MATHEMATICAL MODELING TO DEVELOP A SIMPLE NANO TO MACRO STRUCTURE CONCRETE - BASED MODEL

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A simple concrete - based structure model is proposed by developing it from nano to macro structure. In this model, the structure is divided into four levels and each level is represented by a parametric model. The parameters of the four based structures are identified, in terms of elastic modulus (EM) and poisson's ratio at any time period (t) at Calcium silicate hydrates (CSH), cement paste, mortar and concrete levels. Then, by integrating the proposed model with Bazant – Baweja (B3) model, the compressive strength (CS) and EM of concrete at different curing periods is estimated. Further, it is analyzed and validated by other international models such as B3 model alone, Comite Euro – International Du Beton (CEB) model and Indian standards (IS) method. Few tests were done to investigate the CS of concrete with the inclusion of 25% fly ash (fa) and varying ratios of waste foundry sand (WFS) – 0, 25, 50, 75 and 100%. The results are compared with the obtained values by other models and validated with the experimental results. It is found that the proposed model (PM) i.e., Multiscale modeling (MS) can be used reliably integrated with the other models and builds the interaction between the various matrix to estimate and study the strength parameters of the concrete. MS is a new technique which is based on the mathematical formulation, it doesn't require any earlier data about the mechanical properties of the concrete except the intrinsic values of the cement-based materials and mix details to evaluate the strength of the concrete.

Keywords: *Concrete, international models, strength parameters, elastic modulus, poisson's ratio, parametric model*

Highlights:

- Mathematical modeling is used for describing the compressive strength of concrete
- The model is used to predict the elastic modulus of concrete from microstructure
- Compressive strength of concrete was estimated using prediction models
- Proposed model requires only the mix design details and intrinsic properties

1. Introduction

As it is well known that concrete is a heterogenous material varying with length scales in the multiscale modeling [1]. In multiscale modeling there are four levels which consist of CSH phase, large portlandite (CH) phase, mortar and concrete phase also termed as microscale to macroscale. CSH (calcium silicate hydrates) is one of the major parts in the microscale, which mainly deals with two categories in the nanoscale namely, low density (LD) and high density (HD) based on the size of the particles [2]. The origin of creep and can also be studied by understanding the growth of the nanostructure of concrete. To evaluate the creep of concrete the strength parameters are the important factor. They have investigated that the establishment of creep is due to the reorganization of CSH particles, firmly packed densities present in the cement paste matrix [3]. The porosity of gel is occurred due to the hydration of particles in which there is an increment in water – cement ratio (w/c). Nanoindentation tests were carried out by sub stoichiometries w/c varying between 0.15 to 0.40. It showed a good correlation between the microstructure and mechanical properties of concrete [4]. In this paper, it mainly focuses the determination of elastic modulus and poisson's ratio at each level where the chemical constituents can be identified. The cement – based homogenized models are adopted to develop the micro level to macro level [5]. The creep of shotcrete by using multiscale was studied and investigated to determine the basic creep of concrete [6]. Macroscopic creep tests were carried out to know the viscous properties of creep at finer scales. Further, the proposed model was validated to the B3 models. Due the hardening effect of inclusion, the CSH phases are improvised to the macroscale level. It can be improved by taking the curing temperature into account as one of the important factors in the compliance of creep other than T_o=20°C. From the observation, it was stated that the relative humidity and the degree of hydration plays a vital role in the magnitude and direction of creep. Using waste products with varying w/c ratios in the production of concrete, there was a development in the durability and strength properties of concrete [7-16]. Researchers have studied on the strength factors and effects due to the abrasive action by utilizing waste foundry sand with varying ratios. From the observation, it was noted that the compressive strength of concrete gave the best results at the age of 28 days with 15% of WFS [17]. They had investigated the behavior of concrete by replacing WFS with cement during the production of concrete. Several tests were conducted and also by adopting the B3

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model, ACI method, IS method to estimate the strength parameters of the concrete. From the results, it was detected that 30% and 20% of waste foundry sand can be used for 0.4 and 0.5 w/c to improvise the compressive strength of the concrete [18]. Many researchers have also studied on the various waste products to improvise the strength of the concrete in an economical way by adopting the recycled aggregates with different ratio's during the production of the concrete. The durability and strength parameters are also studied [19-21].

2.Multiscale modeling

Concrete is a heterogeneous material with a varying large scale which comprises of cement, aggregates with some amount of water. CSH phase develops the hydration process in the cement paste. In this model, the cement – based materials consider with four levels as represented in Fig. 1.

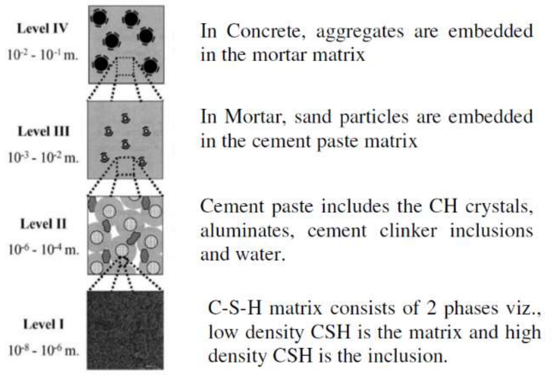

Fig. 1 - Multi-scale microstructure of concrete [22].

In the level I, the CSH phase ranges from 10^{-8} to 10^{-6}m which is the smallest scale. CSH matrix includes with two phases such as low density (LD) and high density (HD) in which HD will be the stiffer inclusion phase and LD will be the lighter phase. In the level II, cement paste consists of CSH, large portlandite crystals (CH), aluminates and macro porosity with greater w/c (>0.4). In the level III, cement mortar phase consists of the inclusion of fine aggregates in a spherical form (< 2 mm) and interfacial transition zone (ITZ) is embedded in the cement paste matrix. At this stage, it also includes the volume fractions of air voids, wfs, fa, water voids. In this study, the ITZ is not considered. At the level IV, concrete phase inclusion the coarse aggregates (> 2 mm) with ITZ are embedded in the mortar matrix. The elastic modulus and poisson's ratio of concrete at each level is determined by using the Mori – Tanaka (MT) scheme and Self – Consistent (SC) scheme by providing volume fractions, shear moduli and bulk moduli as the input factors. This proposed model requires only the mix details, reaction of kinetic model and the intrinsic properties such as elastic properties of cement paste and change in chemical volume. The Mori – Tanaka scheme is used at the level I, III and IV to evaluate the homogenized values of bulk modulus (K_{hom}^{est}) and shear modulus (μ_{hom}^{est}), which are obtained from the following equations:

$$\frac{K_{hom}^{est}}{K_m} = 1 + f_I \frac{(K_I/K_m)-1}{1+\propto_m^{est}(1-f_I)(K_I/K_m-1)} \quad [1]$$

$$\frac{\mu_{hom}^{est}}{\mu_m} = 1 + f_I \frac{\mu_I-\mu_m}{1+\beta_m^{est}(1-f_I)(\mu_I/\mu_m-1)} \quad [2]$$

$$\propto_m^{est} = \frac{3K_m}{3K_m+4\mu_m} \quad [3]$$

$$\beta_m^{est} = \frac{6(K_m+2\mu_m)}{5(3K_m+4\mu_m)} \quad [4]$$

Where, *m* and *I* indicate the matrix and inclusion of particles. *K,* μ and *f* denotes the bulk moduli, shear moduli and volume fractions of matrix and inclusion respectively.

$$E_{hom}^{est} = \frac{9K_{hom}^{est}\mu_{hom}^{est}}{3K_{hom}^{est}+\mu_{hom}^{est}} \quad [5]$$

$$\gamma_{hom}^{est} = \frac{3K_{hom}^{est}-2\mu_{hom}^{est}}{6K_{hom}^{est}+2\mu_{hom}^{est}} \quad [6]$$

The above equations give the homogenized elastic modulus and poisson's ratio at each level. The Self – Consistent scheme is used only in the level II i.e., a cement paste level, which is more coherent to determine the homogenized bulk modulus (K_{hom}^{est}) and shear modulus (μ_{hom}^{est}) which are obtained by using the following equations by including the volume fractions of the phases

$$K_{hom}^{est} = \sum_r K_r f_r \left(1 +\propto_0^{est}\left(\frac{K_r}{K_0}-1\right)\right)^{-1} * \left[\sum_r f_r \left(1 +\propto_0^{est}\left(\frac{K_r}{K_0}-1\right)\right)^{-1}\right]^{-1} \quad [7]$$

$$\mu_0^{est} = \sum_r f_r \mu_r \left(1 + \beta_0^{est}\left(\frac{\mu_r}{\mu_0}-1\right)\right)^{-1} * \left[\sum_r f_r \left(1 + \beta_0^{est}\left(\frac{\mu_r}{\mu_0}-1\right)\right)^{-1}\right]^{-1} \quad [8]$$

In the CSH level, the volume fractions are determined by using the following equations:

$$f_m = \frac{V_{LD}}{V_{LD}+V_{HD}} \quad [9]$$

$$f_I = \frac{V_{HD}}{V_{LD}+V_{HD}} = 1 - f_m \quad [10]$$

Where, V_{LD} and V_{HD} are denoted as the low density and high density of C-S-H volume fractions which can be determined using a hydration kinetics model [22].

$$V_{LD}(t) = V_{C-S-H}^{C_3S}\left(\xi_{C_3S}^{*} - \left(\xi_{C_3S}^{*} - \xi_{C_3S}^{*}(t)\right)_+\right) + V_{C-S-H}^{C_2S}\left(\xi_{C_2S}^{*} - \left(\xi_{C_2S}^{*} - \xi_{C_2S}^{*}(t)\right)_+\right) \quad [11]$$

$V_{HD}(t) = V_{C-S-H}^{C_3S}\left(\xi_{C_3S}(t) - \xi_{C_3S}^{*}\right)_{+}$
$V_{C-S-H}^{C_2S}\left(\xi_{C_2S}(t) - \xi_{C_2S}^{*}\right)_{+}$ [12]

Where, $V_{C-S-H}^{C_3S}$ and $V_{C-S-H}^{C_2S}$ are the asymptotic values of the volume occupied by the reaction products of the hydration of C_3S and C_2S in the C-S-H phase. In the cement paste level, the Self – Consistent scheme is used by including the volume fractions such as air voids, water voids, aluminates, CSH and CH to evaluate the elastic properties at each level.

$$f_m = \frac{V_{LD}+V_{HD}+V_A}{V_{II}} \quad [13]$$

$$f_I = \frac{V_{CH}}{V_{II}} \quad [14]$$

$$V_{II} = V_c^0 + V_w^0 = \left(V_c^0 + V_{fa}^0\right) * \left(1 + {\left(\rho_c + \rho_{fa}\right)}\Big/{\rho_w} * \frac{w}{c}\right) \quad [15]$$

where, V_A and V_{CH} are the volume fractions of aluminates and CH, respectively. V_{II} is the total volume of the typical volume portion at Level II. The cement-to-water density ratio is denoted as $\frac{\rho_c}{\rho_w}$ and water-to-cement ratio as $\frac{w}{c}$. In the mortar level, the sand particles are included in the cement paste. The volume fractions are provided by using the following equations:

$$f_I = \frac{s/\rho_s}{c/\rho_c + w/\rho_w + s/\rho_s + wfs/\rho_{wfs} + fa/\rho_{fa}} \quad [16]$$

$$f_m = 1 - f_I \quad [17]$$

Similarly, in the concrete level, the inclusion material is considered as the gravel in the mortar matrix. Where, s is the sand content, c is the cement paste, w is the water content, ρ_s, ρ_c and ρ_w are the mass densities of sand, cement and water, respectively. In this paper, MS is introduced by developing the matrix from CSH level to concrete level by knowing the CSH and CH of low density, high density and poisson's ratio. The above-mentioned empirical formulae are used in order to estimate the elastic modulus and poisson's ratio at each phase.

3.International models

In this study, further B3 model and CEB model are used to assess the compressive strength of the concrete for different curing periods. B3 model relates to the mathematical report, which is mainly used in the simplex and as well as the complex structures. This model was developed in the year 1997. Further, it was modified in the 1991 and was named as a BP – KX model. This model gives the clear information about the creep compliance. In order to evaluate the creep, the strength parameters are the important factors. The inaccurate values of inelastic modulus can be reduced by adopting the compliance functions. By integrating with multiscale modeling, the elastic modulus at any time (t) and mean compressive strength at 28 days can be determined by using the following equation:

$$E_{cmt} = E_{cm28}\left(\frac{t}{(4+0.85t)}\right)^{0.5} \quad [18]$$

$$E_{cm28} = 4734\sqrt{f_{cm28}} \quad [19]$$

To have a clear idea about the proposed method i.e., Multiscale modeling (MS), three stages are been considered first and foremost by developing the MS from CSH level to concrete level for estimating the poisson's ratio and elastic modulus at each level. Second stage is to determine the compressive strength of concrete using B3 model and CEB model for various proportions of by-products. Third stage is where the B3 model is integrated with the MS to evaluate the strength of the concrete. The proposed method doesn't involve with any previous data regarding the mechanical properties of concrete.

CEB model is also named as CEB MC90-99 in the year 1990 and further with slight modifications it was revised in the year 1999 to differentiate the autogenous shrinkage and the drying shrinkage by Muller and Hilsdorf. The modulus of elasticity at the age of 28 days and at any time (t) (N/mm^2) can be found by using the equation:

$$E_{cmt0} = E_{cm28}\exp\left[\frac{s}{2}\left(1 - \sqrt{\frac{28}{t_0/t_1}}\right)\right] \quad [20]$$

$$E_{cm28} = 21500\sqrt[3]{\frac{f_{cm28}}{f_{cm0}}} \quad [21]$$

where, s is the coefficient widely used for the type of cement, t_o is the age of concrete at loading (days), t_1 = 1 day (constant), f_{cm28} and f_{cm0} is the mean compressive cylinder strength of concrete at 28 days (N/mm^2) and at the age of loading which is taken as constant (10 N/mm^2) respectively.

As per IS method, the elastic modulus of concrete can be determined by using the following equation:

$$E = 5000\sqrt{f_{ck}} \quad [22]$$

4.Results and discussion

The compressive strength of concrete was tested at a varying curing period, such as 3, 7, 28, 56, 90, 100 and 150 days for the w/c – 0.5 with different proportions of fly ash (fa) and waste foundry sand (wfs) as shown in the Fig. 2.

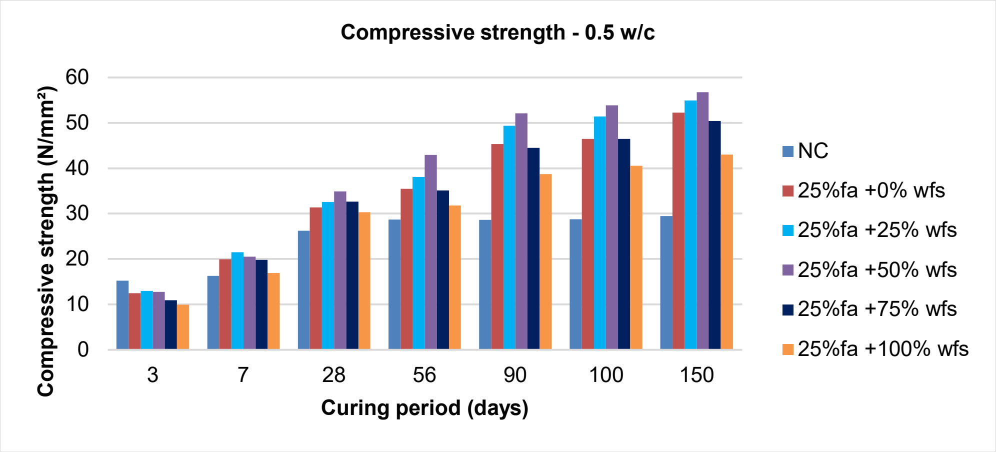

Fig. 2 - Comparison of compressive strength with the different proportions.

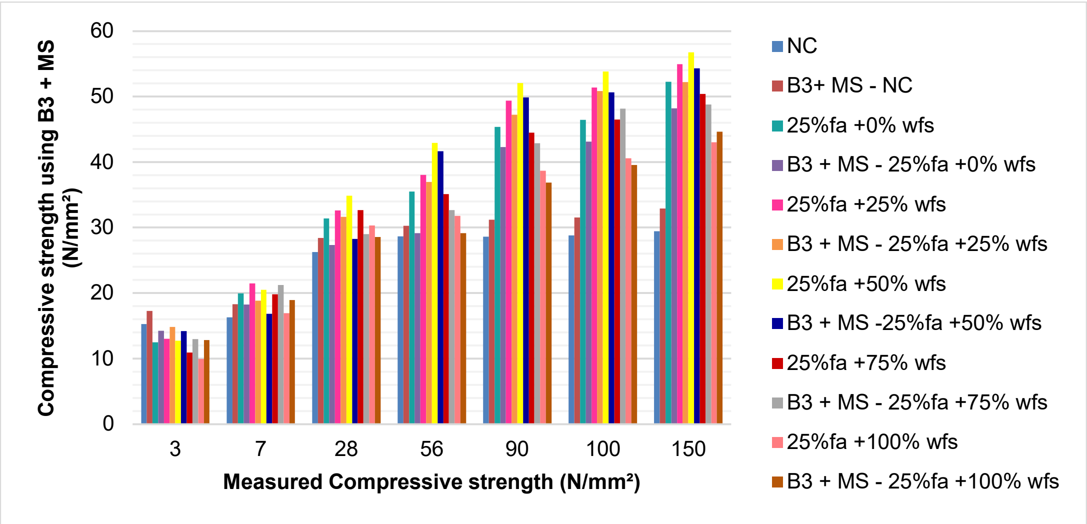

Fig. 3 - Comparison of computed and measured compressive strength with the different experimental data.

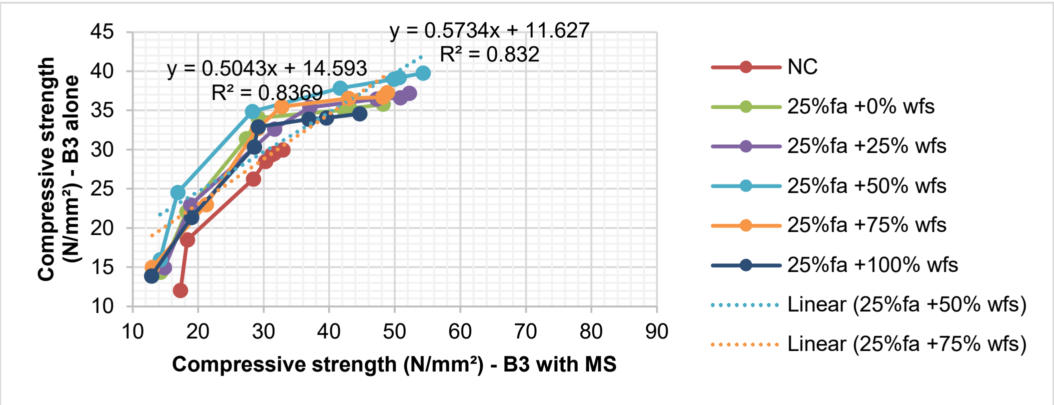

Fig. 4 - Compressive strength of concrete by using B3 model and B3 integrated with multiscale modeling (MS).

To improvise the strength of the concrete, the waste by-products such as fly ash and waste foundry sand can be utilized during the production of concrete by replacing it with cement and river sand respectively. These by-products are easily available and economical too. From the outcomes, it is observed that the usage of 25% of fa with 50% and 75% of wfs is optimum. From the Fig. 3, the compressive strength of concrete using proposed model proportions was compared with the different experimental data.

From the results, it is noted that for the normal concrete (NC) using proposed model and measured value, the compressive strength of concrete was about 28.44 N/mm² and 26.25 N/mm² respectively. There is a least variation of

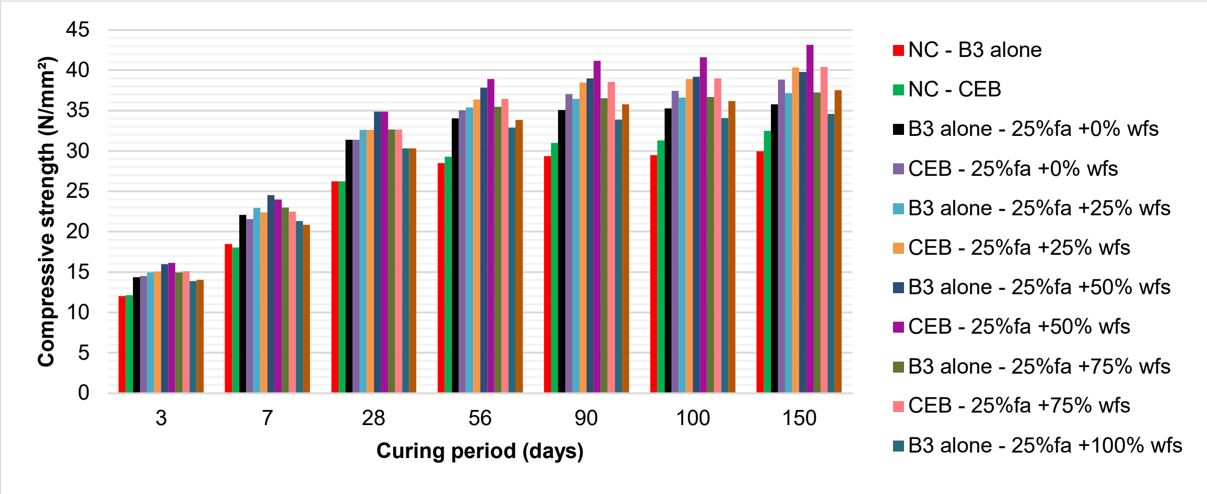

Fig. 5 - Compressive strength of concrete by using B3 model and CEB model.

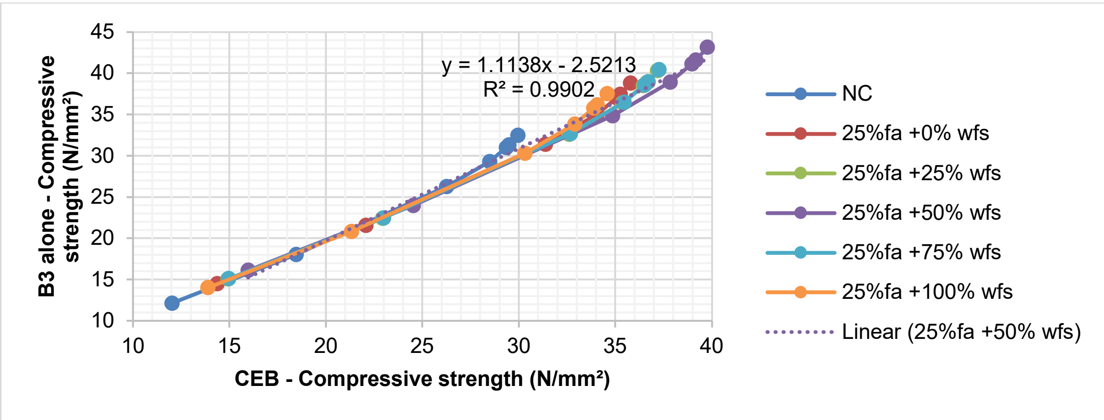

Fig. 6 - Relationship between B3 model and CEB model.

about 7.7% when compared with the measured strength of concrete at the age of 28 days. Similarly, by utilizing the 25% of wfs with 25% of fa, the strength of the concrete was found to be nearly 3% to 5% increase in variation at the age of 28 days when compared with the normal concrete. By using 75% and 100% of wfs with 25% of fa, there was an increase in strength of concrete with a variation of about 3% to 5%. It is also suggested that the usage of 50% and 75% of wfs can be used in the making of concrete to improvise the strength properties of it. The proposed model gives the better results when compared to the NC with a discrepancy of about 3 to 5% overall by having only the intrinsic values of cement materials and the mix design details, the compressive strength of concrete can be evaluated with the help of Multiscale modeling (MS). From the Fig. 4, it is observed that, the compressive strength for the NC with B3+MS having 50% was found to be closer when compared with the B3 model alone with an increase in variation of about 9% at the age of 56 days. With the usage of 50% and 75% of wfs, the strength of concrete using MS was found to be an increase in the variation of about 1% to 5% when compared with the B3 model alone. Similarly, at the age of 90 days and 150 days, the strength of concrete using the B3 model with MS and B3 alone, there was a tremendous increase in strength having an incremental variation of about 15% to 20%, this is mainly due to the increase in the elastic modulus of concrete, which is evaluated at any time period (t) by considering the MS. In this figure it also represents the relation between the computed compressive strength using the B3 model with MS and B3 alone for the w/c – 0.5, the line of regression was used to describe the relationship between these models. It was observed that the computed strength of concrete gave the satisfactory correlation between them (R^2=0.83). The compressive strength of concrete was obtained and validated by using the B3 model and the CEB model as shown in the Fig. 5.

At the age of 56 days, the NC was found to be 29.29 N/mm² by using CEB and 28.48 N/mm² for B3 model, where there is at least variation of about 2.7%. Similarly, by using the 25% of wfs with 25% fa, it was found that there is an incremental variation of 5.7% when compared with the CEB model at the age of 90 days. Using 50% and 75% of wfs, the

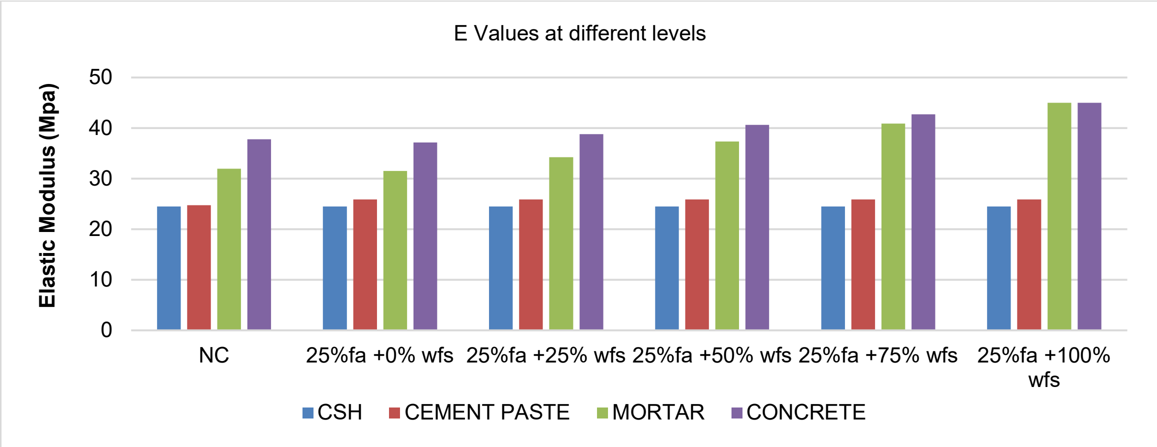

Fig. 7 - Comparison of elastic values at each level using MS

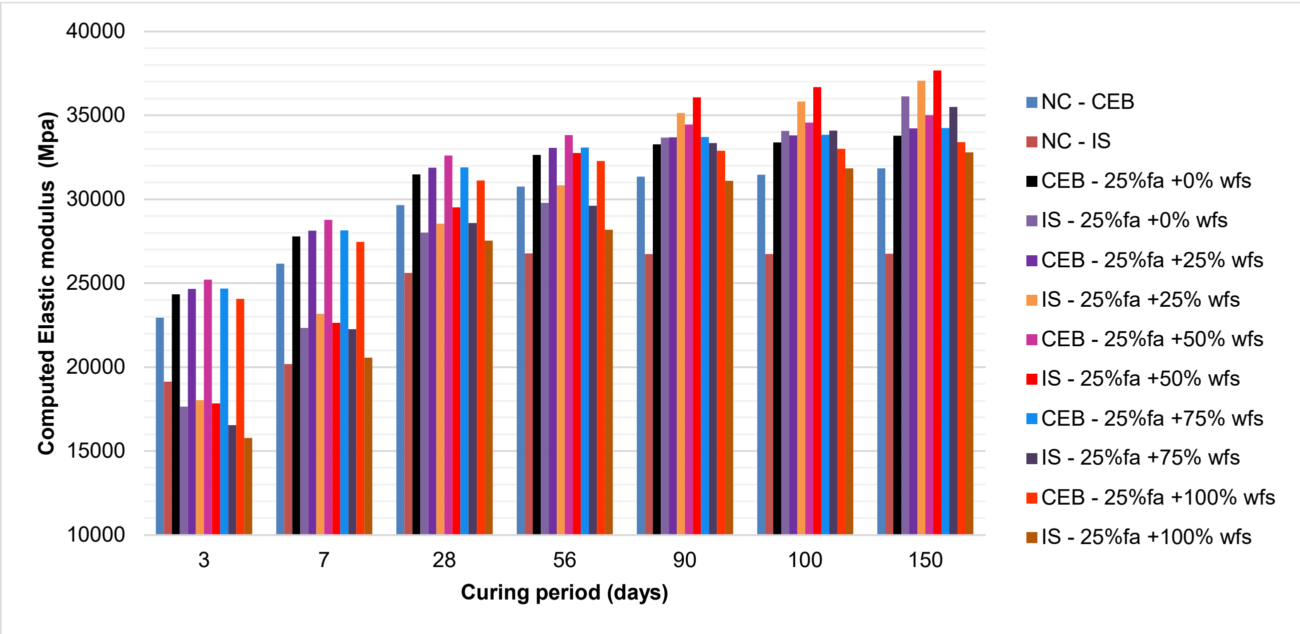

Fig. 8 - Comparison of computed elastic values by using CEB model and IS method

variation of strength between these models ranges between 5.6% to 5.8% respectively. There is an increase in strength of the concrete using CEB model when compared with the B3 model, this is mainly due to the elastic modulus of concrete estimated at any time (t), type of cement and mean compressive strength of concrete when loading starts at the age t_o. The correlation between these two models is represented in the Fig. 6 by introducing the line of regression which provides the better results (R^2=0.9902).

Using MS, the homogenized elastic modulus and poisson's ratio is obtained from the nano to the macro level of concrete [23] and the values are represented in the graph as shown in the Fig. 7. There is an increase in the elastic modulus of concrete due to the inclusion of volume fractions such as air, water, voids, wfs, fa, sand and gravel which, is implanted in the level II, III and IV.

Using MS, the elastic modulus can be estimated at any time period (t) just by providing the mix details of concrete at the initial stage of designing. With the help of elastic modulus of concrete, further the compressive strength of concrete at any time (t) were determined by integrating it with the MS. Using the CEB model and IS method, the elastic modulus of concrete is obtained and the same is represented in the Fig. 8. It is observed that there is a higher discrepancy of 6.7% when compared with IS method at the age of 56 days by utilizing 25% of wfs with 25% of fa. The CEB model is carried out to determine the elastic modulus of concrete by taking the compressive strength of concrete at 28 days into account. Similarly, by using 50% and 75% of wfs in the concrete the strength of the concrete increases with 1.5% to 6% respectively when validated with the CEB model.

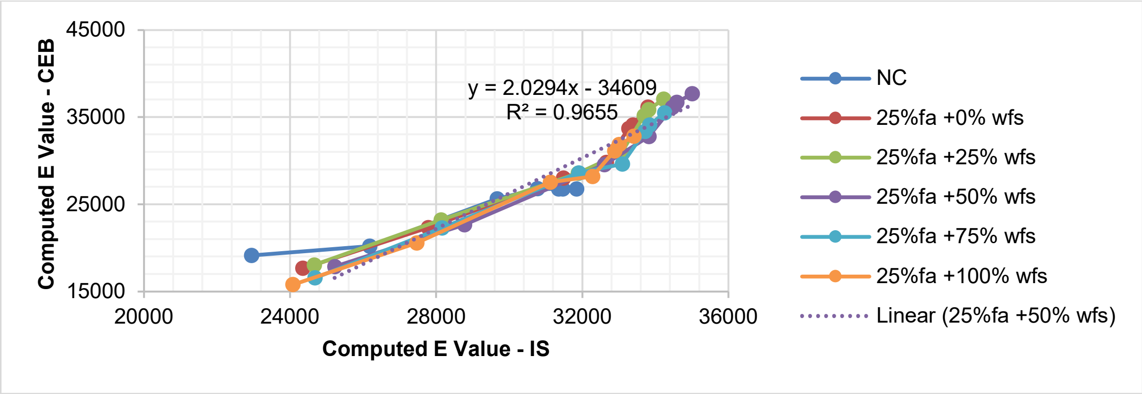

Fig. 9 - Relationship between the computed elastic values by using CEB model and IS method.

The Fig. 9 represents the correlation between the CEB model and IS method by plotting a linear line of regression, from the graph it is noted that these two models provides the better values (R^2=0.9655).

5.Conclusion

Based on the proposed model and experimental results, the following are the conclusions derived by incorporating the various by-products in this study.

- From the measured compressive strength, it was found that there is an increase in the compressive strength of concrete, which varied between 10% to 12.5% for the w/c 0.5 with different mixes.
- The proposed model requires only the mix details and the intrinsic values of cement material parameters to establish the elastic modulus of concrete and poisson's ratio at each level.
- The B3 model is integrated with the MS to evaluate the compressive strength of concrete at any time (t) and it was found to be there is an increase in discrepancy of about 3% to 5% when compared with the experimental results.
- By comparing the compressive strength of the concrete using B3 model and CEB model, there is a variation of about 2% to 8% by using the 50% and 75% of wfs with 25% of fa.
- There is a slightly higher variation in the elastic modulus of concrete, which is mainly depends on the compressive strength of concrete, impact of complete hydration in the concrete and negotiation of interfacial transition zone (ITZ).
- From the experimental results, it is also suggested that the use of 50% and 75% of wfs along with 25% of fa can be extensively used during the making of concrete without disturbing the Indian standards.

Compliance with ethical standards:

Conflict of interest: On behalf of all authors, the corresponding author states that there is no conflict of interest.

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