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PREDICTING THE COMPRESSIVE STRENGTH OF FLY ASH BASED GEOPOLYMERS BY ANFIS MODELS

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Abstract- Fly ash-based geopolymers are widely used material as precast and cast in situ round the world. But several factors influence its mechanical strength. Therefore, this work was designed to incorporate such factors in the prediction of mechanical strength through Artificial intelligence. In this work, four parameters were incorporated such as: (i) curing temperature (20, 60 and, 100 °C), (ii) molarity of NaOH solution (8-16), (iii) alkali particle to precursor ratio (0.3–0.5) and (iv) Sodium silica to sodium hydroxide ratio (2–3). Adaptive neuro fuzzy inference system (ANFIS) was used for optimization in order to predict the corresponding compressive strength as output of geopolymer. A large database was used for purpose of training and after worth testing the model as required by ANFIS model. Analytical results by ANFIS were used to construct relationship between mechanical property as output e.g. compressive strength of geopolymers and different constituent parameters. It was observed that training and testing errors were in acceptable range (about 9%). Developed ANFIS model was used to prepare geopolymers which contains low calcium and it is FA based sustainable material, with compressive strength ranging from 25–35 MPa. Hence, validating the significance of the artificial-intelligence based modeling approach ANFIS to bring forth a novel application for design of low calcium, FA based-geopolymers.

Keywords- Hybrid Model, Adaptive Neuro Fuzzy Inference System (ANFIS), Influencing parameters, Fly Ash-based geopolymers, Optimization.

1 Introduction

Implementation of artificial intelligence (AI) based machine learning techniques have been demonstrated to be extremely useful for an ample scope of legitimate non-linear complications as shown from recently conducted relevant researches [1]. Various approaches based on Artificial intelligence have been implemented to check and integrate behavior of different parameters involved in non-linear pattern of mechanical properties. Different approaches are used for this purpose, for example artificial neural network based modelling which performs similar to the neurons of human brain, fuzzy systems, combination of neural network and fuzzy system named as neuro fuzzy system based modeling technique (NFS) and genetic fuzzy systems appeared to be vastly used in construction domain and management applications including simulation of constituent parameters attribute and modulation of nonlinear problems [2]. These modeling techniques have been used to simulate the non-linear and complicated behavior of sustainable materials e.g. to determining the Concrete mix proportions, estimation of compressive strength and other participating parameters for different sustainable construction materials [3]. In this paper AI based method e.g. Adaptive Neuro fuzzy inference system (ANFIS) is utilized to analyze the effect related to different elements involved in characterizes development for example part of alkali to precursor ratio (A/P), ratio of sodium silica to solution of sodium hydroxide (SS/SH), curing temperature for curing the sample under consideration represented as (T) and molarity (M) on compressive strength (F_c') as output. In order to counter problems related to non-linear functionality and complexity of various materials Jang presented model based on



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combination of neural network and fuzzified systems that is neuro fuzzy inference system [11]. Jang used this system for simulation of hugely nonlinear and comparatively complicated functions. An ANFIS is a hybrid model of ANN and Fuzzy system, this advanced fuzzy inference system (FIS) combines the knowledge reasoning and interpretation of FIS and ANN's ability of learning to direct information from inputs into an output [3]. The most salient aspect of ANFIS is its ability to educate itself, learn from previous knowledge or experimentation and extraction or depiction of knowledge from previously performed experiments or examples [4]. Which makes it most powerful tool to deal with inadequate data. NFS consists of combinations of models which bring together the self-learning aspect of ANN and knowledge presenting feature of fuzzy systems. NFS can be divided into two types e.g. type-1 NFS & type-2 NFS, depending upon fuzzy methods used. Mamdani and sugeno are two main categories in type-I and type- II which are based on fuzzy system whereas, type-II can further broke down into two sets as general based type-2 and interval type-2 based on fuzzy systems. In Mamdani type fuzzy system each of the two, the precedent and consequent of rules are composed of fuzzy sets [5]. Sugeno type systems however, uses the precedent sets as fuzzified values while the upcoming successive parameters are always work as functions of inputs parameters that can either be zero value or any other prime order depending upon the nature of upcoming parameter. Sugeno type fuzzy frameworks are more exact and computationally productive that is the reason generally NFS are carried out utilizing sugeno type fuzzy framework [1].

The absolute salient attribute of ANFIS is its capability to learn it self and to extract relative information from previously available database from various experiments, which makes it the most powerful tool to deal with insufficient or poor data. These features of ANFIS model make it easy to study and analyze procedure to estimate or predict relative output for some certain inputs. Depending upon the behavioral impact of vital parameters on the compressive strength as output consideration for geopolymers, the ANFIS model was utilized for its first, to predict the mechanical property e.g. Compressive strength along with validation by comparison with another model as well as by the experimental data.

2 Research Framework

2.1 Simulation by Adaptive Neuro Fuzzy Inference System

While using ANFIS tool in apps from MATLAB different parameters e.g. A/P, SS/SH, M and T are selected as input. All input data is further distributed in to two different parts. One part for training the system and other for testing outputs. Working methodology of ANFIS model is elaborated in Figure 1.

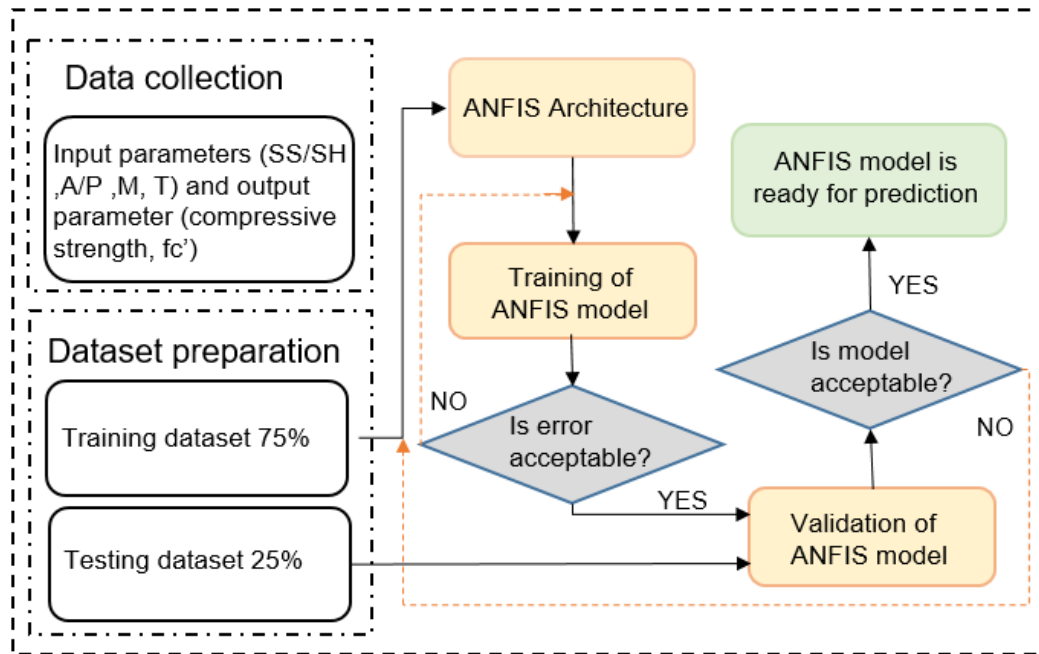


Figure 1 working methodology of ANFIS model

2.2 Mix design database

For the purpose of evaluating the compressive strength and to analyze the behavioral effect of various participating parameters, the database is selected from a study, where a machine learning modelling modeling method e.g. multivariate adaptive regression spline (MARS) model was utilized to access the design mix to prepare geopolymers from mixing different parts for desired compressive strength. For ANFIS model, about 75% part from whole dataset is selected for the training purpose and after completion of training the remaining 25% part is selected for testing the data against previous experiments and ANFIS model (Table 1 of Ref [6]).



2.3 Optimization by ANFIS

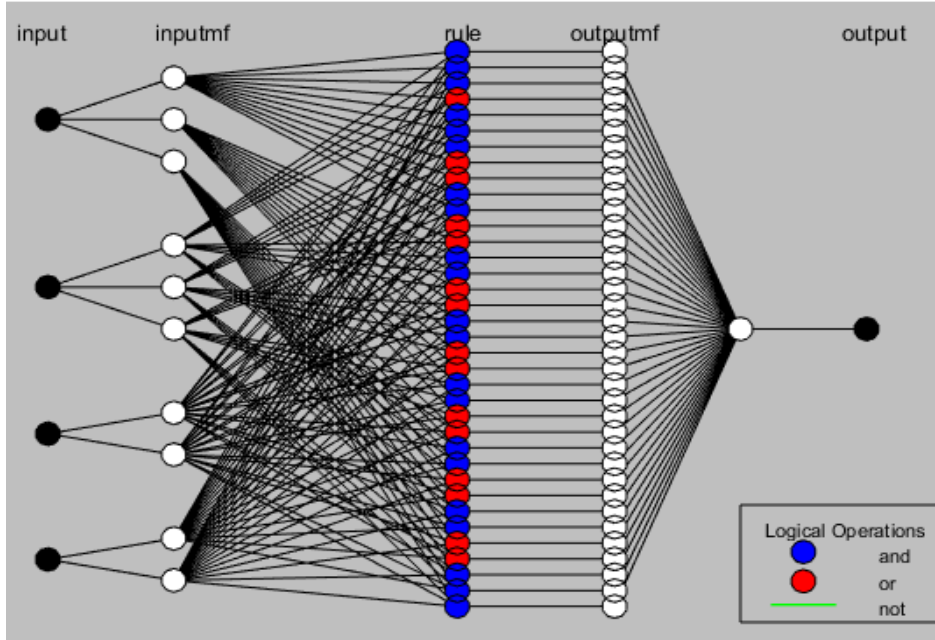


Figure 1: Model Representation of ANFIS Structure

There are five very important adjustments which are made in ANFIS for modeling which are number of input membership functions (MF), type of input and output membership function, method of optimization and number of iterations or total number of epochs. Triangularmf, trapezoidalmf, bell shapedmf, gaussianmf and sigmoidmf are types of MF for input parameters. For output MF we have either constant or linear MF. There are two types of optimization methods e.g. Hybrid and backpropagation[7][3][8]. After studying different researches for this purpose we have utilized triangular type of input MF with three MF for SS/SH & Alk/P and two MF for molarity and temperature each. Output MF was selected as constant. Hybrid optimization method gives less testing and training error where as no. of epochs were 500. Figure 2 shows model representation of ANFIS structure.

3 Results

For the purpose of evaluating the performance of developed predictive model, a variety of performance estimation parameters are used which includes coefficient of relation (R), root mean square error (RMSE) and mean absolute error (MAE). These methods are widely used to validate prediction problems in different machine learning models [9][10].

$$R = \frac{\sum_{i=1}^n (V_{ai} - \bar{V}_a)(V_{pi} - \bar{V}_p)}{\sqrt{\sum_{i=1}^n (V_{ai} - \bar{V}_a)^2} \sqrt{\sum_{i=1}^n (V_{pi} - \bar{V}_p)^2}} \quad (1)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (V_{ai} - V_{pi})^2}{n}} \quad (2)$$

$$MAE = \frac{\sum_{i=1}^n |V_{ai} - V_{pi}|}{n} \quad (3)$$

V_{ai} & V_{pi} are existent and estimated numeric values for compressive strengths, \bar{V}_a & \bar{V}_p are the absolute mean values of existent V_{ai} and estimated V_{pi} values whereas 'n' is the total number of experiments previously conducted for purpose



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under consideration. Diminutive values for root mean error and mean absolute error indicates better correlation between compressive strength extracted from database and optimized compressive strength value. Predicted values for training exhibit better correlation with actual compressive strength obtained from experiments then values predicted from model testing. Values calculated for correlation coefficient, root mean square and Mean absolute error are provided in table 1. R^2 should be in range of 0.7 to 1 which shows better fitting of original and optimized compressive strength and yields better software for estimating compressive strength from existing database. Here we have satisfying relation for R^2 as depicted in table 1. Diminutive values for RMSE and MAE leading to little deviation of predicted values from actual values is a function of limited database which is extracted from existing literature.

Table 1 Error values for training and testing using ANFIS model

		Correlation co. (MPa)	Root mean Square (MPa)	Mean absolute error (MPa)
Training Process	ANFIS	0.74	2.806	0.348
Testing Process	ANFIS	0.90	5.533	1.106

A line graph consisting of scatter plot comprising existent and estimated values for compressive strength for training and testing data regimes are presented in Figure 3. Variation in existent and estimated compressive strength is also represented in Figure 4. Straight line shows when actual values are exactly same to predicted values.

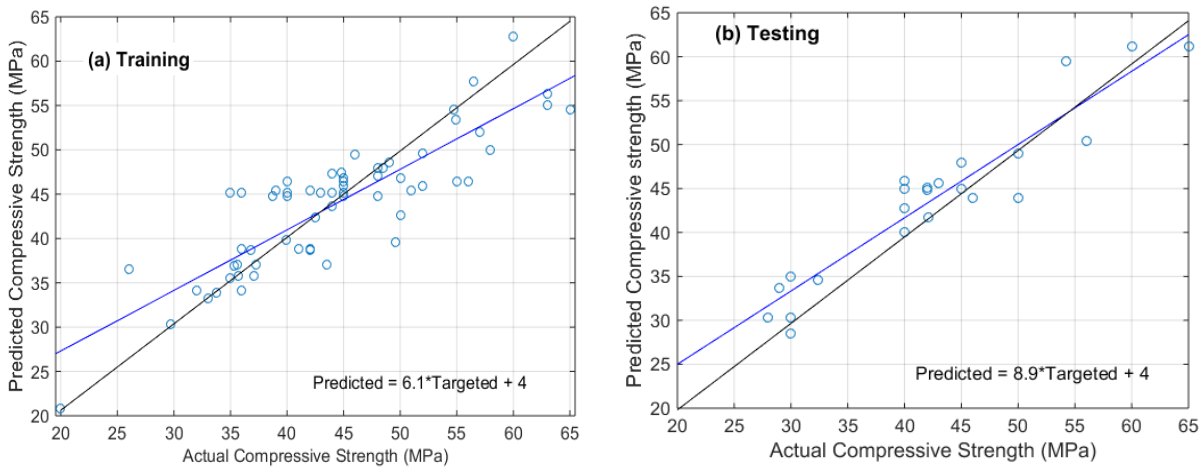


Figure 3 Scatter plot showing variance in predicted compressive strength w.r.t experimentally estimated compressive strength extracted from database for training and testing



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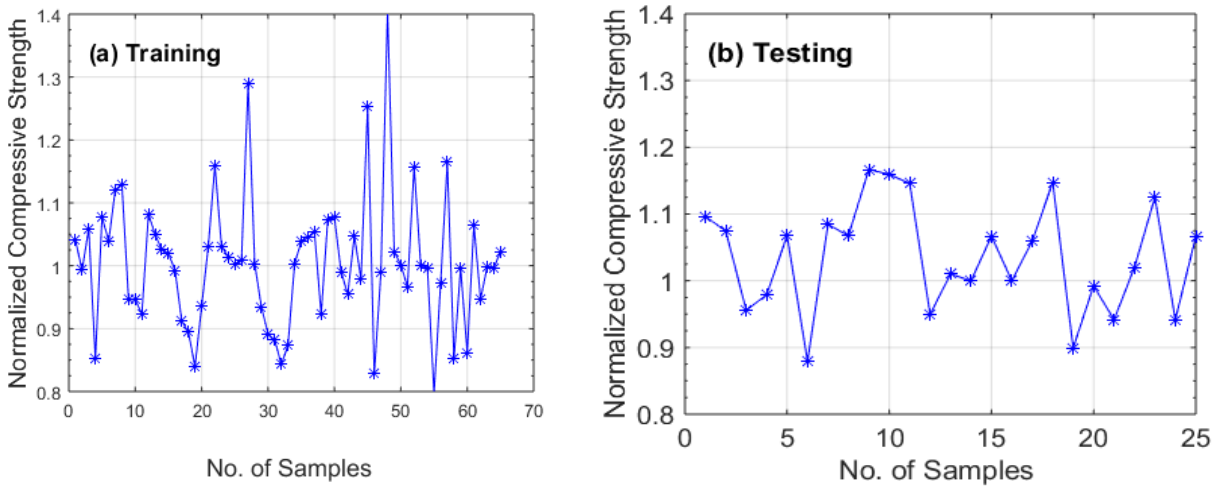


Figure 4 Compressive strength represented graphically as normalized for training and testing data set regimes

3.1 Combined influence of Parameters

Contour plots

Various contour plots extracted from trained and tested ANFIS model are shown in figures which elaborates relation of all four parameters with f_c' . These plots can be used to find out designing parameters and there values for our required strength of geopolymers.

Effect of alkali/precursor ratio

Figure 5(b, e, & f) shows effect of alkali/ precursor ratio and relationship of this ratio with SS/SH, molarity and temperature. Figure 5b shows that for a range of 0.2-1 with increasing ratio compressive strength of f_c' also increases. Figure 5e show for lower Alk/P ratio combined with higher SS/SH ratio can result in increased compressive strength. Figure presents that for a certain fixed amount of molarity, if value for Alk/P ratio changes then different f_c' can be obtained.

Effect of sodium silicate/ sodium hydroxide ratio

Figure 5(e) shows a strong relationship between SS/SH and Alk/P. For a range of 1-3 a higher range of compressive strength can be achieved for Alk/P ranging 0.6-0.7. SS/SH is also related to molarity which is shown in figures (h).

Effect of NAOH molarity

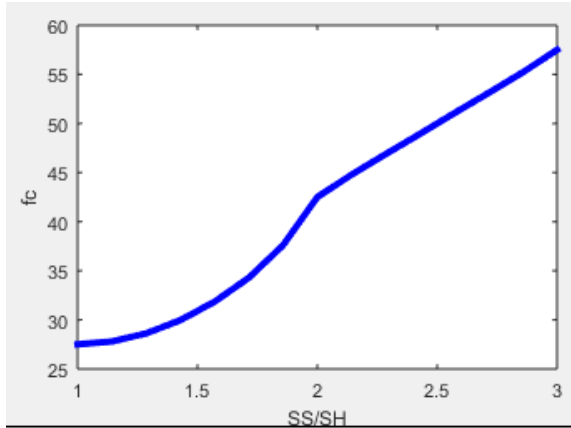
Figure 5d, f and g shows that for a specific value of molarity, a large number of various compressive strengths can be achieved by just changing values for Alk/p and SS/SH ratios. It can be seen from above figures that even for high value of compressive strength can be achieved by changing SS/SH and Alk/P even for reduced molarity. Whereas, overall trend (figure f) shows that by increasing molar value compressive strength decreases.

Effect of temperature

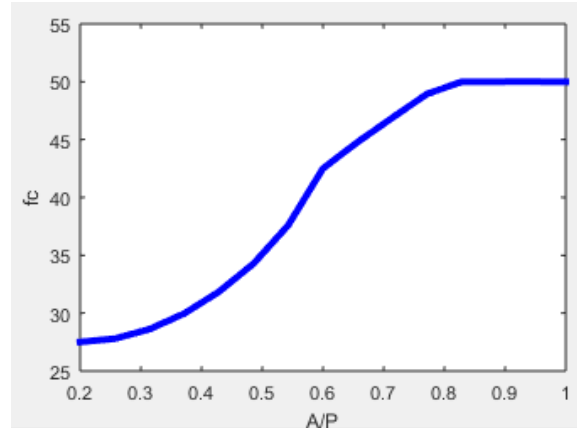
There exist a promising impact of temperature on compressive strength of geopolymers. For elevated temperatures initial setting time reduces but strength get increases as shown in figure c and g.



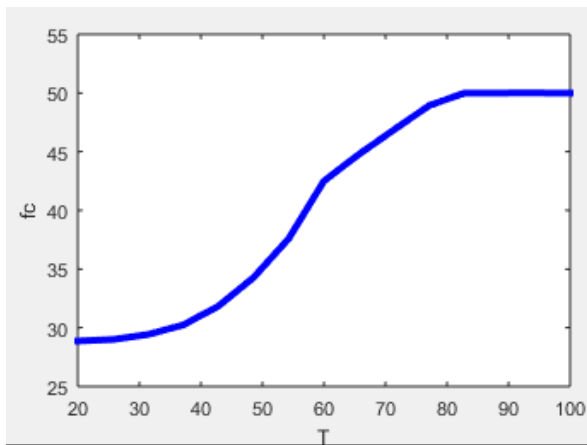
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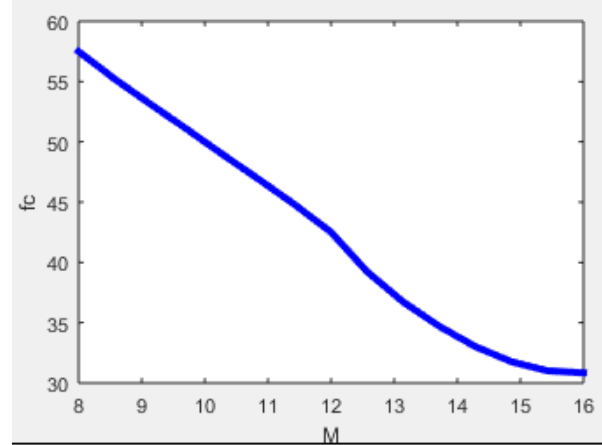
(a)



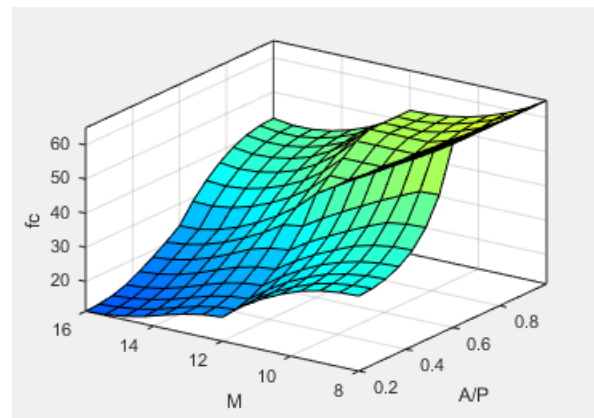
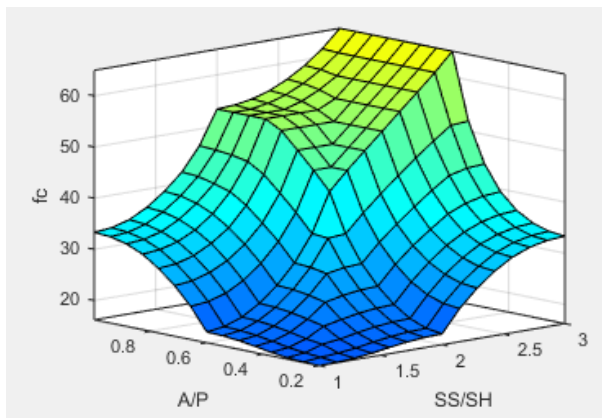
(b)



(c)



(d)





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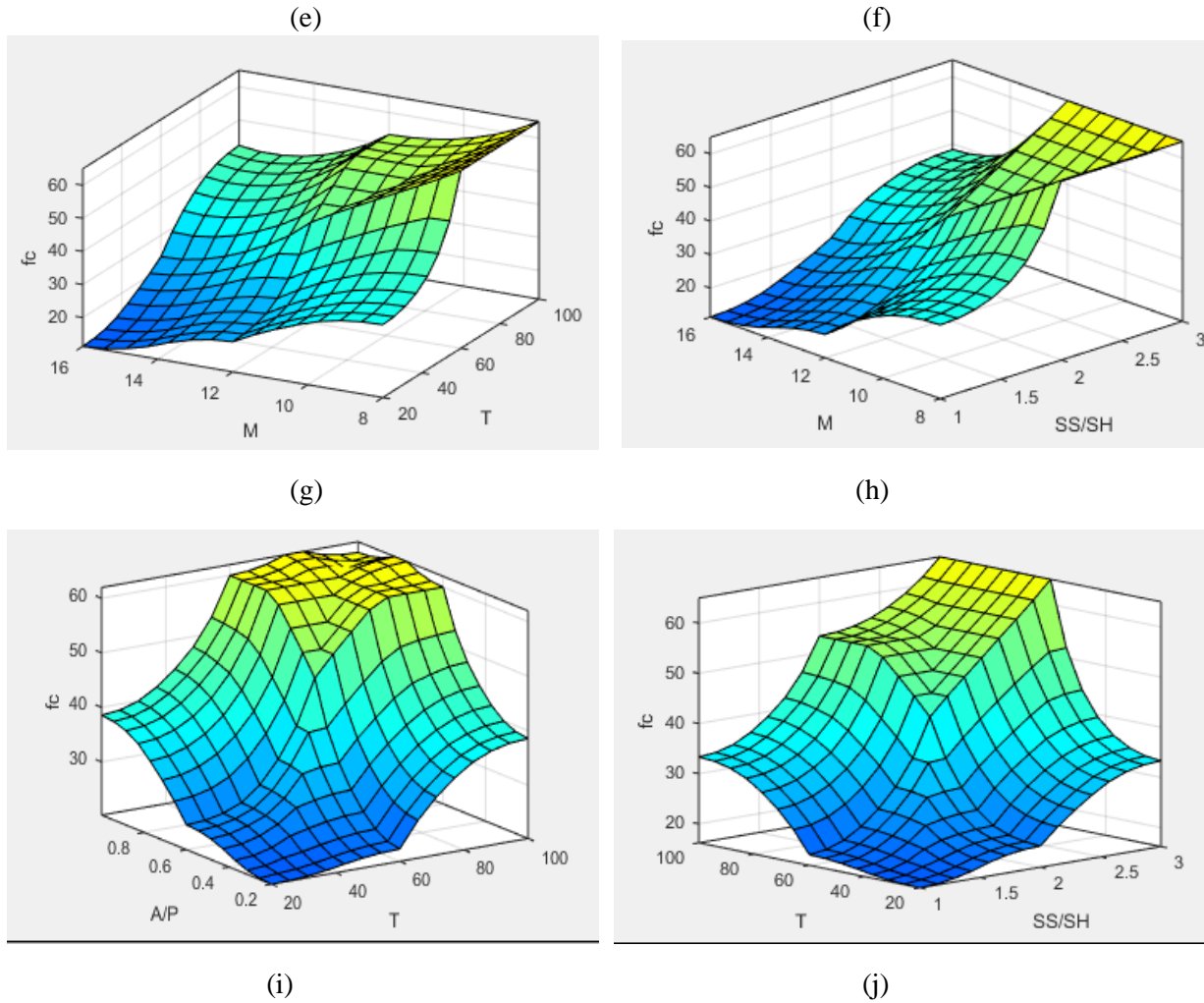


Figure 5 Relationship of different parameters w.r.t compressive strength (f_c')

4 Conclusions

Artificial intelligent based modeling method e.g. ANFIS is used for optimization and design of geopolymer consisting low calcium part and which is Fly ash based with nominal compressive strength ranging from 25 to 35MPa.

After running the model the training error was found out around 8.45 which is considerably less for the same database. Hence a better machine learning approach was utilized to design a geopolymers

ANFIS model was utilized to construct contour plots for presentation of correlation among four key input parameters with compressive strength (f_c'). From these contour plots influence of each parameter in combination with other three parameters was assessed and mix design for different compressive strengths (20-35 MPa) were developed.

The experimental results showed compressive strength values in a range of 20 to 33 MPa for the geopolymers paste at ambient and heat curing with optimal compressive strength is attained for A/P = 0.4 and SS/SH = 2.5.



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The validation of model was done by computing the estimated compressive strength by keeping all the parameters same as for the experiment. The predicted compressive strength values are in good agreement with those calculated by the experiments. Hence ANFIS can be used for mix design of geopolymers pastes.

The experimental results, for checking by ANFIS with compressive strength above 35MPa represent strong agreement with the optimized compressive strength. Hence, constructed contour plots can be implemented for design of low calcium FA-based geopolymers.

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