Chapter 4

Application of Artificial Neural Network for Strength Retrieval of Stabilized Red Mud

4.1 Introduction

This study explored the performance of artificial neural network to predict the unconfined compressive strength of stabilized red mud based on two different approaches. It is well known that the major restrictions for a neural network based model is availability of sufficient data set for good neural network training is required. If the data set available for training is insufficient, the neural network model will not work. There is still no unique formula and thumb rule available in the literature regarding the number of data sets needed for training the neural networks, and it solely depends upon the nature of problem and quality data set. The number of data optimization problem is still an important issue in the neural network application[209]. However, it is not possible sometimes to conduct such large number of experiments for the time-bound important project. In order to overcome such constraints, authors have tried to develop an ANN model based on an experimental designed approach (DOE) and analyze the efficiency of an ANN model with fewer well-design data. From the literature review, it is seen that very few works have been reported on use of design of experiment for studying the engineering properties of artificially cemented soil. However, Experimental designed approach has been successfully applied in other areas for to obtain an optimized solution for the response [178, 179, 181–183, 185]. The present work is an attempt to fill the gap of past studies on stabilized red mud. In this chapter, experimental designed artificial neural network (ANN) model is developed and compared with those of conventional designed ANN model for the assessment of the unconfined compressive strength. Finally, equations have also been proposed for predicting the unconfined compressive strength (UCS) using the neural network, and Part of the work have been published as [3].

4.2 Overview of Artificial neural network

Artificial neural network is a machine learning system that is inspired by the models of biological neurons of the human brain during the problem-solving procedures. Collection of data, normalization, and splitting of data, selection of types of network architecture, numbers of hidden layers and neurons, selection of activation function, training, and validation of the neural network are the important steps for the successful application of artificial neural network. The chapter 2, Sec 2.8.4 summarizes

[3] **S. Kumar and A. Prasad**, Strength retrieval of artificially cemented bauxite residue using machine learning: an alternative design approach based on response surface methodology," *Neural Computing and Applications*, pp. 1-14, 2018

the detailed study about theory and work procedure of artificial neural network. Feed back neural network spreading (FFBPANN) was used in this study. In this procedure, the input layer neurons pass on their information to each neuron of the hidden layer with their weights. The weighted inputs of each input layer neurons are added and compute the output through transfer functions at each hidden layer. The output values at hidden layer nodes become the input values for the corresponding nodes of the output layer. Finally, the output layer nodes calculate the final output equivalent to their input. Based on the target and calculated output value, the error is computed [237].

4.2.1 Optimization of Initial ANN Model

One of the essential steps of neural network design is the selection of the appropriate number of hidden layers and the number of neurons. The larger number of neurons extends the time for formation while the fewer neurons leads to insufficient network training. There is no unique approach available for the selection of the optimal number of the hidden neuron. However, few researchers suggested guidelines that would be sufficient to model neural network problem in the selection of the numbers of hidden neurons and layers [188, 238]. With respect to the number of hidden neurons, 75% or 2/3rd of inputs, the twice input layer size, the square root of the number of input and output, between the average and the sum of the input and output nodes, or the minimum of root mean square error was recommended [239–243]. Because of the above, a single hidden layer with two numbers of hidden neurons was adopted in the present study. Bayesian regularization as a training function (*trainbr*) with tan-sigmoid transfer function at hidden and output layers was used for modeling the neural network. An ANN toolbox in MATLAB software was implemented to create, train, test, validate, and simulate the ANN models.

4.2.2 Database Preparation

In this study, data sets obtained through conventional and experimental designed (DOE) approach were used to train and test the artificial neural network model. Proportioning of datasets is an important step in the execution of artificial neural network and is solely based on their principles, nature, goals, and algorithmic and computational complexity. Proper proportioning of datasets is needed so that the artificial neural network could train the model with all datasets patterns to achieve a meaningful response. The prime goal of data proportioning is to minimize the error and take care of over-fitting. In the present study, Trial-and-Error (generate and test) method is used to split the dataset for training and testing and the optimum is found at 70% and 30% respectively[243]. In this present study, 180 data sets with three replication obtained from laboratory test using conventional and experimental designed (DOE) approach were used to develop the artificial neural network models. Detailed discussions on input selection and planning for laboratory tests have been included in chapter 2. Table 4.5 shows the range of input and output parameters with descriptive statistics considered for conventional design approach. In Table 4.5 we can see that three parameters are used to predict the unconfined

TABLE 4.1: Range of input and output parameters with descriptive statistics considered for conventional design approach

Parameters	(w) %	(t) days	γ_d (kN/m^3)	L (%)	Lv	η (%)	η/Lv'	UCS (kPa)
Min	26	7	13	3	1.584	48.362	39.54	430.71
Max	30	60	15.5	11	6.447	57.897	55.85	4692.97
Mean	28.00	31.67	14.38	7.00	3.90	52.74	45.94	1775.23
Median	28.00	28.00	14.50	7.00	3.97	52.35	45.69	1695.73
Std dev	1.64	21.85	0.96	2.84	1.52	3.18	3.99	855.81
Count	180.00	180	180	180	180	180	180	180

compressive strength(UCS) of the stabilized red mud, namely molding moisture content(w), curing time(t) and porosity / volumetric lime(η/Lv'). Furthermore, the

ANN model was also developed in the following section, with data sets based on an experimentally designed approach.

4.3 Description of Design of Experiment

Proper selection of points where the response is to be estimated is one of the leading steps for the design of the experiment. Various design of experiment methods is available based on different ways of mapping independent factors. As discussed in Chapter 2, several methods can be applied for experiment design. There are different methods of experimentation, but each method has its own merits and repercussions. The selection of a suitable experimental design is an important step and depends exclusively on the nature, objectives, objective and complexity of the experiment. In this study, response surface methodology (central composite and the Box Behnken) method are selected based on the suitability of the present problem. The range of input as well as their coded level was chosen according to the possible unit weight reached in the field using different compaction efforts and are presented in Table 4.6. As depicted in Table 2, the terms -1, 0, and 1 refer to the lowest, middle, and the highest actual value of the input parameter respectively and used for the design of the experiment. In view of the above, 20 and 17 experiments using faced central

TABLE 4.2: Range of the input parameters in terms of coded and actual factors

Input Parameter	Range		
	-1	0	1
w (%)	26	28	30
t (Day)	7	34	60
η/Lv'	40	48	56

composite ($FCCD$) and Box-Behnken (BBD) design methods respectively were

TABLE 4.3: Design matrix of input and response based on experimental designed approach

Central composite design (CCD)					Box-Behnken design (BBD)				
Run No.	w	t	(η/LV')	Measured UCS	Run No.	w	t	(η/LV')	Measured UCS
1	0	0	0	1380.51	1	0	1	1	1159.95
2	0	0	0	1349.15	2	-1	0	1	803.31
3	0	0	1	750.153	3	1	-1	0	853.785
4	0	-1	0	951.25	4	-1	0	-1	3096.31
5	0	0	0	1324.39	5	-1	1	0	1871.27
6	0	1	0	1886.44	6	0	-1	-1	1785.51
7	-1	-1	-1	2123.27	7	0	0	0	1380.51
8	0	0	-1	3308.91	8	0	0	0	1349.15
9	-1	1	-1	3744.34	9	0	0	0	1392.28
10	-1	0	0	1348.64	10	1	0	1	735.93
11	1	-1	1	500.04	11	1	1	0	1901.375
12	-1	1	1	1136.84	12	0	0	0	1392.28
13	1	1	-1	4692.97	13	1	0	-1	3408.09
14	0	0	0	1392.28	14	0	-1	1	437.88
15	0	0	0	1405.26	15	0	1	-1	4461.02
16	1	0	0	1480.57	16	0	0	0	1337.06
17	0	0	0	1337.06	17	-1	-1	0	942.71
18	-1	-1	1	430.71					
19	1	1	1	847.896					
20	1	-1	-1	2407.332					

carried out in the laboratory for determining the unconfined compressive strength of stabilized red mud specimens. Design – Expert 10, an optimization statistical software package, was used for the design of experiment for central composite design and Box-Behnken design methods, and the results are presented in Table4.7.

4.4 Results and Discussion

4.4.1 Conventional Approach ANN Model

In the present investigation, 180 data sets obtained through conventional experimental approach were used to develop the artificial neural network model. The 135 data out of 180 (75%) data sets were used as the training data sets for the model and the remaining 45 (25%) as test data sets. The scatter plot between measured and predicted values of unconfined compressive strength (q_u) is presented in Fig. 4.1. From Fig. 4.1, it is seen that the predicted values of unconfined compressive

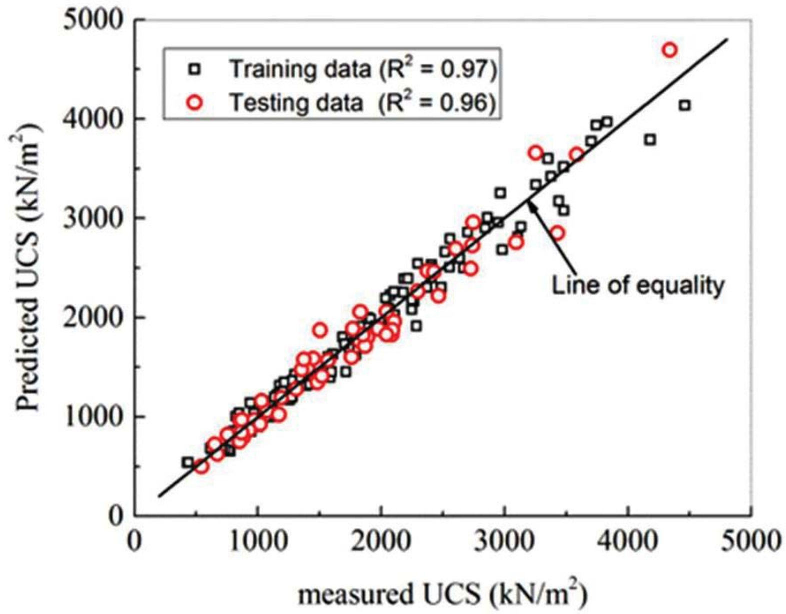


FIGURE 4.1: Scatter plot between measured and predicted values of unconfined compressive strength (q_u) based on conventional designed ANN model

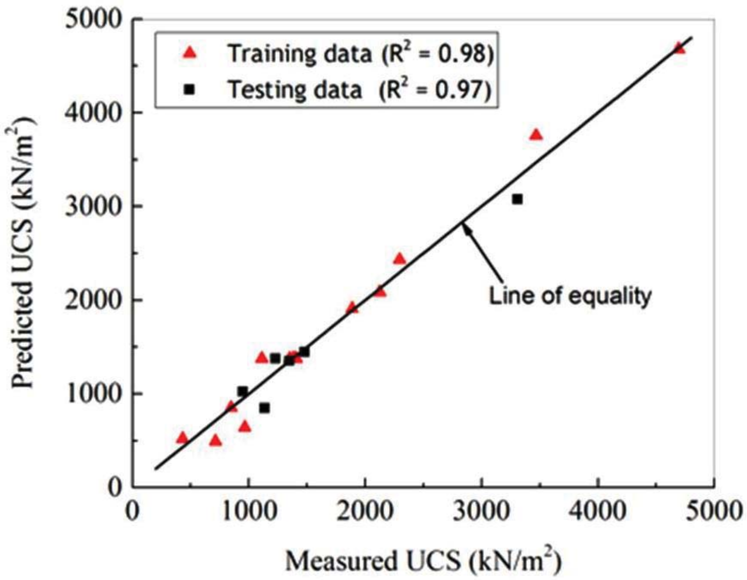
strength using artificial neural network algorithms are close enough to the observed values. For example, the coefficient of determination (R2) for training and testing data sets are close to unity, and that supports the validity of proposed ANN model. Further, various statistical parameters to check the adequacy of the proposed model is discussed in detail in the subsequent section. Based on the trained neural network, final weights and biases may be employed to develop the predictive equation.

4.4.2 Experimental Designed ANN model

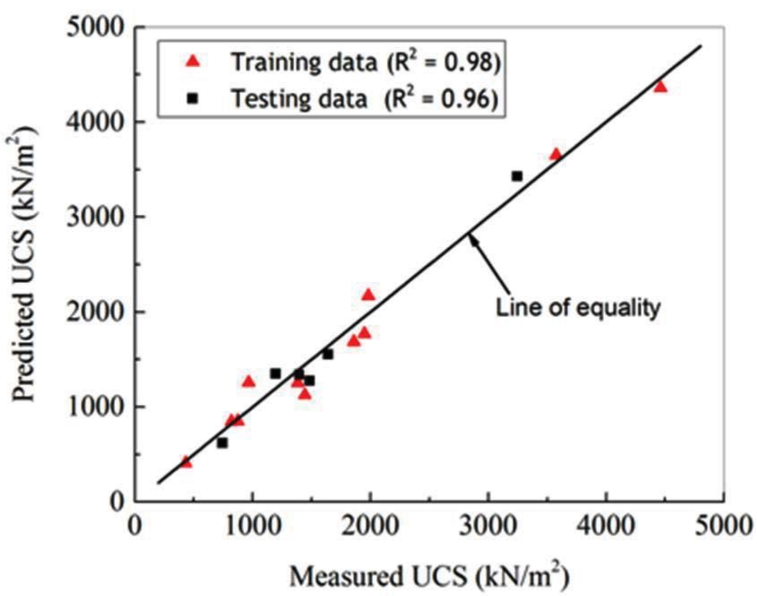
In this segment, the artificial neural network model was trained with 20 and 17 optimized data set obtained by central composite design (CCD) and Box-Behnken design (BBD) methodology respectively. The scatter plots between measured and predicted values of the unconfined compressive strength of stabilized red mud are presented in Fig.4.2. From Fig.4.2, it is evident that the results obtained from CCD and BBD methods are in good agreement with the experimental values. The weights and biases based on the trained network can be efficiently used for sensitivity analysis and developing model equation and are presented in subsequent sections.

4.4.3 Performance Study

From previous sections, it is seen that different models can be successfully developed based on conventionally designed and response surface methodology designed artificial neural network. Now, the important steps are to check the functionality of the various predictive models over the conventional designed actual experimental data sets. The scatter plot of measured and predicted unconfined compressive strength of stabilized red mud based on conventional designed, central composite designed and Box-Behnken designed neural network models are presented in Fig. 4.3. From Fig. 4.3, it is observed that the predicted unconfined compressive strengths are in good agreement with the measured unconfined compressive strengths which confirms that the response surface methodology designed model works well as compared to the conventional model but with significantly less numbers of data sets. Further, to check the adequacy of the proposed models, the study of statistical parameters such as maximum absolute error (MAE), average absolute error (AAE), root mean square error ($RMSE$), mean absolute percentage error ($MAPE$) and coefficient of



(a)



(b)

FIGURE 4.2: Scatter plot between measured and predicted values of unconfined compressive strength (q_u) based on model (a) central composite design and(b) Box-Behnken design ANN model

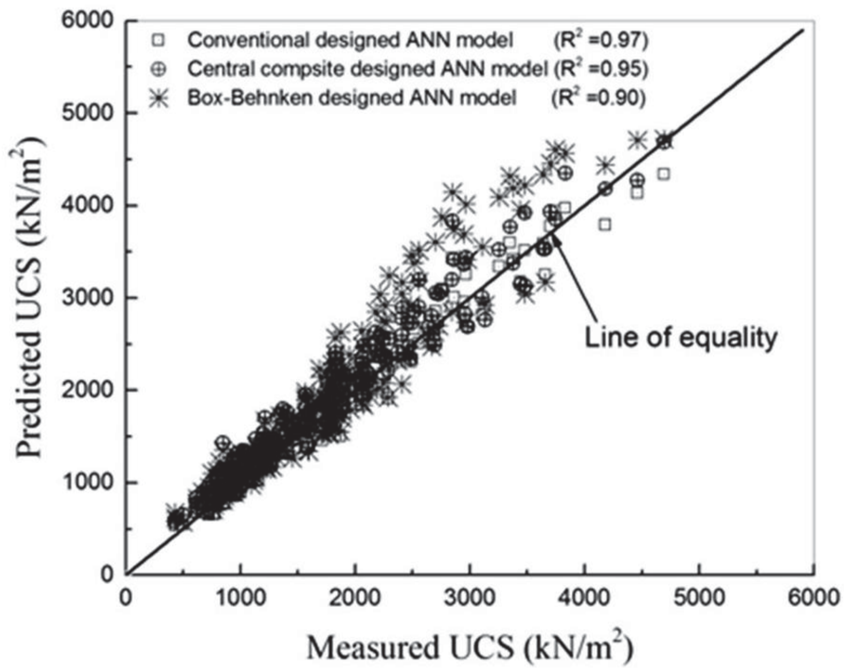


FIGURE 4.3: Variation of predicted vs. measured unconfined compressive strength for stabilized red mud based on conventional, central composite and Box-Behnken designed ANN models

determination (R^2) is quite necessary. Table 4.4 presents the statistical parameters for neural network models based on the conventional designed ($CONVDANN$), central composite designed ($CCDANN$) and Box-Behnken designed ($BBDANN$) methodology.

From Table 4.4, It can be seen that R-squared (R^2) is comparable with all designed approach. For example, R^2 by conventional designed neural network model is 0.97 that changes to 0.95 and 0.90 with central composite and Box-Behnken designed ANN models respectively. $MAPE$ measures the prediction accuracy of proposed equations. It states that the proposed predictive model will be excellent, fair and poor fit with the actual data set if the error is less than 10%, 10%-20% and

Table 4.4: Statistical performance for the conventional designed experimental data sets in UCS based on conventional and response surface methodology designed ANN models

Description	CONVDANN Model	CCDANN Model	BBDANN Model
R^2	0.974	0.954	0.901
MAE	580.53	987.17	1295.302
RMSE	151.122	254.016	395.156
AAE	116.42	202.96	288.302
MAPE	6.96	13.43	16.22

higher than 20% respectively. The values of $MAPE$ are 6.96, 13.43 and 16.22 that shows that the proposed ANN models are working excellent with conventional design approach and good with central composite and Box-Behnken designed approaches. However, the main advantage of the application of response surface methodology over conventional approach is that the number of experiments in case of response surface methodology approach is relatively much less than that in the conventional approach. For example, in the present study, the number of experiments used to successfully develop the predictive equations based on conventional, central composite and Box-Behnken designed approaches are 180, 20 and 17 respectively. Therefore, from the above study, it can be concluded that response surface methodology designed approach may be considered as an alternative over conventional designed approach for estimating the unconfined compressive strength that not only reduces the experimentation time but also saves the resources.

4.4.4 Neural Interpretation Diagram

Neural interpretation diagram (NID) is a visual interpretation for the relation between input parameter and response based on connections of weights among neurons [244]. Weight and bias of the trained neural network based on different approach are presented in Tables (4.5-4.7) .

Table 4.5: Final connection weights and biases based on conventional designed ANN

Neurons	Weights				Biases	
	Input 1	Input 2	Input 3	Output	*bhk*	b_0
1	-0.086	-0.272	1.049	-1.122	1.410	0.531
2	-0.006	0.412	-0.616	0.441	-0.165	-

Table 4.6: Final connection weights and biases based on central composite designed ANN

Neurons	Weights				Biases	
	Input 1	Input 2	Input 3	Output	*bhk*	b_0
1	-0.010	0.161	-0.294	0.098	0.098	0.035
1	0.088	0.382	-0.993	0.899	-0.87	-

Table 4.7: Final connection weights and biases based on Box-Behnken designed ANN model

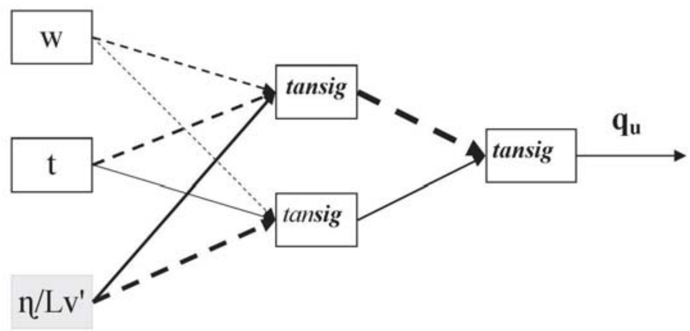
Neurons	Weights				Biases	
	Input 1	Input 2	Input 3	Output	*bhk*	b_0
1	0.0859	0.672	-1.495	0.935	-1.535	0.0823
2	0.0483	-0.317	0.372	-0.503	-0.413	-

The magnitude and direction of weights between layers are represented by different line pattern. Positive weights are represented by solid lines and negative weights by dashed lines, whereas, the thickness of lines represents their magnitude. Positive and negative effect of any individual input parameter on the response follows simple multiplication rule. Different pattern schemes are also considered for the presentation of input. The white and gray rectangle represents the positive and negative effect of input on output respectively. For example, the effect of any particular input parameter will be positive only if the positive or negative magnitude of weights will be present at both the level (input–hidden and hidden-output level). Whereas, alternate positive and negative or vice versa of input–hidden and hidden-output represents the adverse effect of the particular input parameter on the response. Neural interpretation diagrams based on weights and biases are shown in

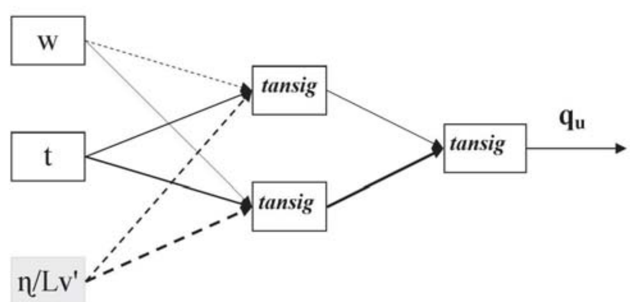
Fig.4.4. A study of Fig.4.4 depicts that moisture content (w) and curing time (t) have positive contribution, whereas, porosity/volumetric lime (η/Lv') has negative contribution on the unconfined compressive strength of stabilized red mud and the same can also be observed from the experimental results presented in 3.

4.4.5 Sensitivity Analysis

Sensitivity analysis is carried out to find the relative contribution of inputs parameters by analyzing the weight of trained neural network and assistance in the selection of relevant input parameters for the development of optimal model equation. It also evaluates how the independent parameters influence the response under given situations.Connection-weight approach has been adopted here to compute the relative importance of a particular input factor on the response (output) [245]. The relative importance has been evaluated by simply adding the product of weights of input layer to hidden layer and hidden layer to output layer for the corresponding input. Fig.4.5 shows the relative importance of input parameters on the response. From Fig.4.5, it is revealed that the input parameter porosity/volumetric lime (η/Lv') has the maximum contribution on unconfined compressive strength followed by curing time (t) and moisture content (w). Further, it is also observed that the contribution of individual input parameters to the output by central composite designed and Box-Behnken design methodology designed ANN models shows an equivalent performance over the conventional designed ANN models but with relatively small data set. Hence, the proposed model based on response surface methodology may be very effective as compared to conventional designed experimental approach for developing a predictive model.



(a)



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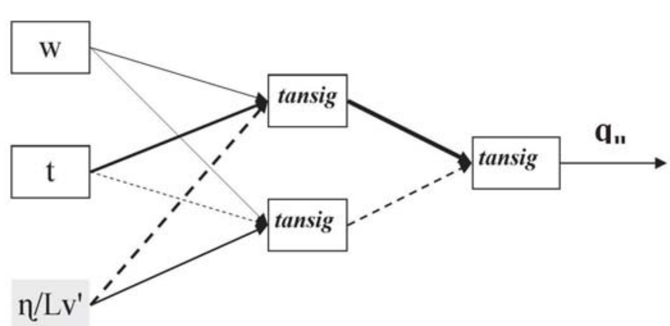

(c)

FIGURE 4.4: Neural interpretation diagrams based on (a) Conventional (b) Central composite and (c) Box-Behnken designed ANN model

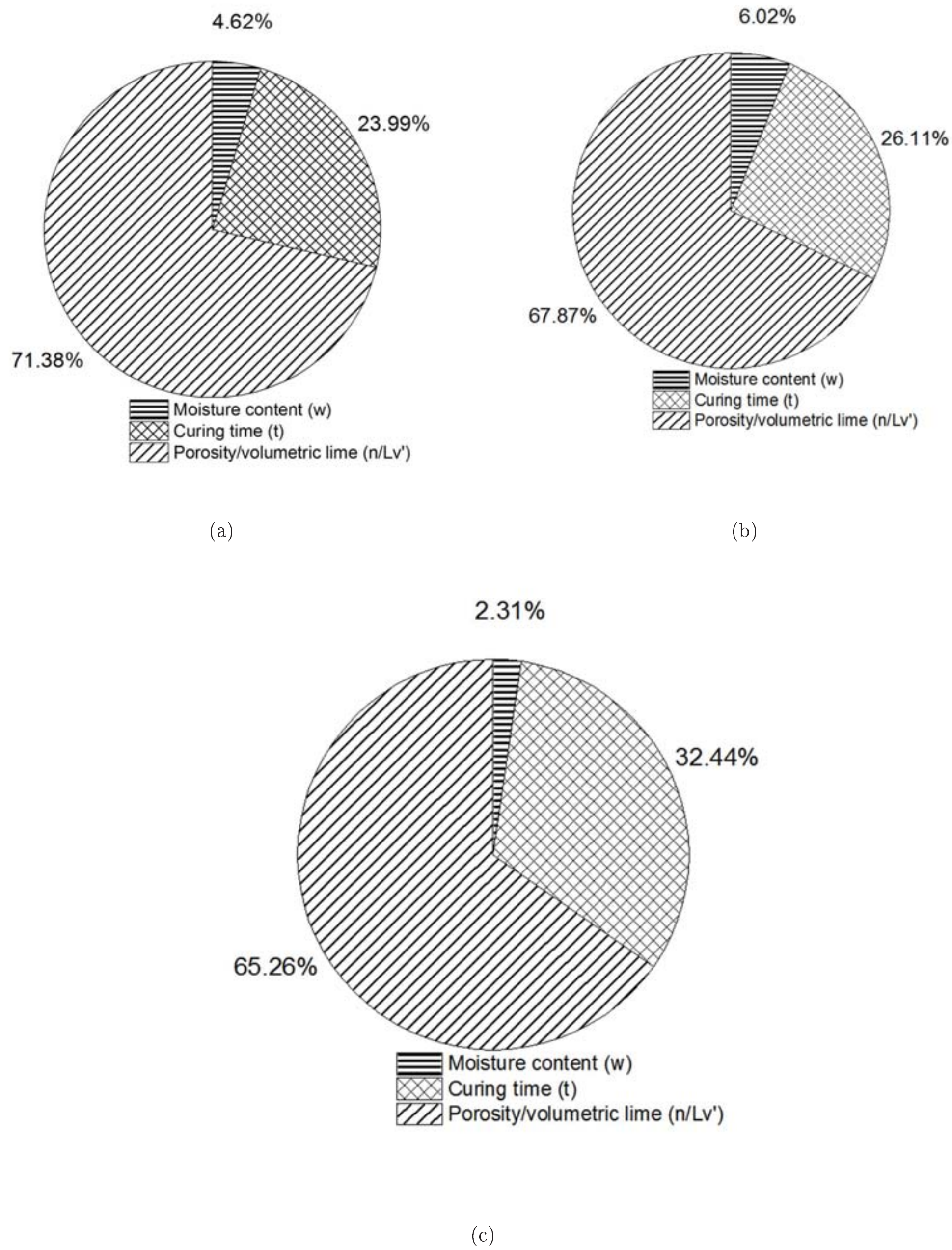

FIGURE 4.5: Relative contribution of input parameters on response based on (a) Conventional (b) Central composite and (c) Box-Behnken designed ANN model

4.4.6 Development of ANN Model Equations

Finally the important and main steps is to frame/establish an model equation based on the weights and biases based on the trained neural network that can be used as reference by researchers and academicians. The step by step procedure for ANN model equation are discussed in Chapter 2, Sec.2.8.3. However, for the sake of completeness and ready reference, the basic mathematical equation in terms of input and output is presented herein.

$$q_{un} = f\left\{b_0 + \sum_{k=1}^{h}\left[w_k \times f\left(\sum_{i=1}^{m} w_{ik}X_i\right)\right]\right\} \tag{4.1}$$

where,

q_{un} = model unconfined compressive strength in the range [-1, 1],

bo = bias at the output layer, w_k = connection weight between kth neuron in the hidden layer and single output neuron,

b_{hk} = bias at the k_{th} neuron in the hidden layer,

m = number of input variables,

h = number of hidden layers,

w_{ik} = connection weight between i^{th} input variable and k_{th} = neuron in the hidden layer,

X_i = normalized input variable i in the range [-1, 1],

K = number of neurons in the input layer, and f = transfer function.

From Sec. 4.4.3, it is seen that the ANN model equations based on response methodology (CCD and BBD) could be an alternative approach for estimating unconfined compressive strength of stabilized red mud. Using the values of final weights and biases the following expression may be written to reach the correlation of output (q_u) with the input parameters (t, w and $\eta/Lv^{'}$).

Case 1: Equation based on central composite designed artificial neural network as per weights and biases given in Table 4.6:

$$A_1 = 0.098 - 0.010w + 0.161t - 0.294\frac{\eta}{Lv'} \tag{4.2}$$

$$A_2 = -0.87 + 0.088w + 0.382t - 0.993\frac{\eta}{Lv'} \tag{4.3}$$

$$B = 0.035 + 0.098 \times \frac{(e^{A_1} - e^{-A_1})}{(e^{A_1} + e^{-A_1})} + 0.899 \times \frac{(e^{A_2} - e^{-A_2})}{(e^{A_2} + e^{-A_2})} \tag{4.4}$$

$$q_{un} = \frac{(e^{B} - e^{-B})}{(e^{B} + e^{-B})} \tag{4.5}$$

$$q_{up} = 0.5(q_{un} + 1)(q_{umax} - q_{umin}) + q_{umin} \tag{4.6}$$

Case 2: Equation based on Box-Behnken designed artificial neural network as per weights and biases given in Table 4.7:

$$A_1 = -1.535 + 0.0859w + 0.672t - 1.495\frac{\eta}{Lv'} \tag{4.7}$$

$$A_2 = -0.0483 - 0.317w + 0.317t - 0.372\frac{\eta}{Lv'} \tag{4.8}$$

$$B = 0.0823 + 0.935 \times \frac{(e^{A_1} - e^{-A_1})}{(e^{A_1} + e^{-A_1})} - 0.503 \times \frac{(e^{A_2} - e^{-A_2})}{(e^{A_2} + e^{-A_2})} \tag{4.9}$$

$$q_{un} = \frac{(e^{B} - e^{-B})}{(e^{B} + e^{-B})} \tag{4.10}$$

$$q_{up} = 0.5(q_{un} + 1)(q_{umax} - q_{umin}) + q_{umin} \tag{4.11}$$

Where, A_1, A_2 are the weighted input of hidden neurons 1 and 2, B is the weighted input at output neuron, q_{un} = model unconfined compressive strength in the range -1 to 1, q_{up} = predicted unconfined compressive strength base on ANN model, and q_{umax} and q_{umin} are the maximum and the minimum values of unconfined compressive strength in the data set. Finally, the value of unconfined compressive strength of stabilized red mud is computed using Eqs.4.6 and4.11 for the range of studies. However, further study is required to check the applicability of design of experiment for the generalization of the result.

4.4.7 Summary

In the present chapter, different artificial neural network models are developed based on conventional as well as the experimental designed approach for the prediction of the unconfined compressive strength of stabilized red mud. The results obtained from experimental designed ANN models are close to the conventional designed ANN model. Hence, the proposed ANN models may be useful tool where the generation of data set is expensive, time-consuming and tedious. Sensitivity analysis based on connection weight approach shows that porosity/volumetric lime (η/Lv') has the maximum contribution over unconfined compressive strength followed by curing time (t) and moisture content (w). From neural interpretation diagram, it is seen that the unconfined compressive strength of stabilized red mud increases with the increase in moisture content and curing time, whereas, it decreases with the increase in porosity/volumetric lime. Finally, a predictive equation based on the training dataset of response surface methodology designed artificial neural network is also presented that can be used for the estimation of the unconfined compressive strength of stabilized red mud.

Chapter 5

Application Potential of Stabilized Red Mud

5.1 General

A waste material can only be used as building and construction material when the end product satisfies strength criteria, durability and leachate (leaching of harmful elements) characteristics. From Chapter 3, it is seen that stabilized red mud has good strength such as unconfined compressive strength($460 \leq q_u \leq 4350$ kPa), split tensile strength ($60 \leq q_u \leq 750$ kPa), satisfactory durability (loss in mass ≤ 30 %) and having leaching of harmful metals in within permissible limits for the range of studies ($3 \leq L \leq 11$ % , $13 \leq \gamma_d \leq 15.5\ kN/m^3$, $26 \leq t \leq 60\ days$ and $13 \leq w \leq 30$ %). After fulfillment of these criteria, the stabilized red mud may be used in different civil engineering applications such as pavement materials, unfired bricks etc.