Study of Analytical Simulation of MNC Composites: Techniques and Influencing Factors

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***Abstract*— This article focuses on how the behavior of cement matrices is influenced by the water-cement ratio and the percentage of nano clay in concrete mixes. Due to the high costs associated with experimental analysis, an initial simulation is conducted to evaluate the behavior of montmorillonite nano clay (MNC) in cementitious materials. Simulations utilize representative volume element (RVE) techniques, leading to the creation of two regression equations to characterize compressive strength and flexural strength based on the two variables. Ultimately, this study provides valuable insights into MNC-cement composites, aiming to reduce the need for macro reinforcement in construction and to facilitate more efficient and cost-effective concrete designs.**

Keywords *– Montmorillonite Nano Clay (MNC); MNC Cement Composite; RVE; Compressive Strength, Flexural Strength*

I. Introduction

Nanofibers are anticipated to gain popularity as a cementitious material due to their exceptional mechanical properties, high electrical and thermal conductivity, and unique morphology. This chapter explores the incorporation of Montmorillonite Nano Clay (MNC) to enhance the properties of cementitious materials. An analytical simulation was performed using ANSYS 15.0, utilizing the finite element method to reduce costs and minimize the number of experimental trials.

The study introduces the concept of the Representative Volume Element (RVE), defined as the smallest volume capable of yielding measurements that accurately represent the entire material. Following the creation of the RVE model for nano-cementitious materials, optimization was conducted focusing on two key factors: the water-cement ratio and the proportion of nanofibers. This thesis analyzes RVE data and formulates equations for predicting compressive and flexural strengths. A parametric equation was derived from RVE analysis to identify essential design parameters for developing appropriate rational equations.

The primary focus of this study is to identify the optimal percentages of nanofibers to incorporate into cementitious materials to boost strength at the micro level. Various proportions of nanofibers, relative to cement weight, were tested through the casting of beams and cubes to assess their impact on reducing micro-cracks and improving the overall performance of the composite structure.

Research indicates that Montmorillonite nano clay (MNC) has excellent mechanical properties that strengthen nano cementitious materials, thanks to its unique structure. For example, [1] Ta-Peng Chang et al. (2007) showed that Portland pozzolana cement reacts with the silicon dioxide in MNCs, forming a gel matrix that enhances MNC-cement paste properties.

In 2021, [2] Niu, Xu-Jing, and colleagues presented nano clay and calcined nano clay, emphasizing their pozzolanic activity and their role in stabilizing pozzolanic bridging and filling effects. [3] Ayesha Kausar et al. (2023) identified nano clay as an energy-efficient material with applications in diverse sectors such as aerospace and electronics. [4] Irshidat M. R. et al. (2018) investigated the strength enhancement achieved with 2% hydrophilic nano clay in cement paste, noting its positive effects on permeability and flowability, which aid in better dispersion of nanofibers. [5] K M Ali provided insights into the microstructural features of nano clay, presenting experimental findings on the mechanical and microstructural properties of nano cementitious materials. [6] Bunea et al. (2023) reviewed the benefits of titanium dioxide and nano clay cement composites, focusing on their strength and durability for environmental and social applications. [7] Tao Zheng et al. (2017) explored how MNC can improve the dispersion of polycarboxylate ether, enhancing the absorption and fluidity of cementitious materials. [8] F. Uddin (2008) investigated the additive, bonding, and filling capabilities of MNC, highlighting its growing popularity compared to other nanofibers. He also pointed out the cost advantages of MNC over alternatives like CNTs, CNFs, and GNPs, while discussing the availability of Montmorillonite clay structures.

Research on MNC primarily concentrates on its properties, with some studies exploring the optimal nanofiber percentage to improve strength parameters. However, these studies reveal several gaps. Firstly, they often neglect the water-cement ratios used in composite construction. Secondly, they tend to focus only on mechanical properties, ignoring microscopic physical parameters. This study therefore seeks to fill these gaps by examining analytically mechanical characteristics of MNC cement composites, incorporating two distinct water-cement ratios and varying percentages of nanofibers.

II. Materials

The analytical simulation has been prepared based on the properties of Portland Pozzolona Cement (Grade II) and Montmorillonite Nano Clay (MNC). The chemical composition and physical characteristics of pozzolona cement are governed by IS:8112-2013 and IS:4031 respectively. **Table 1** describes the chemical and physical components of cement adopted for the study. Two types of properties are described; one is physical, and the other is chemical. **[Fig. 1(a)]** shows a sample of Portland cement.

Table 1*: *Chemical and Physical Components of PPC

	Basic Constituents	Weight (%)
Chemical Properties	Calcium Oxide (CaO)	63.28
	Silica Dioxide (SiO_2)	20.22
	Aluminum Oxide (Al_2O_3)	4.9
	Iron Oxide (Fe_2O_3)	3.3
	Sodium Oxide (Na_2O)	0.98
	Magnesium Oxide (MgO)	2.1
	Sulphuric Anhydride (SO_3)	1.6
	Insoluble Residue	0.2
	Loss On Ignition	1.6
	Chloride Content	0.01
	Alkali Content	0.008
	Oxide Component	**Weight (%)**
	Tricalcium Silicate (C_3S)	63.4376
	Dicalcium Silicate (C_2S)	16.2
	Tricalcium Aluminate (C_3A)	7.41
Physical Properties	**Particulars**	**Range**
	Fineness	290 m^2/kg
	Normal Consistency	32 %
	Specific Gravity	2.87
	Initial Setting Time	110 min
	Final Setting Time	240 min
	Compressive Strength 72 ± 1 h	12 MPa
	Compressive Strength 168 ± 2 h	23 MPa
	Compressive Strength 672 ± 4 h	36 MPa
	Soundness by Autoclave	0.8

On the other hand, Montmorillonite Nano Clay (MNC) **[Fig. 1(b)]** shows a plate-like structure composed of multiple layers of silica, which aids in its dispersion in solutions and enhances material strength. Upon dispersion, these layers become fully separated, exhibiting an impressive aspect ratio, making MNC an effective conductor. It possesses excellent thermal and optical properties, and its chemical composition contributes to the formation of composite structures while improving strength characteristics.

MNC consists of multilayers that are 1 nm thick, with diameters of 1 µm and lengths of 10 µm. As a porous material, it absorbs water and exhibits strong electrical conductivity. Its physical structure consists of tetrahedral and octahedral sheet layers, made up of magnesium or aluminum and hydroxyl ions. These layers are bonded together through electrostatic or Van Der Waals forces. **Table 2** outlines the various properties of Montmorillonite Nano Clay.

Fig.1 (a)	Fig.1 (b)
Portland Pozzolona Cement	Montmorillonite Nano Clay

Figure 1*: *Type of Cementitious Materials

Table 2*: *Physical Components of MNC

	Particulars	MNC
Physical Properties	Length (µm)	10
	Thickness (nm)	1
	Diameter (µm)	1
	Purity	99.9%
	Weight (g/mol)	202.185
	Density (gm/cm^3)	1.3
	Surface Area (m^2/g)	220-270
	Morphology	Flakes
	Specific Gravity (g/cm^3)	2.6
	Electrical Conductivity (S/m)	25
	pH	8.5
	Moisture Content	12%
	Layers	1nm thick

III. Analytical Study

A. RVE Model Generation

Simulations have been performed to study the behaviour of nano-cementitious materials. While experimental analysis is crucial for understanding the properties of these materials, the costs associated with such trials can be prohibitively high. To reduce these costs, some simulations employed ANSYS 15.0 and the concept of 3D Representative Volume Element (RVE), which defines the smallest volume that can provide measurements representative of the entire material. The simulation findings demonstrated that adding nanofibers enhances strength, with optimal improvements of 0.3%, 0.28%, and 0.2% for MNC cementitious materials, respectively. [9] Three types of RVE models are generally considered: Hexagonal RVE, Square RVE, and Cylindrical RVE, as illustrated in **[Fig. 2(a)].**

In this simulation model, Montmorillonite Nano Clay (MNC) is incorporated into the cementitious material at various percentages. This study introduces the square RVE model, as shown in **[Fig. 2(b)]**.

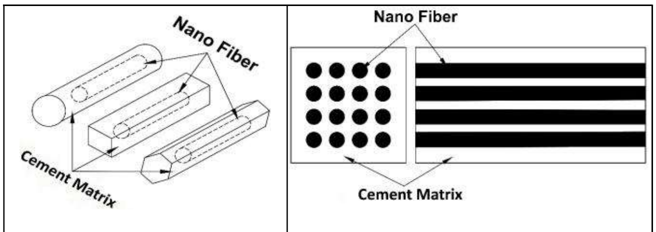

Fig.2 (a)	Fig.2 (b)

Figure 2*: *RVE Representation* - (a) *RVE Model Types*; (b) *MNC Nanofiber With Cement Composites

Here, various percentages of MNCs are introduced (0 to 0.4% by weight of cement). Multiple numbers of Square, Hexagonal, and Cylindrical RVE models are prepared with various percentages, and a comparative result show that square RVE gives a better response than others. Here, the square RVE model is adopted. The property of nanofiber is considered from Sigma Aldrich, and it is used to generate the RVE model in ANSYS 15. The properties of cement are tested in the Laboratory of NIT, Durgapur. 150 design points are selected by random selection with different percentages of nanofibers and various water-cement ratios, as per **[Fig. 3(a)]**.

The cement matrix is selected as a target element for both instances, and nanofibers are chosen as a contact element. Here, bonded contacts are considered. After selecting the related element, the meshing and boundary conditions are adopted. The mesh pattern adopted for the numerical study is shown in **[Fig. 3(b)]**.

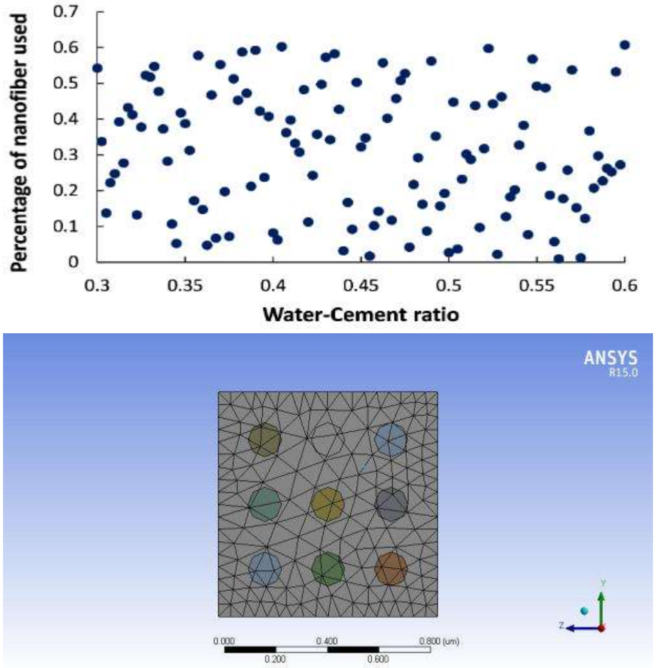

Figure 3*: *RVE Representation* - (a) *Design Key Point from Random Sample Technique*; (b) *Meshing of RVE Model

The size of RVE model and property of nanofiber are tabulated in **Table 3(a)** and **Table 3(b)**.

Table 3(a)*: *Physical Components of RVE Model Size

Dimensions	Range
Width and Height of the cement matrix, 'a'	850 nm
Length of the matrix, 'L'	10 µm
The outer diameter of the Length	130 nm
The thickness of MNC	60 nm
The inner diameter of MNC	70 nm

Table 3(b)*: *Properties of Montmorillonite Nano Clay

Properties of MNC	Range
Length (µm)	10 µm
Density (kg/m^3)	1300-1370
Specific Surface Area (m^2/g)	220-270
Electrical Conductivity (MV)	25

Table 4*: *Concentration of MNC Nano Fibers

Number of Nanofibers	Concentration of Nanofiber (by Weight of Cement)
1	0.02
4	0.08
6	0.1
8	0.15
9	0.17
12	0.22
15	0.28
18	0.34

In the present study work, eight types of RVE models are prepared using Finite Element simulation, as detailed in **Table 4**. These models are used to study the interactions of nanofibers with the matrix, such as the load transfer mechanism and stress distributions along the interfaces, or to evaluate the effective material properties of the composites.

Several models are constructed with various percentages of nano reinforcement (0.01% to 0.3%). Different models with the same geometrical configuration but different nanofiber percentages (by cement weight) have been developed. The nanofibers are assumed to be uniformly distributed over the entire volume. After meshing the models and defining the boundary conditions, the models are analyzed using 3-Dimensional solid elements with the following assumptions:

(i) The material is isotropic. At each amalgamation point, cracking is allowed in three orthogonal directions.

(ii) In the case of cracking at an amalgamation point, it is simulated by altering material properties.

The RVE model sample for various nanofiber percentages is presented in **[Fig. 3(c)]** to **[Fig. 3(e)]**. After confirming the boundary condition and mesh pattern, a comparative study is carried out based on the data generated through the analysis of various models.

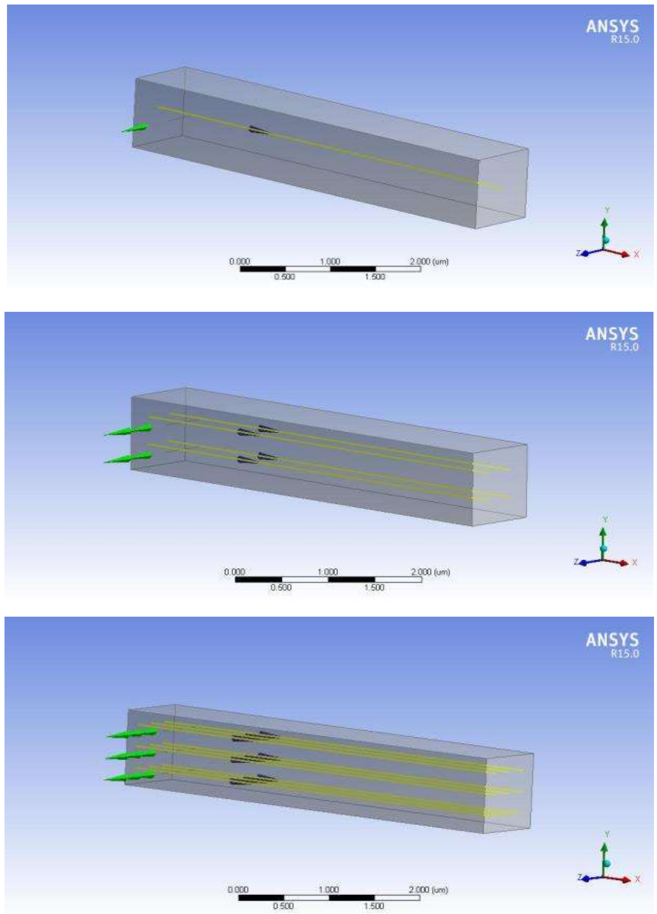

Figure 3*: (c) *RVE model with 0.02%*; (d) *RVE model with 0.1%*; (e) *RVE model with 0.17% of Nanofiber

[Fig. 4(a)] to **[Fig. 4(c)]** shows the analysis of stress-strain and load-displacement patterns when 0.02% of nanofiber is introduced. **[Fig. 4(a)]** shows the stress diagram when 0.02% nanofiber is introduced with cementitious material. **[Fig. 4(b)]** shows the strain diagram, and **[Fig. 4(c)]** represents the displacement diagram with 0.02 percentage of MNC.

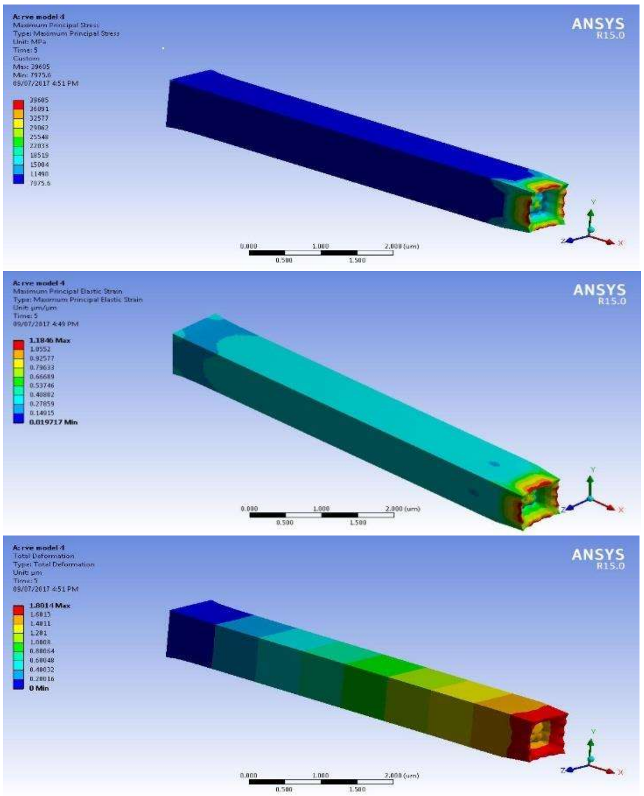

Figure 4*: (a) *Stress Diagram*; (b) *Strain Diagram*; (c) *Displacement Diagram with 0.02% of Nanofiber

The stress diagram, strain diagram, and displacement results with 0.1 percentage MNC RVE model are represented in **[Fig. 5(a)]** to **[Fig. 5(c)]**.

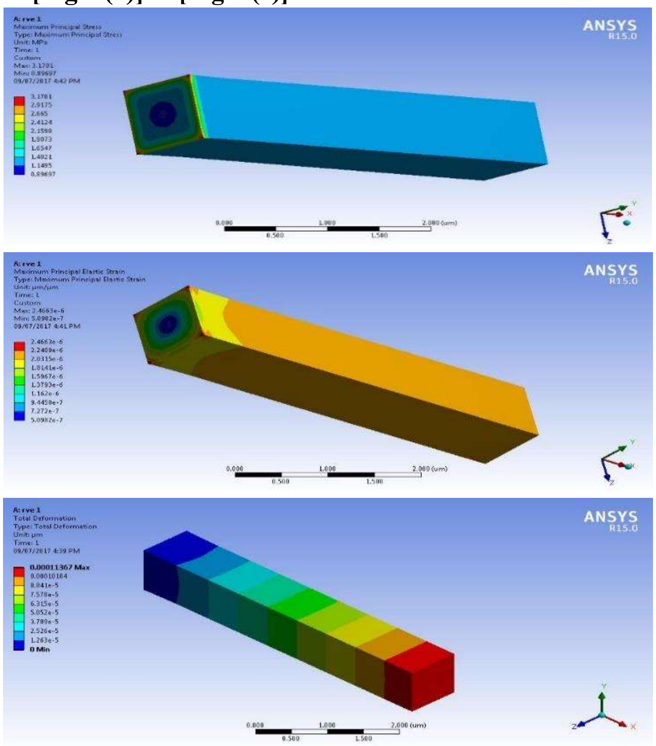

Figure 5*: (a) *Stress Diagram*; (b) *Strain Diagram*; (c) *Displacement Diagram with 0.1% of Nanofiber

Similarly, **[Fig. 6(a)]** to **[Fig. 6(c)]** also means the same for 0.17 percent MNC nanofiber RVE model. Afterwards, a mechanical analysis is studied for MNC nanofiber. **[Fig. 7(a)]** describes the flexural strength behavior of cementitious material with MNC. The compressive strength of MNC is illustrated in **[Fig. 7(b)]**, respectively. [10] The analytical study shows that increasing MNC up to 0.17 percent increases the mechanical properties of cementitious material.

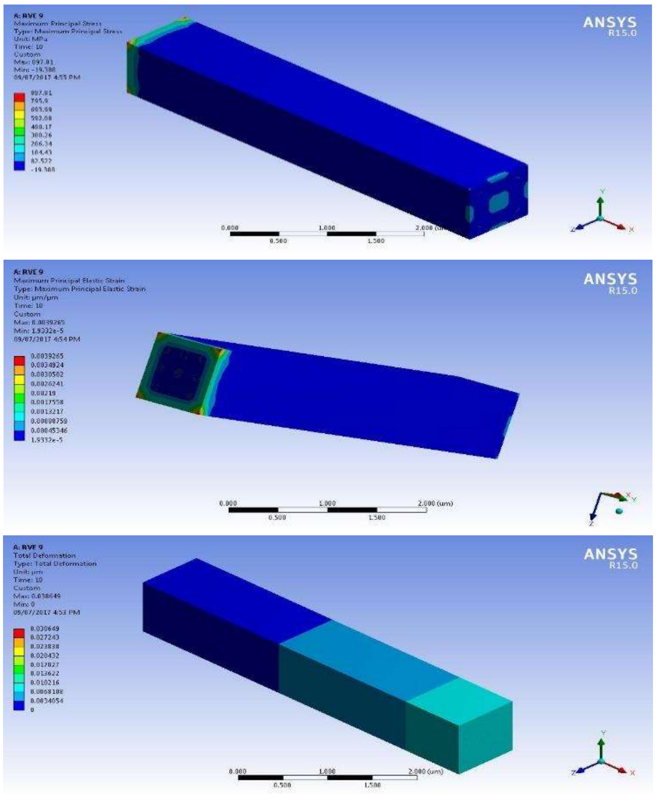

Figure 6*: (a) *Stress Diagram*; (b) *Strain Diagram*; (c) *Displacement Diagram with 0.17% of Nanofiber

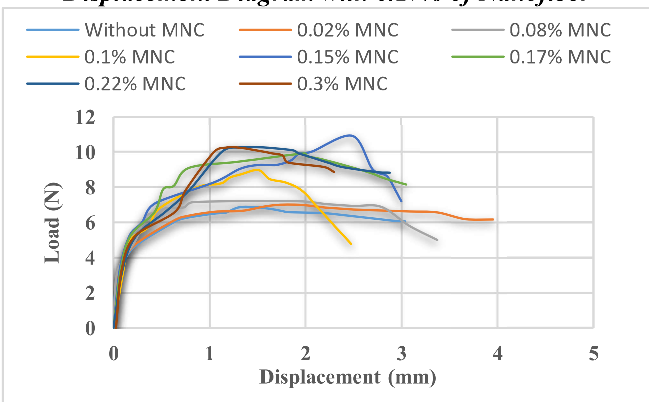

Figure 7*: (a) *Graphical Representation of Flexural Strength Behaviour of Cementitious Material with MNC

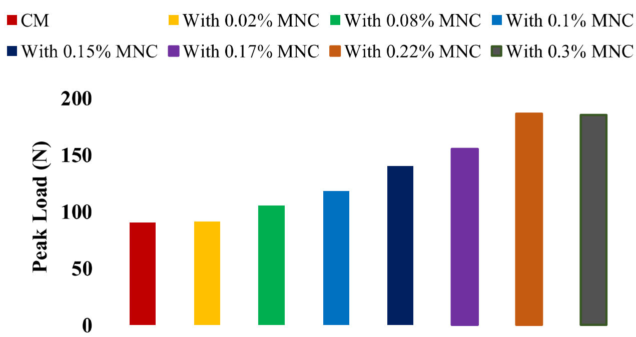

Figure 7*: (b) *Graphical Representation of Compressive Strength Behaviour of Cementitious Material with MNC

B. REGRESSION EQUATION

After getting compressive strength and 150 design key points, a parametric assessment is prepared through Systat Table Curve 3D with two variables: Water-Cement Ratio and Nanofiber Percentage [11]. [12] K. Raoufi generated a parametric evaluation of mortar under thermal loading . Two equations are generated, where **Equation (1)** is representing the compressive strength, while **Equation (2)** is representing the tensile or flexural strength of nano cementitious material.

$$\sigma_c = \frac{a_1+a_2x+a_3x^2+a_4y}{1+b_1x+b_2y+b_3y^2} \quad \text{--------- (1)}$$

$$\sigma_f = \frac{a_1+a_2x+a_3y+a_4y^2+a_5y^3}{1+b_1x+b_2y} \quad \text{--------- (2)}$$

Where, x and y are two variables, x denotes the water-cement ratio, and y denotes the nanofiber percentage. **Table 5(a)** defines the co-efficient used in Equation (1), and **Table 5(b)** establishes the Equation (2) parameter.

Table 5(a)*: *Coefficients a_i and b_i for Compressive Strength* (σ_c) *with Standard Error and the* (R^2) *Value

Coefficient	Value	Standard Error	R^2
a_1	18	0.056323868	0.91234399
a_2	-2	0.034335378	
a_3	-21	0.093422789	
a_4	1	0.052248222	
b_1	-0.98	0.009867521	
b_2	-1	0.086729065	
b_3	-5	0.000654329	

Table 5(b)*: *Coefficients a_i and b_i for Flexural Strength* (σ_f) *with Standard Error and the* (R^2) *Value

Coefficient	Value	Standard Error	R^2
a_1	0.8	0.001325358	0.95433665
a_2	7	0.008976543	
a_3	25	0.012332438	
a_4	3	0.097844234	
a_5	-18	0.044532258	
b_1	-1.2	0.076342267	
b_2	-2.1	0.005623421	

Two surface plots are prepared for compressive(σ_c) and tensile strength (σ_f) parameters with 150 key design points concerning water-cement ratio and nanofiber percentage, shown in **[Fig. 8(a)]** and **[Fig. 8(b)]**.

[Fig. 8(a)] represents the Regression Equation's Surface Plots for the strength for **'x'** (Water-Cement Ratio), and **'y'** (MNC Percentage) of MNC-CM cementitious material for determining compressive strength, and **[Fig. 8(b)]**) represents the same for flexural strength.

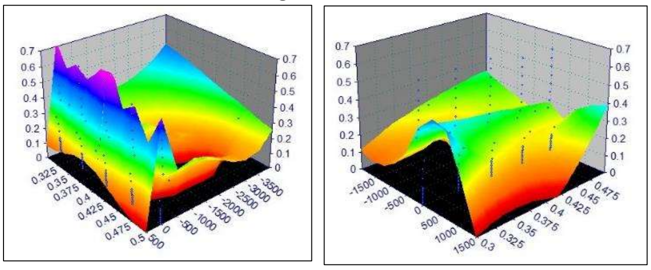

Figure 8*: *Graphical Representation of Regression Equation's Surface Plot* – (a) *Compressive Strength*; (b) *Flexural Strength

IV. CONCLUSION

This study focused on determining the optimum water-cement ratio and optimum percentage of nanofiber for MNC-type nano-cementitious material. Two consecutive analytical results, i.e., RVE and regression equation, are compared in this thesis to get the exact analysis. In this study, various percentages of MNC-CM are mixed as a reinforcement with the cement matrix. The generated equation reduces the time of design and gives an economical design. The subsequent conclusion can be drawn as presented below.

1. The current study contains regression equations for defining the strength characteristics of a nano-cementitious material with various water-cement ratios that can be gladly accepted for design resolutions.
2. The analytical study shows that optimum content of 0.17 percent of Nano Clay gives the optimum load vs deflection characteristics for flexural strength of RVE model.
3. The study also shows that RVE model having optimum content of 0.22 percent of Nano Clay gives the Maximum Compressive Strength compared to the other models with different proportions.
4. In future reference, it can be proposed that the Multi-objective optimization studies could be done using MATLAB by minimizing and maximizing both stresses together to define a suitable strength.

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