Modelling the Shear Flow Behaviour of Cement Paste Using Machine Learning –XGBoost

Dhanya Sathyan1*, Govind D2, Rajesh C B3, Gopikrishnan K4, G Aswath Kannan5, Jayanth Mahadevan5

1Assistant Professor, Department of Civil Engineering, Amrita School of Engineering, Coimbatore, Amrita Vishwa Vidyapeetham, India. *Corresponding Author: email: s_dhanya@cb.amrita.edu

2Assistant Professor, Centre for Computational Engineering & Networking, Amrita School of Engineering, Coimbatore, Amrita Vishwa Vidyapeetham, India. email: d_govind@cb.amrita.edu

3Assistant Professor, Department of Electronics and Communication Engineering, Amrita School of Engineering, Coimbatore, Amrita Vishwa Vidyapeetham, India. email: cb_rajesh@cb.amrita.edu

4Undergraduate student, Department of Electronics and Communication Engineering, Amrita School of Engineering, Coimbatore, Amrita Vishwa Vidyapeetham, India. email: gopikrishnanka99@gmail.com

5Undergraduate student, Department of Civil Engineering, Amrita School of Engineering, Coimbatore, Amrita Vishwa Vidyapeetham, India. email: g.aswathk@gmail.com, jayanthkeshu11@gmail.com

Abstract: In recent years machine learning is considered as a highly effective and widely used tool to predict the behaviour of complex and heterogeneous problems. In this paper, the behaviour of superplasticised cement paste is assessed by XGBoost, which is accepted to accomplish the state-of-the-art results on many machine learning challenges. The data required for the development of model is formulated experimentally by conducting rheological tests on cement pastes using a temperature controlled Coaxial Cylinder Viscometer. Various parameters like amount of cement, superplasticiser, water and test temperature are taken as input parameters and the behaviour is assessed by taking rheological characteristics like yield stress and plastic viscosity as output parameters. Out of the 252 data formulated experimentally 85% are used for training and the remaining is for testing the efficacy of the network. From the results it is observed that the model developed using XGBoost is a promising tool for the solution of highly complex and heterogeneous civil engineering problems, which otherwise is highly tedious and time consuming in nature.

1. Introduction
The rapid growth in the construction sector demands the need for concrete with high flowability and strength. This requires the usage of superplasticizers in concrete. Rheology is the study concerning the flow and change of shape of the matter when subjected to an applied force. Flow behaviour of concrete mix is mainly represented by the cement paste phase. Rheological properties of the mix
changes with temperature, ingredient type and dosage, mixing method, mixing sequence etc. Rheological studies of the cement matrix help in studying its fresh stage property and give idea about the hardened stage properties.

The effects of shear rate and mixing methods on the rheological behaviour of cement paste were studied by Williams et al. (1999). Hand mixed, high shear mixed and paddle mixed pastes were used for this study. With increase in pre-shear rate a reduction in plastic viscosity is observed. Effect of modified polyacrylic superplasticisers on rheological properties of Portland cement pastes was studied by Papo and Piani (2004). Steric hindrance effect of side chain of polyacrylic superplasticisers is also observed in this study.

The role of excess water to solid surface area ratio on the rheology of cement paste was studied by Wong and Kwan (2008) through cement paste samples made with different proportions of condensed silica fume (CSF), fuel ash, cement and different water contents. With increase in excess water to solid surface area ratio there is a reduction in rheological parameter values.

Influence of superplasticizer dosage and sequence of mixing of the cement paste on the rheological performance at different test temperature was studied by Altable and Casanova et al. (2006). Delayed addition of superplasticizer is found to be better for a better rheological performance. Increase in yield stress and decrease in plastic viscosity was observed with increase in temperature. Up to a certain dosage of superplasticizer, there is a decrease in plastic viscosity of the paste which was observed with increase in superplasticizer dosage.

The influence of the cement characteristic on the rheology of the cement paste was studied by Vikan et al. (2007). Three different types of plasticizers namely polyether grafted polyacrylate, naphthalenesulphonate-formaldehyde condensate and lignosulphonate have been tested on 6 different types of cement. It was found that flow resistance of the cement paste increases with increase in C3A content and C3S content and the surface area of the cement.

Coupled effect of temperature and time on the plastic viscosity and yield stress of superplasticized OPC cement paste was studied by Martini and Nehdi (2009). In a linear fashion the rheological parameters increase with time and temperature. Up to saturation dosage of admixtures, it was observed that the yield stress and plastic viscosity decreases with admixture dosage. But not much change in the performance was observed after the saturation dosage of superplasticizer.

Through rotational viscometry measurement as well as by the use of the flow table test, the rheological property of superplasticized alkali-activated fly ash paste was studied by Criado et al. (2009). Flow table spread, yield stress and plastic viscosity of the different mixes were measured. It was also observed that for studying the rheological behaviour of cement paste, the viscometer study was more accurate method than that of flow table test. PCE based superplasticizers were found to be the efficient admixture to the new cementitious pastes.

By extracting mortar from SCC mix, effect of time, superplasticizer dosage and temperature on the rheology of flowable mortar was studied by Petit et al. (2005, 2006, 2007, 2009 and 2010). With time and temperature, change in yield stress and plastic viscosity is observed. Compared to the mixes with silica fume, mixes made with fly ash showed less change in the rheological parameter with time and temperature.

Fernandez and Casanova (2006) has reported a similar observation about the variation of viscosity with temperature in the rheological studies conducted on the OPC Paste. Combined effect of time and temperature on the fluidity of ordinary portland cement paste and mortar was studied by Kong et al. (2013). With increase in time and temperature increase in plastic viscosity and yield stress was observed. Decrease in spread diameter of the mortar with time and temperature is also reported in this study.

Analysis and modelling of flow behaviour cement paste and SCC was reported in many previous studies (Dhanya et al 2018, Dhanya et al 2018, Sindu et al 2018, Dhanya et al 2018, Aravind et al 2018).
The present paper reports a study on assessing the flow behaviour of cement paste at different temperature using machine learning technique. The developed model can reduce the large amount of time, material and labour required to perform the trial tests to arrive at the optimum behaviour.

2. Experimental Investigations
Cement paste were prepared using four brands of Portland Pozzolana Cement (C1, C2, C3, C4) and superplasticizer from four different families (Polycarboxylate Ether, Sulphonated Melamine Formaldehyde, Sulphonated Naphthalene Formaldehyde and Lignosulphates). The properties of cement and superplasticizer used for the study are listed in Table 1 and 2. A water binder ratio of 0.37 was adopted in this study. Test was performed at three different temperature i.e 15, 27 and 35°C. Two loading and unloading cycles were imposed by increasing, and later decreasing the shear rate. The response of downward curve of the second cycle is used for determining the rheological parameters. Rheological parameters obtained at constant test temperature by fitting the second cycle downward flow curves using Bingham model and Herschel Bulkley model are compared.

### Table 1. Physical properties of cement

| Property                      | C1  | C2  | C3  | C4  |
|-------------------------------|-----|-----|-----|-----|
| Fineness (%)                  | 3.50| 5.40| 6   | 6.4 |
| Specific Gravity              | 2.85| 2.80| 2.80| 2.72|
| Standard Consistency (%)      | 35.5| 36  | 37  | 37  |
| Initial Setting Time (minutes)| 160 | 110 | 142 | 75  |
| Final Setting Time (minutes)  | 220 | 185 | 194 | 155 |

### Table 2. Properties of superplasticisers

| SP   | Density (g/cc) | Solid Content (%) | pH |
|------|----------------|-------------------|----|
| PCE1 | 1.11           | 36.67             | 6  |
| PCE2 | 1.07           | 29.85             | ≥ 6|
| SNF1 | 1.21           | 37.43             | 7-8|
| SNF2 | 1.21           | 37.83             | 7-8|
| LS1  | 1.15           | 30.05             | ≥ 6|
| LS2  | 1.17           | 31.61             | ≥ 6|
| SMF  | 1.23           | 33.06             | 7  |

Viscometer test was done to study the rheological properties of cement. The test was done in a temperature controlled digital coaxial cylinder viscometer as shown in Fig 1, which has a variable speed capability and easy programmability of shear rates. Coaxial cylinder viscometer was used in this case because well-defined shear stress and shear rate data was required for a small volume of sample(cement) used for testing. The equipment was loaded with the step wise shear rate cycle (Fig 2) adopted in a previous study by Robert et al (2018) programmed using the RheoCalc software. The cement paste was loaded into the coaxial cylinder of the viscometer with the amount of water added being the consistency of cement. The torque sensor applies shear rate depending on the cycle setup and shear stress is measured in the process by the viscometer. The step wise loading system consisted of two loading and unloading cycles with shear rate applied in five steps, in increments of 5rpm for every 10 second interval with the maximum speed of the spindle set at 65 rpm. The descending curve...
of the second cycle of the loading system was taken for analysis. The analysis was done using the SigmaPlot software to find the Plastic viscosity and yield stress. The data was gathered by the Rheocalc software and was fed into the SigmaPlot software. The Bingham and Herschel-Buckley modified Newtonian equations were considered for the analysis, for its two and three parameter structures respectively.

In Bingham model, \( \tau = \tau_0 + \eta \dot{\gamma} \)

\( \tau \) represents shear stress in N/mm\(^2\), \( \dot{\gamma} \) represents shear rate, \( \tau_0 \) represents yield stress in Pa, \( \eta \) represents plastic viscosity in Pa s

Whereas in Herschel-Buckley model, \( \tau = \tau_0 + K(\dot{\gamma})^n \)

\( K \) represents consistency index, \( n \) represents the flow index or the degree of non-Newtonian flow, \( \dot{\gamma} \) represents shear rate

**Fig 1 Viscometer**

**Fig 2 Stepwise Loading Pattern**

### 2.1 Analytical Modelling

Machine Learning is a subset of Artificial Intelligence that enables a computer or a machine to perform certain tasks without the need for explicit instructions. This is achieved by creating a statistical model based on a set of data that is available beforehand (known as the ‘training data’) and
this process is called training. During the training process, the model being developed is altered based on the output that the input data parameters (features) provide and a certain loss function that is directly proportional to the absolute difference between the predicted outputs and the actual value. A simple loss function is given as follows:

\[
\frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2
\]

where \( m \) is the number of data samples available, \( x^{(i)} \) being the input parameters, \( h_\theta(x^{(i)}) \) being the predicted values and \( y^{(i)} \) the actual output provided in the training dataset. On testing it out on a ‘validation dataset’, and after obtaining the desired accuracy, the model can be deployed and used to predict the output when ‘test data’ is fed as input.

In the present paper, XGBoost (Extreme Gradient Boosting) is employed in developing a model to predict the values of yield stress and plastic viscosity where ingredients quantity and temperature is given as the input parameter(Tianqi Chen & Carlos Guestrin). XGBoost is an optimized distributed gradient library and is one of the best when it comes to regression problems, i.e. those problems whose outputs vary over a continuous range of values. XGBoost is an ensemble additive model that is composed of several base learners and the ensembles being trees.

At each iteration, a function is chosen at each base learner that minimizes the absolute value of the loss function. In gradient boosting, at each iteration, the value by which the model is to be modified is obtained by fitting a base learner to the negative gradient of loss function of the previous iteration’s value. In XGBoost, several base learners or functions are explored and tried out and an appropriate function that minimizes the loss function is taken into consideration. But a problem arises here as the loss function has to be calculated for every base learner, which is computationally expensive. Hence, XGBoost employs the Taylor series to approximate the value of the loss function for each base learner.

To create a tree of base learners that gives the model with the highest accuracy and the lowest loss function, XGBoost employs a greedy algorithm in figuring out the branches with the lowest loss, wherein after each node encountered, the corresponding nodes are split into left and right nodes and the split with the minimum loss function is taken into consideration and the reduction in loss is also noted.

The model is created and then trained on the training data and can be used to predict the output on the testing data.

3. Results and Discussion

Figure 3 and Figure 4 presents the comparison of the actual and predicted values corresponding to yield stress and plastic viscosity. Out of the 252 data tested nearly 35-40 data are taken for testing the model. The solid line in the figures represents the condition where the actual values are equal to predicted values. From Figure 3 and 4, it is observed that the predicted values are almost matching with the actual values corresponding to majority test data. It is observed that for low values of yield stress the prediction is better compared to higher values. This may be due to the small number of data corresponding to higher yield stress values. Unlike yield stress values, predicted plastic viscosity shows slight variations from the actual values, but with an allowable limit.
Fig. 3 Predicted Vs Actual Values – Yield Stress

Fig. 4 Predicted Vs Actual Values – Plastic Viscosity
4. Conclusions
The present paper reports the study carried out using machine learning to assess the rheological characteristics of cement paste. XGBoost (Extreme Gradient Boosting) is used in developing the model. The input parameters consist of dosages of cement, superplasticizer, water and test temperatures and the output parameters are the rheological characteristics like yield stress and plastic viscosity.
From the test results it is observed that the developed model predicts the rheological characteristics with required accuracy. During the development of the model it is observed that the prediction can be further improved by the addition of more data for training, which is a major challenge faced.
The developed model can thus be used to eliminate the long test procedures involved in finding the behaviour of superplasticized cement paste which is otherwise tedious and highly timeconsuming involving lot of experimental procedures.

5. References
[1]. David, A Williams, Aaron, W Saak and Hamlin, M Jennings (1999). “The influence of mixing on the rheology of fresh cement paste.” Cement and concrete research, 29, 1491-1496.
[2]. Adriano Papo and Luciano Piani (2004). “Effect of various superplasticisers on the rheological properties of portland cement pastes.” Cement and concrete research, 34, 2097-2101.
[3]. WongHHC and Kwan, A.K.H. (2008). “Rheology of cement paste: Role of excess water to solid surface area ratio.” Journal of materials in civil engineering, 20(2), 189-197.
[4]. Victor Fernández-Altable and Ignasi Casanova (2006). “Influence of mixing sequence and superplasticiser dosage on the rheological response of cement pastes at different temperatures.” Cement and concrete research, 36, 1222-1230.
[5]. Vikan, H, Justnes, H, Winnefeld, F and Figi, R (2007). “Correlating cement characteristics with rheology of paste.” Cement and concrete research, 37, 1502-1511.
[6]. Martini, S Al and Nehdi, M (2009). “Coupled effect of time and high temperature on rheological properties of cement pastes incorporating various superplasticisers.” Journal of materials in civil engineering, 21(8), 392 - 401.
[7]. Criado, MA Palomo, A, Fernández-Jiménez, and PFG, Banfill (2009). “Alkali activated fly ash: effect of admixtures on paste rheology.” Rheologica acta, 48(4), 447-455.
[8]. Petit, J. Y, Wirquin, E and DuthoitB. (2005). “Influence of temperature on the yield value of highly flowable micromortars made with sulfonatebased superplasticizer.” Cement and concrete research, 35, 256 - 266.
[9]. Petit, JY, Khayat, KH and Wirquin, E (2006). “Coupled effect of time and temperature on variations of yield value of highly flowable mortar.” Cement and concrete research, 36,832-841.
[10]. Petit, JY, Wirquin, E, Vanhove, Y and Khayat, K (2007). “Yield stress and viscosity equations for mortars and self-consolidating concrete.” Cement and concrete research, 37,655-670.
[11]. Petit, JY, Khayat, KH and Wirquin, E (2009). “Coupled effect of time and temperature on variations of plastic viscosity of highly flowable mortar.” Cement and concrete research, 39, 165–170.
[12]. Petit, JY, Wirquin, E and Kamal H Khayat (2010). “Effect of temperature on the rheology of flowable mortars.” *Cement and Concrete Composites*, 32, 43-53.

[13]. Kong, X, Zhang, Y and Hou, S (2013). “Study on the rheological properties of portland cement pastes with polycarboxylatesuperplasticizers.” *Rheologica Acta*, 52, 707-718.

[14]. Dhanya Sathyan, K B Anand, Aravind J Prakash and Pemjith B (2018), “Modelling of fresh and hardened stage properties of self-compacting concrete using random kitchen sink algorithm”, *International journal of concrete structures and materials*, Springer, DOI 10.1186/s40069-018-0246-7.

[15]. Rojin C Robert, Dhanya Sathyan, K B Anand (2018), “Effect of superplasticizers on the rheological properties of fly ash incorporated cement paste”, *Material today proceeding, Volume 5, Issue 11, Part 3, 2018, Pages 23955-23963*

[16]. Dhanya Sathyan, Anand, K.B. and Sindu Menon, M. (2018). “Temperature influence on rheology of superplasticizedpozzolana cement and modelling using random kitchen sink algorithm.” *Journal of materials in civil engineering*, ASCE, DOI: 10.1061/(ASCE) MT.1943-5533.00

[17]. Sindhu Menon M, Dhanya Sathyan, and K B Anand (2017), “Studies on Rheological Properties of Superplasticised PPC Paste, *International Journal of Civil Engineering and Technology.* Volume 8, Issue 10, pp 939–947.

[18]. Dhanya Sathyan, K B Anand, Chinnu Jose and Aravind N R (2018), “Modelling the mini slump spread of superplasticized PPC paste using RLS with the application of random kitchen sink”, *IOP conference series*, Volume 310. DOI:10.1088/1757-899X/310/1/012035.

[19]. Aravind J Prakash, Dhanya Sathyan, K B Anand and Aravind N R (2018), “Comparison of ANN and RKS approaches to model SCC strength, *IOP conference series,* Volume 310. DOI:10.1088/1757-899X/310/1/012037.

[20]. Tianqi Chen, Carlos Guestrin, XGBoost: A Scalable Tree Boosting System, University of Washington