	41.75	-0.0008	-0.003	1.62	-0.0114	0	0.14	0.27
LM 6	51.8	-0.0008	-0.003	1.62	-0.02	0.0017	0.14	0.204
LM 7	52.1	-0.0008	-0.003	1.62	-0.02	0.0043	0.14	0.204
LM 8	31.1	-0.0008	-0.003	15.56	-0.0028	0	0.14	2.145
LM 9	83.67	-0.0008	-0.003	-24.45	-0.0054	0	0.232	0.12
LM 10	42.51	-0.0008	0.0027	25.95	-0.0032	0	0.6004	0.0755
LM 11	47.14	-0.0008	0.0027	15.5	-0.0032	0	0.49	0.097
LM 12	46.45	-0.0008	0.0027	15.5	0.001	0	0.49	0.0647
LM 13	50.54	-0.0008	0.0027	15.5	-0.0004	0	0.49	0.0647
LM 14	53.48	-0.0008	0.1154	10.98	-0.0032	0	0.46	0.06
LM 15	243.06	-0.0008	0.0112	16.13	-0.0032	-0.158	0.45	0.0655
LM 16	42.13	-0.003	-0.001	-49.75	-0.0057	0	0.3535	5.95
LM 17	46.22	-0.003	-0.001	-45.29	-0.0059	0.0099	1.01	0.1326
LM 18	35.1	-0.003	-0.001	-14.062	-0.0059	0.0099	1.01	0.133
LM 19	24.7	-0.003	-0.001	-10.37	-0.0059	0.011	0.99	0.133
LM 20	53.5	-0.003	-0.001	-43.95	-0.01	0.0043	0.853	0.133
LM 21	37.13	-0.0124	-0.001	-18.561	0.0065	0.0079	0.562	0.0736
LM 22	42.9	-0.0124	-0.001	-18.56	0.0065	0.0079	0.6352	0.0439
LM 23	59.5	-0.0186	-0.001	-57.99	0.009	0.0074	0.91	0.0355
LM 24	53.04	-0.0186	-0.001	-52.74	0.009	0.0074	0.91	0.0355
LM 25	41.1	-0.0186	-0.001	-27.23	0.009	0.0133	0.93	0.0355
LM 26	44.61	-0.0186	-0.001	-27.23	0.009	0.0148	0.93	0.0355
LM 27	77.81	-0.0727	-0.001	-45.443	0.0103	0.008	0.64	0.0384
LM 28	110.83	-0.1379	-0.001	-51.52	0.0103	0.008	0.64	0.0384
LM 29	91.1	-0.0809	-0.001	-56.27	0.0103	0.008	0.64	0.0384
LM 30	71.2	-0.0072	-0.001	-8.08	0.0277	-0.0445	0.2857	0.0223
LM 31	476.244	-0.0072	-0.001	-85.69	0.0234	-0.33	0.2857	0.0223

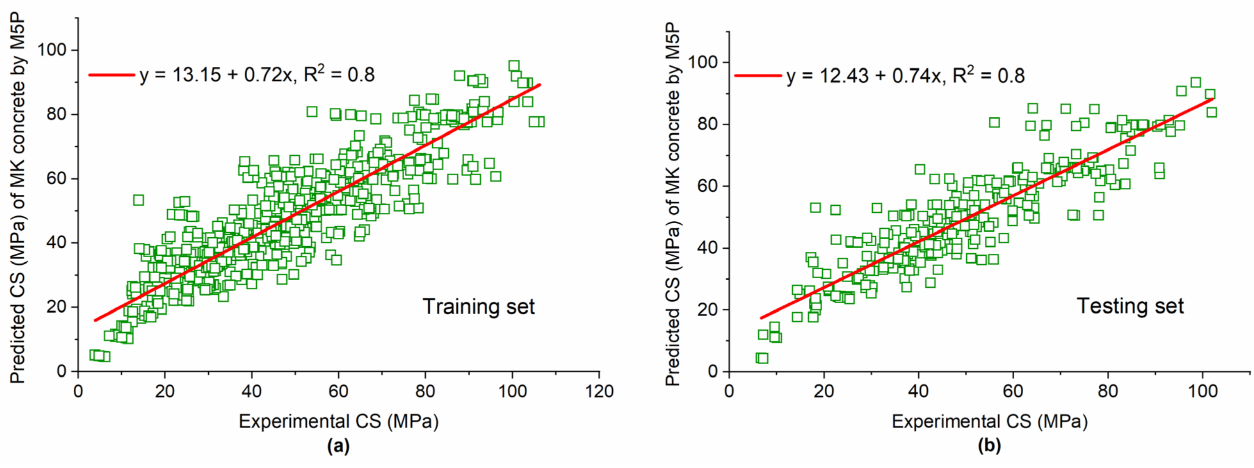

Figure 9: Experimental vs predicted CS of MK concrete by using M5P for (a) training set and (b) testing set.

3.2.2 Comparison of M5P with other modelling techniques

For both the training and testing set, the GEP model showed superior performance followed by M5P, RSM, and linear regression analysis. The value of R^2 for the data sets is 0.8 for M5P while this is 0.82 in the case of GEP as shown in Fig. 10.

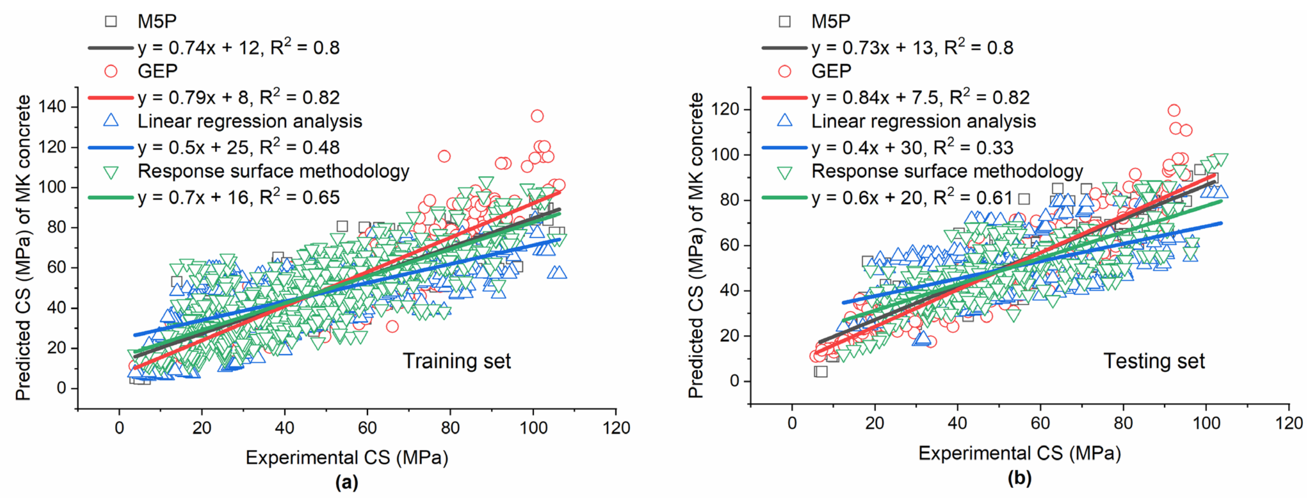

Figure 10: Comparison of M5P with GEP, linear regression analysis and RSM developed for CS of MK concrete for (a) training set and (b) testing set

Although, GEP showed high accuracy for both the data sets, one of the advantages of M5P over GEP is the generation of simple linear models as compared with complex nonlinear equations by GEP (Shah et al., 2022). The linear regression analysis gave $R^2 = 0.48$ for the training set, however, its performance was significantly lower in the testing set. The values of R^2 of RSM for both data sets in the case of MK concrete are lower as compared with FA concrete. The lower values of RSM, RMSE, and MAE for GEP as compared with other modelling techniques also confirm the superiority of GEP for MK concrete as shown in Table 6.

Table 6 Statistical indicators of models developed for estimating CS of MK concrete

Models for CS of MK concrete	Training set			Testing set		
	RMSE	RSE	MAE	RMSE	RSE	MAE
M5P	9.91	0.2	7.4	9.29	0.19	7.1
GEP	9.1	0.18	6.9	8.9	0.18	6.8
Linear regression analysis	16	0.52	13	21	0.78	16
RSM	13	0.35	10.2	14.3	0.41	11.2

3.2.3 Sensitivity and Parametric analysis

The sensitivity analysis of concrete with MK is shown in Fig. 11. Similar to sensitivity analysis results of FA, the top 3 contributing variables are w/b ratio, days and SP content. In Fig. 11, it is also shown that contribution of MK is close to cement (which was not the case for concrete with FA). This is because MK has an early pozzolanic reaction and contributes to CS by reacting with $Ca(OH)_2$. Similar to Fig. 5, the contribution of aggregate to CS is very little.

Fig. 12 shows that CS increases by increasing MK content. The enhancement in CS with MK can be attributed to the filling effect, acceleration of hydration of cement, and the pozzolanic reaction of MK with $Ca(OH)_2$. Due to these effects, Fig. 13 depicts that the microstruscture of cement paste with 15% MK content is more compact and uniform as compared with 0% MK content at 28 days. Higher-strength development was observed at the early ages with MK due to the formation of alumina phases such as C_2ASH_8. MK has a long history as a sustainable material used in concrete as a partial replacement for cement and it is now being used for producing alkali-activated concrete.

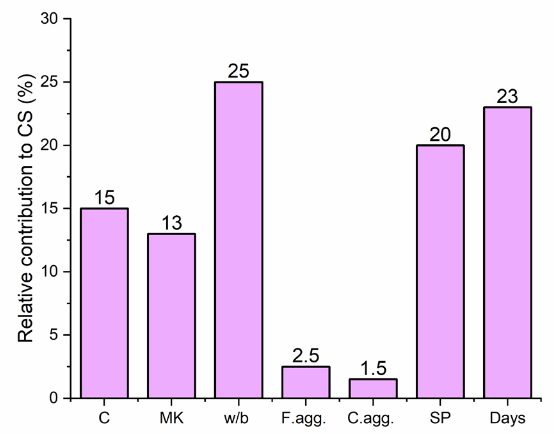

Figure 11: Relative contribution of input parameters on CS with MK

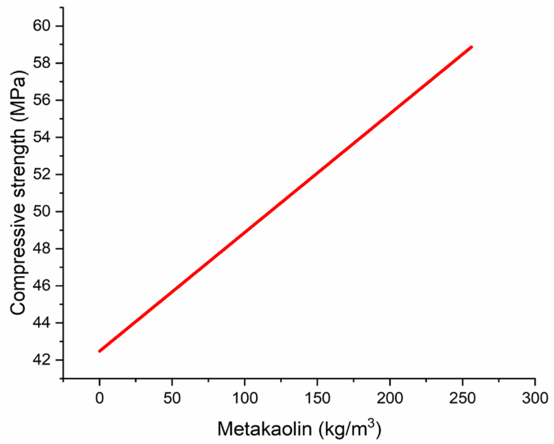

Figure 12: Variation of CS of concrete with MK

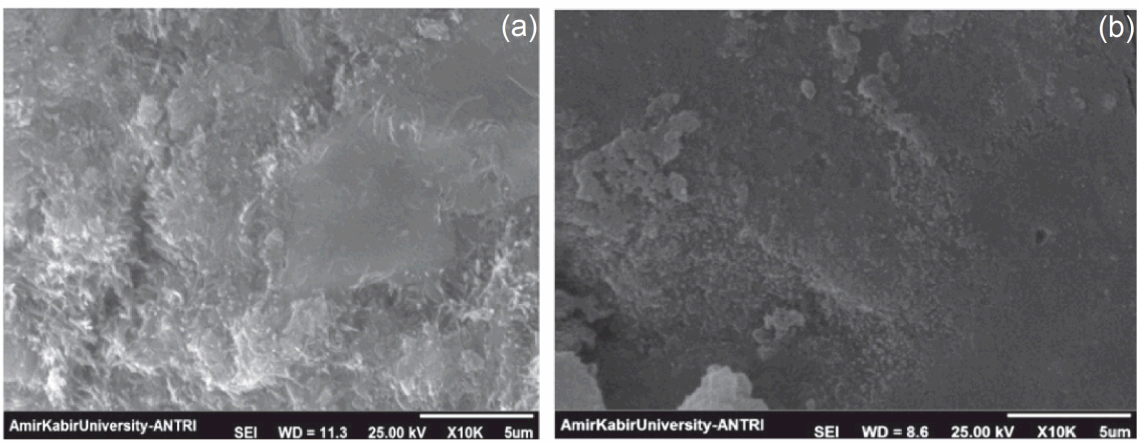

Figure 13: SEM of cement pastes (a) with 0% MK and (b) with 15% MK at 28 days (Fig. obtained from (Ramezanianpour & Jovein, 2012) with permission)

3.3 Silica fume concrete

3.3.1 M5P developed model

The developed model tree structures of M5P for SF concrete are given in Fig. 14 and coefficients of linear models are shown in Table 7.

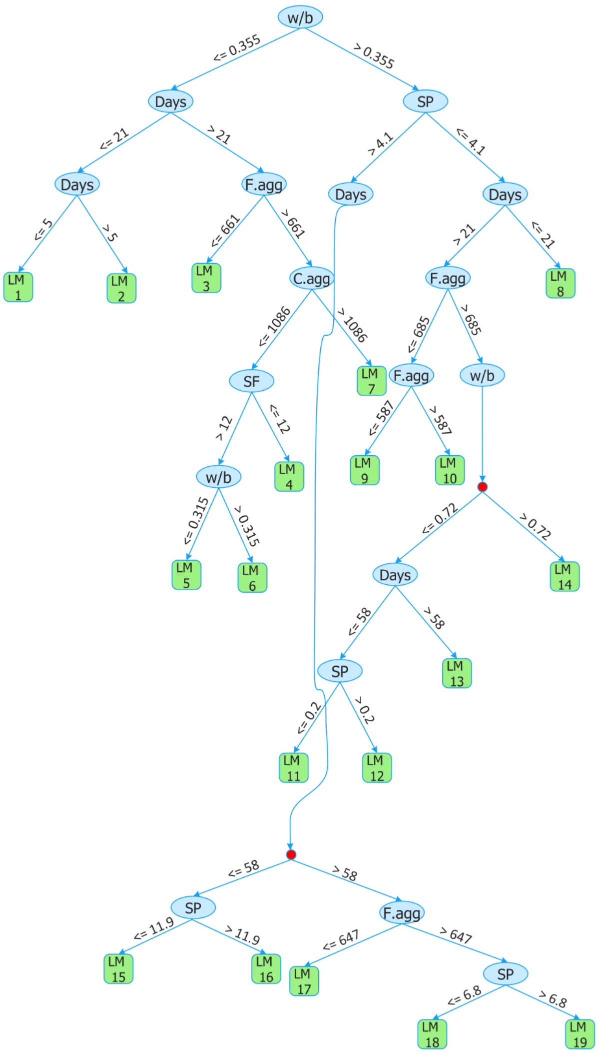

Figure 14: Model tree structures of M5P developed for predicting CS of SF concrete

Table 7 Coefficients of linear models by M5P developed for estimating CS of SF concrete

Linear model	Coefficients							
	a	b	c	d	e	f	g	h
LM 1	-60	-0.0306	-0.01	-94	0.107	0.0605	0.0003	7.3
LM2	164	-0.11	-0.01	-290	0.05	0.0024	0.0003	0.69
LM 3	133	-0.09	0.13	-147	0.0044	0.017	0.0019	0.0235
LM 4	194	-0.087	0	-182	0.0044	-0.0147	0.0019	0.0235
LM 5	197	-0.09	0.04	-185.2	0.0044	-0.0147	0.0019	0.0235
LM 6	201	-0.09	-0.017	-200	0.0044	-0.0147	0.0019	0.0235
LM 7	279	-0.2343	-0.049	-181	0.0044	-0.0215	0.0019	0.0235
LM 8	42	0.012	0	-30	-0.0048	-0.001	0.601	0.729
LM 9	33.55	0.007	-0.015	-18.5	0.032	-0.006	0.87	0.043
LM 10	48	0.007	0.067	-18.5	0.0145	-0.0006	0.87	0.048
LM 11	41	0.0069	-0.053	-7.47	-0.0035	-0.0006	2.72	0.0327
LM 12	43	0.0069	-0.046	-7.47	-0.0035	-0.0006	2.52	0.0327
LM 13	54	0.0069	0.05	-20.5	-0.0035	-0.0006	1.88	0.032
LM 14	46	0.0069	-0.008	-19	-0.0035	-0.0006	1.52	0.04
LM 15	59	0.0015	0	-10.9	-0.0014	-0.0006	-0.3	0.35
LM 16	59	0.0015	0	-10.9	-0.0014	-0.0006	-0.65	0.16
LM 17	71	0.0015	0	-11	-0.0014	-0.0006	0.4	0.035
LM 18	66	0.0015	0	-11	-0.0014	-0.0006	0.52	0.035
LM 19	68	0.0015	0	-11	-0.0014	-0.0006	0.655	0.035

For the development of the M5Pmodel for SF concrete, a different number of instances wastested and it wasobserved that by increasing min. number of instances, the accuracy of the developed model decreased as shown in Fig. 15. There are two ways todecrease the number of linear models: 1) by increasing the minimum number of instances at the leaf node as shown in Fig. 15, however, it will decrease the accuracy of the developed M5P model; 2) by decreasing the number of data points,however, more datapointsshould be included to obtainrobust prediction model.

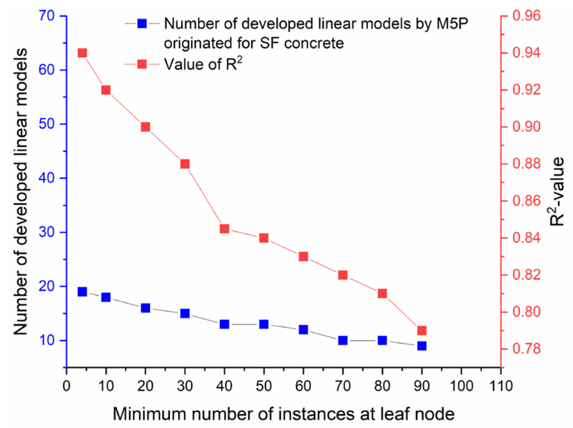

Figure 15: Variation in accuracy of M5P model developed for SF concrete by changing minimum number of instances

The number of generated linear models also decreases by increasing min. number of instances thus resulting in a relatively simple model. Fig. 16 illustrates the relationship between actual and predicted CS by the M5P model developed for SF concrete. In the training set, the high value of R^2 =0.92 indicates that the M5P model trained very well on known data and predicted CS with high accuracy of R^2 = 0.94 on unseen data in the testing set. The high prediction capability of the M5P model for concrete with SF is also confirmed by the value of slope for the training set (0.87) and testing set (0.84) which is close to 1. These values of R^2 are higher as compared with M5P models develop for FA and MK concrete.

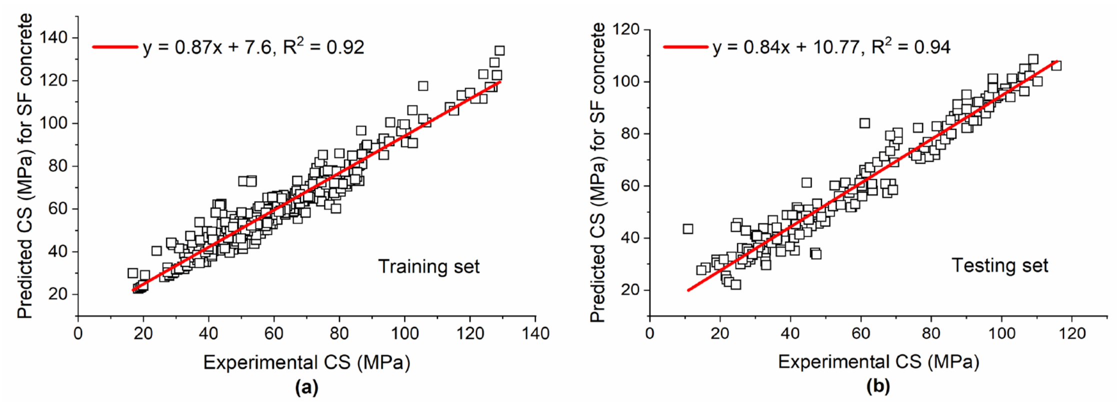

Figure 16: Actual vs estimated CS of concrete with SF by using M5P for (a) training set and (b) testing set

3.3.2 Comparison of M5P with other modelling techniques

The comparison of different modelling techniques for predicting CS of SF concrete is shown in Fig. 16. In the training set, the M5P has shown a greater value of R^2 which is 0.92. This shows that the difference between the actual value and the predicted value is very small. RSM is second most accurate method for estimating CS of SF concrete with R^2 = 0.78 followed by GEP (R^2 = 0.74) and linear regression analysis (R^2 = 0.52). In contrast to the MK database, RSM showed higher accuracy as compared with GEP for the SF database. The mathematical equation generated by RSM may be less complex as compared with the nonlinear equation developed by GEP (Shah et al., 2022). In terms of model accuracies, a similar trend is observed in the case of the testing set as shown in Fig. 17(b). Table 8 also confirms that the accuracy of different models for both data sets is in the order of M5P > RSM > GEP > linear regression analysis.

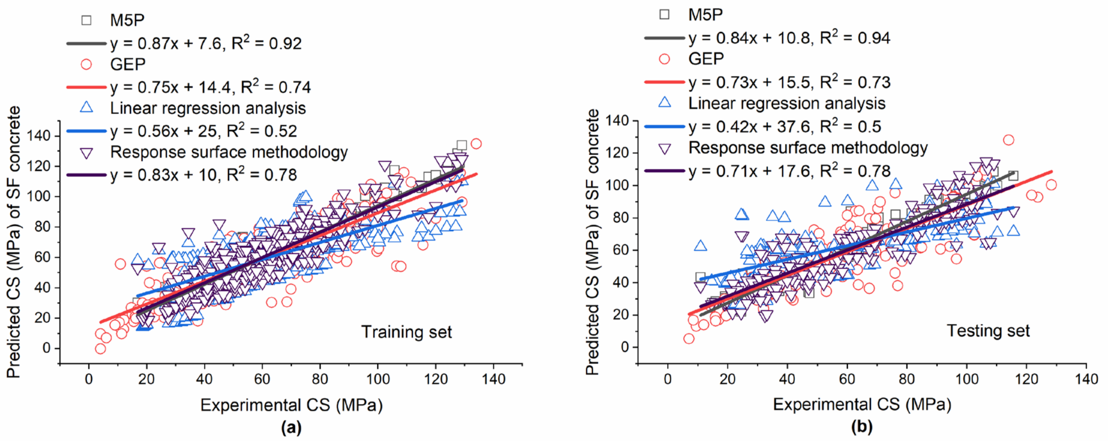

Figure 17: Comparison of M5P model developed for SF concrete with GEP, linear regression analysis and RSM for (a) training set and (b) testing set

Table 8 Statistical indicators of different models developed for CS of SF concrete

Models for CS of SF concrete	Training set			Testing set		
	RMSE	RSE	MAE	RMSE	RSE	MAE
M5P	6.4	0.08	4.9	6.1	0.07	4.7
GEP	13	0.25	9.5	13.1	0.25	9.5
Linear regression analysis	11.3	0.23	8.6	11.2	0.23	8.5
RSM	10.5	0.22	8.3	10.4	0.22	8.2

3.3.3 Sensitivity and Parametric analysis

The sensitivity analysis of concrete with SF is given in Fig. 18. Similar to results of concrete with MK and FA, the top three contributing variables are w/b, days and SP content. Moreover, the figure also shows that contribution of SF and cement is the same which is consistent with Fig. 10. This is because similar to MK, SF also has high initial pozzolanic activities and enhances strength by filler effects and by reacting with hydration product ($Ca(OH)_2$). However, the contribution of fine and coarse aggregate is not significant the same as shown in Figs. 5 and 11.

The CS of concrete increases with the increase in SF content as shown in Fig. 19. This increase in CS with SF content can be attributed to the filling ability of SF due to its ultrafine particles and pozzolanic reaction with calcium hydroxide. Due to these effects, the density of the interfacial transition zone and matrix can be enhanced, thus improving concrete microstructure and mechanical strength (Siddique, 2011). With the addition of SF, it was observed that the interfacial transition zone was less porous with a more homogenous microstructure (Bentur, Goldman, & Cohen, 1987). Nezerka et al. (Nežerka, Bílý, Hrbek, & Fládr, 2019) found a 25% and 65% reduction in the interfacial transition zone with the addition of 10% and 30% SF, respectively. With the addition of 6% and 12% SF, the microstructure of concrete was observed to change from rough, porous, and heterogenous to flat, dense, and homogenous, respectively as shown in Fig. 20 (Lü, Qiu, Zheng, Wang, & Zeng, 2019).

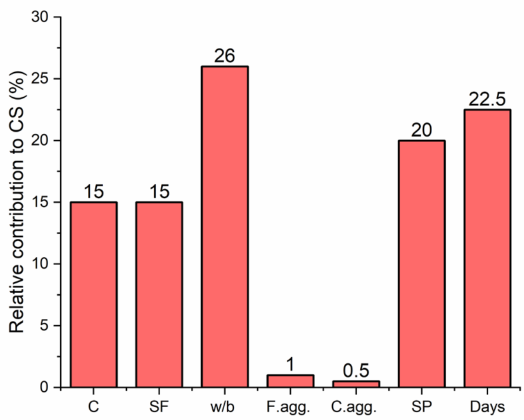

Figure 18: Relative contribution of input parameters on CS with SF

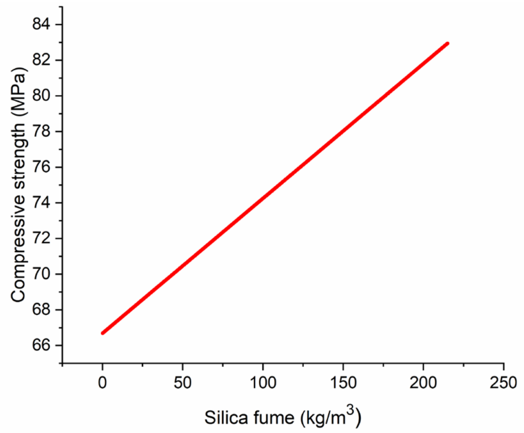

Figure 19: Variation of CS of concrete with SF

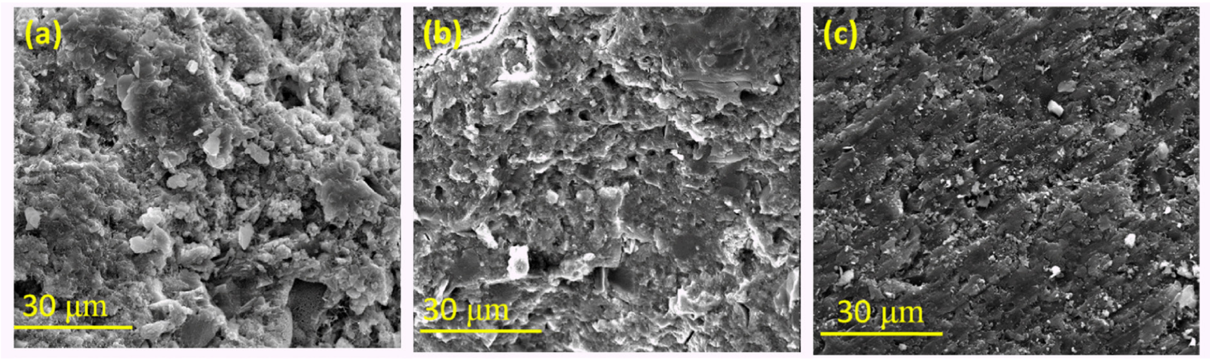

Figure 20: Micro-morphology of surface of concrete at: (a) 0%; (b) 6%; (c) 12% SF content (images obtained from (Lü et al., 2019) with permission)

4 CONCLUSION

In this study, M5P was used to develop simple linear models for the prediction of CS of concrete with FA, MK, and SF. These simple linear mathematical equations can be easily used for practical engineering. The developed M5P models were compared with GEP, linear regression analysis, and RSM. The following conclusions can be drawn from the study:

1. For the FA concrete, the M5P model showed superior accuracy in both training and testing sets as compared with GEP, linear regression analysis, and RSM. Moreover, parametric analysis (PA) showed that by increasing FA content, CS decreased which can be attributed to the slow pozzolanic reaction of FA at early ages.
2. In the case of MK concrete, GEP showed higher performance in terms of the high value of R^2 and low values of RSE, RMSE, and MAE for both training and testing sets as compared with M5P, linear regression analysis and RSM. In addition, PA indicated that by increasing MK content, CS increased linearly because of pozzolanic reaction and filling effects.
3. Similar to FA concrete, M5P showed higher performance for SF concrete and the order of accuracies of developed models is M5P > RSM > GEP > linear regression analysis for both training and testing sets. Similar to MK concrete, by increasing SF content, CS increased linearly which may be attributed to the fast early pozzolanic reaction of SF with calcium hydroxide, and the filling effect due to ultrafine particles of SF.

Author Contributions: Conceptualization, Data curation, Methodology, Investigation, Resources, O Das, Visualization, Writing – review & editing, Al-Saraireh, Majd, Ali.

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