

YOUNG'S MODULUS OF CAEBON NANOTUBESS REINFORCED CONCRETE USING REPRESENTATIVE ELEMENTARY VOLUME METHODOLOGY & ANSYS

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ABSTRACT

The catastrophic failures of concrete structures occur everywhere due to natural calamities such as floods, earthquakes, Tsunamis, cyclones and volcanoes. The man-made disasters due to war and bombing leads to huge amount of property loss and lives. To prevent the occupants and the property, the strong column weak beam theory is adopted in seismic prone areas. However the failures or cracks in structures could never be eliminated. With advent of nanotechnology & its applications in concrete, this research investigation focuses on developing a newer material by reinforcing concrete with CNT fibres and macroscopic CNT bars. Nano technology promises crack free materials and structures that could stand for a millennia. So far the CNTs have been known in the form of powder and recent technologies have projected the possibilities of using CNTs as cables for suspension cable bridges with reduced cross sectional area and the Japanese had proposed space elevators using CNT technology. However the steel is vulnerable to corrosion where as energy dissipation of FRP has low modulus of elasticity when compared with steel. Addressing these drawbacks, this research investigation projects macroscopic CNT bars as reinforcement bars in compression members. Further representative element volume methodology had been used to predict Young's modulus of CNT reinforced concrete implying finite element analysis software.

KEYWORDS: Carbon Nanotubes, Reinforced Concrete, Young's Modulus of Elasticity, Representative Elementary Volume etc.

INTRODUCTION

Nanomaterials and nanotechnologies have been used in a variety of applications, including medical, construction, cars, energy, telecommunications, and informatics. The nanomaterials have special characteristics at nanoscale improving the enhanced capacity of the nanocomposites. The carbon foot print for construction had been reduced in the building constructed using nanocomposites in the particular field. This impinges a positive response of the nanotechnology in construction including the self-cleansing properties of the construction materials.

To enable the use of nanomaterials in construction industry at wide scale, a research is needed to be executed in the following stages: choice of nano materials and their use in construction and elaborate study on its characteristics; the behaviour study of the building elements subjected to loads such as columns, beams, slabs and footings etc., development of design and construction standards of structures reinforced with macroscopic CNT bars; Nanosized particles enhance hydration of cementitious and reinforced concrete substantiating particle packing theory. The power of nanotechnology is to alter the desirable properties at atomic level by manipulation using nanosized particles.

C.RameshBabu (2017), narrated that the recent developments in nano technology had led to the newer nano materials such as nanosilica, nano titanium oxide, nano iron oxide, CNTs and graphene oxides with morphologies 0D, 1D and 2D sheets as reported earlier. Unlike 0D nano

particles, the nanofibres & 2D sheets behave as reinforcing materials to bridge cracks. They provide high aspect ratio and intrinsic strength. The fibres usually provide crack bridging capabilities, improved tensile strength, and toughness. The fibre reinforced concrete have poor compressive strength while the ductility and toughness are good. The nanomaterials excel among other supplements in cement by providing modification at nanoscale.

Carbon nanotubes are classified as 1D nanofibres. When reinforced concrete is impregnated with CNTs, it becomes possible to stop fractures at the nanoscale. As shown in Figure 1, there might be greater emphasis on the uses of reinforced concrete impregnated / reinforced with CNTs employing SWNT (Single Walled Carbon Nano Tubes) and MWNT (Multi Walled Carbon Nano Tubes).

CNTs have a wide range of uses in the realm of nanotechnology. The CNTs were researched by scientists for more than 100 years starting from carbon fibres. Growth of filamentous carbon started from 1889. Carbon Nano Tube is a sheet of graphite rolled up into tube structure. CNTs are categorised into SWNTs and MWNTs, as shown in Figure 1.

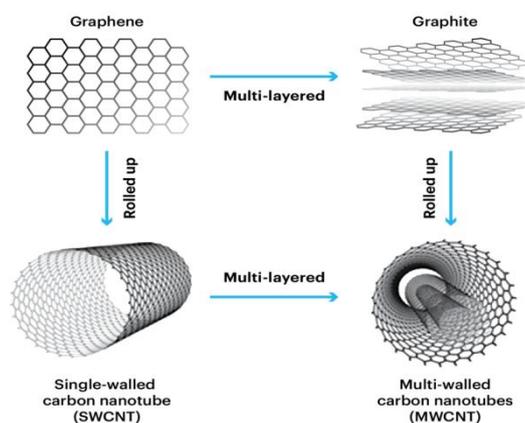


Fig. 1: types of CNTs

SWNTs are made by rolling a single sheet with a diameter close to 1nm, whereas MWNTs are formed by rolling numerous sheets with diameters ranging from 10 to 80 nm. CNTs have Young's moduli ranging from 270 GPa to 1 TPa, tensile strengths ranging from 11 to 200 GPa, and yield strengths ranging from 63 GPa (Sasmal et al. 2013, Sindu et al. 2012). CNTs have five times the Young's modulus of steel (1000 GPa) and 100 times the strength of steel while being one-sixth the weight. Elastic strain capabilities were claimed to be 60 times higher than steel. (Kasthurirangan et al. 2011).

Furthermore, these CNTs are very flexible, with a high yield strength and a low weight. Because of Vander Waal's forces, the CNTs stick together. Various techniques involved in synthesis of CNTs include chemical modification, functionalization, filling and doping. The CNT dominates all technologies including tennis rackets to Li-ion batteries. The Carbon Nanotubes having amazing properties to include as reinforcement starting from biomedical applications to polymer nanocomposites and electronic devices.

The CNTs have different structural integrity such as Arm chair, ZigZag and Chiral as depicted in Figure2. The concrete matrix when impregnated with nano materials such as Carbon Nanotubes (CNTs) exhibit enhanced mechanical properties compared to macroscopic concrete nucleation provided by Calcium – Silicate – Hydrate (CSH) gel. Various methods of dispersion have been proposed for enhancing flexural & compressive strength of CNT reinforced concrete matrix.

The hindrance of agglomeration when stirred with cementitious materials had been found to be eliminated by Cement Hybrid Material popularly mentioned as CHM using multi scaling approach. Other dispersion methodologies discovered are coating CNTs with SiO₂ content along with surface area. The interaction with C₃S (Tri Calcium Silicate) depicted enhanced pozzalonic activity and appreciable morphology of C-S-H gel. Structural elements with reduced cross section and light weight are possible by CNTs. Samuel Chuah et al. (2014) tried deagglomeration of CNTs in cementitious compounds using sonication for 120 minutes along with Nitrogen doped CNTs. To conclude, still scientific investigations are investigating methodologies to avoid formation of threads by CNTs in cement matrix.

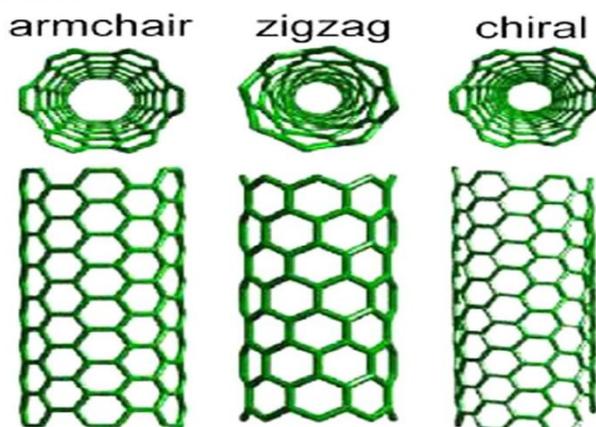


Fig. 2: Arm chair, ZigZag and Chiral CNTs

Samuel Chuah et al. (2014) states that the size of nano particles form seeding units for CSH gel resembling the size of the gel. Among all kinds of nano fillers, Graphene Oxide and CNTs have been showing positivity in enhancing tensile strength and flexural strength.

The Graphene Oxide (GO) has superior aspect ratio, good covalent bonding for hydration of cement. But CNTs are better in load transfer and have improved workability when compared with Graphene Oxide. The CNTs are utilized in construction industry for superior mechanical properties with good workability.

Ramesh Babu (2017) narrated that the synthesis of CNTs using Arc Discharge, Laser Ablation & Chemical vapour deposition had been pronounced in the past research papers. The research on the CNT reinforced cement compounds had been found to be unaffordable due to the manufacturing costs. These fundamental limitations restrict commercial and construction applications. Based on above hindrances in executing research on CNT impregnated concrete or cement matrix, analytical studies are executed.

The macroscopic structures were synthesized using self-assembling technologies in olden days. These were applicable to microscale and nanoscale materials including photonic crystals, nanocomposites and modified DNA structures.

Zhou et al. (2002) proposes that the SWNTs were made hydrophilic and were created up to a dimension of 100 micro metre. The Carbon Nano Tubes can be woven to macroscopic assemblies which would have the inheritance of the individual mother material. The CNT arrays had been discovered by spinning. The fibrous CNTs exhibit extreme tensile strength due to torsional twisting and spinning along the radial direction of fibres. Macroscopic CNTs are preferred as 1D CNT bundle when compared with chirality - pure CNTs (Zhang et al. 2015).

The Raman analysis and SEM image had confirmed uniform CNT array with good morphology. The past researches proved that surfactants with opposite charge will uniformly disperse the CNTs in any matrix.

Past investigations by Jiang et al. (2014) revealed manufacturing SWNTfibres by polyelectrolyte dispersions through stabilization of ether in dimethyl sulfoxide followed by coagulation in aqueous solutions. The produced CNT fibres showed tensilestrength of 124 MPa with Young'smodulus being 1 TPa.

This research investigation aims at the FEM of CNT reinforcedconcrete matrix for 3 gradesof concretenamely M40, M60 & M120 depicting NSC, HSC, and UHSC. The finite element model using ANSYS replicated arbitrarily oriented CNTs for nine fibrevolume fractions from 0.1%to0.9% covering 54 specimens. Upon evaluation of model, longitudinal & transverse Young'smodulus of CNT reinforcedconcrete were arrived. The REV was adopted for the simulations.

These seamless tubes of the twenty-first century have extraordinarily high mechanical qualities and are used in electronics, biology, chemistry, and multifunctional composites. CNTs are rolled graphene sheets with a theoretical strength 100 times that of steel, a specific gravity 1/6th that of steel, an elastic strain of 12%, a Young's modulus of 1TPa, and a tensile strength of 200 GPa. CNTs were discovered to be excellent reinforcing fibers, greatly increasing the mechanical characteristics of any host material. The tensile and flexural strength of cement composites were determined using the law of mixing.

Rouiania et al. (2008) estimated the Young's modulus of CNT reinforced composites. Maria et al. (2014) determined the constitutive relations of CNT reinforced concrete. Assuming concrete nonlinearity and taking interfacial bonding into account. The CNTs in the cement matrix were expected to be evenly distributed and unidirectionally oriented.

Hasan et al. (2014), on the other hand, considered random distribution of nanotubes in cement and generated a new factor proposed for random orientation of CNT in cement matrix. The findings of analytical modeling were found to have a high connection with the outcomes of the experiments. The scientist assumed a distribution function for fibre orientation in the composite and computed effective mechanical characteristics of the fibres depending on their location angle in the composite.

Finally, Hasan et al. (2014) projected the compressive strength of CNT/cement composite using the representative elementary volume (REV) approach. A few analytical models were developed using a unit cell with a single fiber reinforcement. The various modeling techniques used finite element modeling (FEM) to represent CNTs as line elements, hollow cylinders, and solid cylinders. Based on the REV technique and FEM, it was discovered that the coordination of fibers in the matrix reinforced with CNTs follows a certain law. (Yengejeh and colleagues, 2017)

The model's effective Young's modulus decreases almost linearly as the matrix volume percentage increases. The proper dispersion of agglomerated nanotubes is the key difficulty in the CNT reinforced concrete matrix. Many ways have been offered, including the innovative approach WS2 nanoreinforced cement, which demonstrated that nanoparticles might increase the tensile, flexural, and fracture toughness properties of concrete. (Nadivet al. 2015)

Studies have also demonstrated that adding smaller concentrations of CNTs or carbon nanofibres (CNFs) can increase strength, ductility, and fracture toughness. Furthermore, the move to fiber reinforced concrete (FRC) is supported by the fact that individual fibers, rather than small bits of steel, may increase tensile strength. There is a large database on CNT reinforcement and dispersion where researchers employ CNTs in the range of 0.01 to 2%. (Rashad et al. 2017)

This low percentile is sufficient to improve the cement matrix's compressive, tensile, and flexural strength. Macroscopic scale research considers embedding CNTs as reinforcement in a matching volume proportion. To describe the concrete composites, the matrix was simulated using several nonlinear constitutive models. In continuum mechanics, complete bonding between CNTs

and matrix has been claimed after several microscopic scale research illustrating structural morphology of CNT reinforcements. (Wang et al. 2016)

The findings of nano indentation demonstrated that MWCNTs could substantially strengthen the cement paste matrix at the nano scale, increasing the quantity of high stiffness C-S-H gel and lowering porosity. Surface-modified Nanotubes and CSH crystals would result in strong binding strength, resulting in load transmission from the cement matrix to the reinforcement. For random distributions with high CNT concentration, the numerical simulations revealed good agreement between the meshless approach, experiments, and the finite element model. (Wang et al. 2016)

CNTs might be employed as reinforcing bars in concrete, according to RameshBabu et al. (2017). This study focuses on the use of CNTs, both single and multiwalled, as fiber reinforcements for various fibre volume fractions using the representative volume element method (RVE) ranging from 0.1% to 1.0% using the FEA software ANSYS 2023R1 and culminating in a simplified equation for determining the Young's modulus of concrete matrix reinforced with carbon nanotubes.

LITERATURE REVIEW

GhandiRousainia et al. (2008) from Algeria investigated the Young's modulus of a composite reinforced with Single Walled Carbon Nanotubes (SWNT). Using the finite element method, the researcher created a number of modeling approaches and analyses. The study demonstrated the effect and advantages of incorporating SWNT into a concrete matrix. By modeling SWNTs with pipe components in ABAQUS, the FEM was utilized to evaluate the longitudinal elastic modulus of the composite and large scale models. The findings of finite element simulations were confirmed by comparing them to the analytical results (rule of mixtures). Using continuum mechanics, the researcher discovered that 1% SWNT in a concrete matrix enhanced 33% of the Young's modulus of the concrete composite in both single and multiple SWNTs. Even a volume fraction of less than 1% improves the composite's Young's modulus. Finally, the researcher believes that adding SWNTs to concrete in modest and cheap volume fractions improves its mechanical behavior and proposes that additional study is needed, particularly in fracture and tensile behavior.

Chengmin Jiang et al. (2014) produced SWNT fibres from SWNT polyelectrolyte dispersed by crown ether in dimethylsulfoxide & coagulated in the aqueous solution. The manufactured spun CNT fibre showed tensile strength of 124 MPa & Young's modulus of 14 GPa. The CNTs have huge tensile strength owing to their SP² hybridization bonding resembling the atomic structure of diamond.

VijayaBhaskar et al. (2017) projects that the CNTs could be used in varied fields of civil engineering. The mechanical properties can be increased significantly. The interaction between CNTs & cement paste was active. The compressive strength could be increased by flyash mixes. The addition of CNTs in small quantities led to appreciable increase in compressive strength, flexural strength and split tensile strength. The Young's modulus of the CNT reinforced matrix would be greater than the plain cement concrete/mortar.

Tuhi et al. (2018) demonstrated that drawing, winding, and pressing may be used to create horizontally aligned CNT sheets from vertically aligned CNT arrays. CNT diameter reduction would improve the mechanical characteristics of aligned CNT sheets and their composites.

Tao et al. (2019) reported that the CNTs were found to be good at thermal conductivity and electrical conductivity. The mechanical stirring approach, ultrasonic dispersion method, or modification and integrated method might all be used to disperse CNTs/CNFs. The inclusion of CNTs has a significant impact on the mechanical and microscopic properties. The inclusion of

carbon nanotubes can boost compressive and bending strength by 20% on average. Finally, it was discovered that in the case of cementitious matrix microstructure, excellent adhesive performance was recorded between CNTs and the cement matrix. CNTs cover the gaps and fissures, reducing porosity and permeability. The presence of CNTs can transmit stress acting at weaker places such as cracks and pores, hence delaying the formation of cracks. The CNTs also reduce the permeability of the concrete leading to defence against the entry of foreign matter inside the concrete. This enhances the durability of the concrete.

XiaobinSongetal., (2020) studied the effect of CNT dosage, concrete cover thickness, and steel bar diameter on the binding behavior of steel bars and CNT modified concrete. To better imitate the stress state of concrete near steel bars in real constructions, beam specimens were built and evaluated. The results of the tests revealed that at CNT doses of 0.1 wt% and 0.15 wt%, the initial bond strength and peak bond stress could be increased by 37.2% and 49.7%, respectively. It was also revealed that the peak bond stress increased almost linearly with the concrete cover thickness to reinforcing bar diameter ratio, c/d , and altered with CNT dosage synchronously with the uniaxial tensile strength of concrete for a given c/d ratio.

Heeyoung Lee etal. (2020) studied the bonding behavior of composites and reinforcing bars by constructing 20 bond strength test specimens and conducting a pullout test. The compressive strengths of MWCNT-cementitious composites with various MWCNT concentrations were also investigated. The internal structural processes of MWCNT cementitious composites were investigated using mercury intrusion porosimetry (MIP) and field emission scanning electron microscopy (FE-SEM). The results demonstrated that adding 0.5 weight percent MWCNTs to cementitious composites boosted their compressive strength and improved bonding between the cement composite and the reinforcing bar.

Chang Su (2022) investigated saltwater sand concrete (SWSSC) beams reinforced with basalt fiber-reinforced polymer (BFRP) bars for marine durability. To extend the lifetime of the SWSSC beams, carbon nanotube (CNT)-modified BFRP longitudinal bars, CNT-modified BFRP stirrups, and sand-coated BFRP stirrups were employed to replace steel bars and normal BFRP bars. Furthermore, the durability of CNT-modified BFRP bars in a SWSSC environment was investigated, as was the binding strength between CNT-modified BFRP bars/sand-coated BFRP bars and SWSSC in a marine environment. The results demonstrated that the CNT modification successfully delayed the rate of tensile strength degradation of the BFRP bar and the bond strength between the BFRP bar and SWSSC concrete in the marine environment.

Lee, Dongmin, et al. (2023) explore the binding behavior of rebar implanted in cementitious composites including polyvinyl alcohol (PVA) fibers and carbon nanotubes (CNTs). The results of the experiments demonstrated that when the rebar diameter or CNTs mix ratio was reduced, the binding strength of the rebar increased. Based on the test results, a new, basic model was constructed that takes into consideration the rebar diameter as well as the CNTs mix ratio. When the test results were compared, it was observed that the proposed model successfully predicted the bond behavior of a rebar implanted in PVA cementitious composites with or without CNTs, including the bond strength and related slip.

OBJECTIVES OF THE STUDY

- To find Young's modulus of CNT reinforced concrete using Representative Elementary Volume (REV) methodology & FEA software ANSYS.

**DETERMINATION OF YOUNG'S MODULUS OF CNTRC
 REV METHOD**

According to Pellisou et al. (2009), REV is the smallest representation of a composite with spatially constant macroscopic constitutive representation, and it may be precise enough for constitutive relation and response. In order to replace a heterogeneous material with a homogeneous material, the chosen volume must be big enough to reflect the microstructure and small enough to analyze analytically.

The REV would reproduce the composite's elastic constant and fiber volume fraction. This study discovered the REV by reinforcing hollow CNTs in the concrete matrix without any additional e-material with fibre volume fractions ranging from 0.10% to 0.90%.The constructed finite element model represented a random distribution of CNTs that reproduced the orientation of any concrete structural member, reinforced or unreinforced with steel bars.

COMPUTATIONAL MICROMECHANICS

The elastic characteristics of composites may be shown in the form of Young's modulus E, Shear modulus G, and Poisson's ratio (Barbero et al. 2014). Heterogeneous composites need a wide range of material characteristics, and determining these qualities experimentally is time-consuming and expensive. Analytical homogenization might be used instead of experimentation.

The analytical models would differ substantially, displaying complicated and accurate models. The composites' stiffness U and compliance Z tensors are-

$$U = \sum T_i U^i R^i; \sum T_i R^i = I; = \sum T_i Z_i B^i \text{ and } \sum T_i B^i = I \dots\dots\dots(1)$$

Where, T_i = volume fraction of the i^{th} phase of composite

U_i = stiffness of the i^{th} phase of the composite

Z_i = compliancetensors of i^{th} phase of composite

I = 6 x 6 identity matrix.

R_i = strain of i^{th} phase

B_i = stressconcentration tensors of the i^{th} phase.

$I = f, m$ represents the fibre and matrix phases in fiber reinforced composites. The stiffness tensor is transversely isotropic in most composites with random fiber orientation. There is just one axis of symmetry in this type of transversely isotropic material. It is characterized by five constants. Barbero et al. (2014) propose three representative volume elements (RVE) for a composite material with a periodic, square fiber array, as shown in Figure 3.

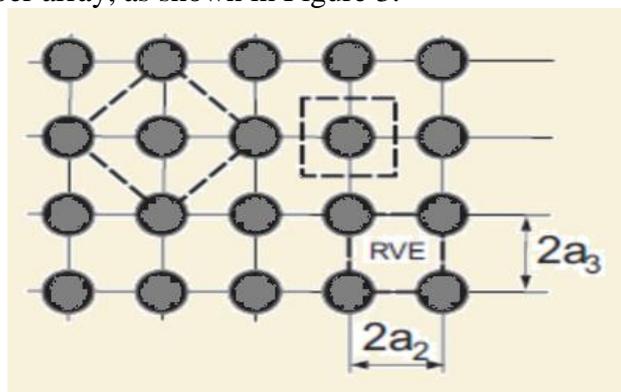


Figure 3: Three possible REV

$$D_{11} = \lambda_m + 2\mu_m - \frac{v_f}{j} \left[\frac{A_3^2}{\mu_m^2} - \frac{2A_6A_3}{g\mu_m^2} - \frac{aA_3}{\mu_m^c} + \frac{A_6^2 - A_7^2}{g^2\mu_m^2} - \frac{A_6a + A_7b}{g\mu_m^c} + \frac{a^2 - b^2}{4c^2} \right] \dots\dots\dots(2)$$

$$D_{12} = \lambda_m + \frac{v_f}{j} \left[\frac{A_3}{2\mu_m^c} - \frac{A_6 - A_7}{2g\mu_m^c} + \frac{a+b}{4c^2} \right] \dots\dots\dots(3)$$

$$D_{23} = \lambda_m + \frac{v_f}{j} \left[\frac{A_7 a}{2g\mu_m^c} + \frac{ba+b^2}{4c^2} \right] \dots\dots\dots(4)$$

$$D_{22} = \lambda_m - 2\mu_m - \frac{v_f}{j} \left[-\frac{aA_3}{2\mu_m^c} + \frac{aA_6}{2g\mu_m^c} + \frac{a^2-b^2}{4c^2} \right] \dots\dots\dots(5)$$

$$D_{44} = \mu_m - V_f \left[-2\frac{A_3}{\mu_m} + (\mu_m - \mu_f)^{-1} + \frac{4A_7}{\mu_m(2-2\mu_m)} \right]^{-1} \dots\dots\dots(6)$$

$$D_{66} = \mu_m - V_f \left[-\frac{A_3}{\mu_m} + (\mu_m - \mu_f)^{-1} \right]^{-1} \dots\dots\dots(7)$$

$$J = \frac{aA_3^2}{2\mu_m^2 c} - \frac{aA_6 A_3}{g\mu_m^2} + \frac{a(A_6^2 - A_7^2)}{2cg^2\mu_m^2} + \frac{A_3(b^2 - a^2)}{2\mu_m c^2} + \frac{A_6(a^2 - b^2) + a_7(ab + b^2)}{2\mu_m c^2 g} + \frac{(a^3 - 2b^3 - 3ab^2)}{8c^3} \dots\dots\dots(8)$$

To analyze all of the components of the stiffness tensor of the given composite, the composite with periodic microstructure might be represented by Fourier series. Also, according to Barbero, composites with randomly oriented fibers have transversely isotropic characteristics, and the microstructure has square symmetry, hence the stiffness tensor has six distinct coefficients provided by six Equations (2) to (7). (Barbero et al. 2014)

Where,

$$a = \mu_f - \mu_m - 2\mu_f \mu_m + V_f \dots\dots\dots(9)$$

$$b = -\mu_f V_m + \mu_f V_f + 2\mu_f V_m V_f - 2\mu_m V_m V_f \dots\dots\dots(10)$$

$$c = (\mu_m - \mu_f)(\mu_f - \mu_m + \mu_f V_f - \mu_m V_m + 2\mu_m V_f - 2\mu_m V_m + 2\mu_m V_m V_f - 2\mu_f V_m V_f) \dots\dots\dots(11)$$

$$g = (2 - 2V_m) \dots\dots\dots(12)$$

The letters (V)m and (V)f stand for matrix and fiber, respectively. Barbero stated that the constants for the composite reinforced with cylindrical, long, and circular fibers placed in a square array along the x-axis with $a_2 = a_3$ are:

$$A_3 = 0.49 - 0.47V_f - 0.02V_f^2 \dots\dots\dots(13)$$

$$A_6 = 0.368 - 0.14V_f - 0.27V_f^2 \dots\dots\dots(14)$$

$$A_7 = 0.12 - 0.32V_f + 0.23V_f^2 \dots\dots\dots(15)$$

Because of the periodic design, the resultant tensor A^* would have a square array. Because most composites have random fiber orientation, resulting in a transversely isotropic stiffness tensor with independent constants of 5, the values of Young's modulus of elasticity E and shear modulus G might be calculated using the coefficients of tensor A^* . Most of the time, uniform fiber orientation in a concrete matrix is unattainable, thus a random microstructure is assumed, resulting in transversely isotropic at the mesoscale.

FINITE ELEMENT MODELING

The finite element modeling was based on the narrative of computational micromechanics by Barbero et al. (2014). The representative volume element (RVE) with dimensions $2a_1 \times 2a_2 \times 2a_3$ was chosen for study, and 1/8th of the RVE was simulated using ANSYS 2023R1, as shown in figure 4.

The mesh volume has a maximum of 172 elements and 330 nodes. This type of modeling favored precise replication of the CNT reinforced concrete matrix with random orientation for all concrete types, including NSC, HSC, and UHSC. The nanotubes were hollow and arranged without the use of any additional substance. The volume fractions were calculated based on the volume of the concrete matrix. Figure 6 depicts the terms $2a_1$ along the z direction, $2a_2$ along the x direction, and $2a_3$ along the y direction. The boundary conditions were set to $x = y = z = 0$; then a uniform displacement was applied along the z direction.

The FEA model and its constituents were found to be macroscopically orthotropic as a result of the boundary conditions indicated. For different fibre volume fractions ranging from 0.1% to 0.9%, the SOLID 65 element was utilized to model the concrete matrix, followed by random orientation of CNTs. The simulated model could predict the Young's modulus of a CNT reinforced concrete matrix in both the transverse and longitudinal directions, as well as the composite's Poisson ratio and shear moduli. The diameter of the single walled carbon nanotubes (SWNTs) was estimated to be 3nm, with a Young's modulus of 1TPa and a Poisson's ratio of 0.22. The same feature was found in multiple walled carbon nanotubes (MWNTs), which had a diameter of 100nm.

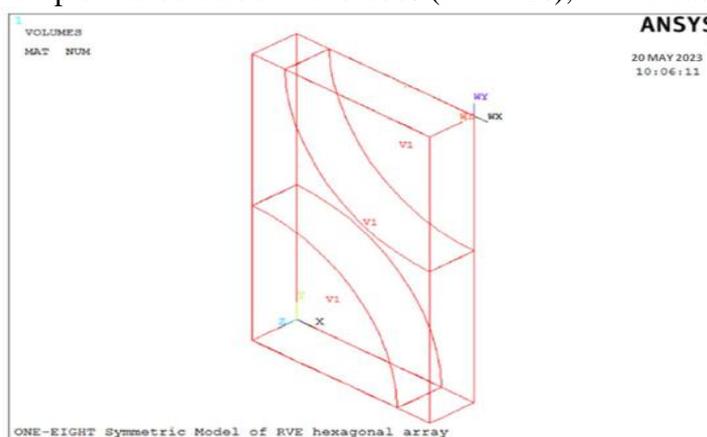


Figure 4: OneEighth symmetric model of REV

Figure 4 shows the ninth model of the simulated volume generated by the finite element modeling program ANSYS 2023R1. The concrete grade ranged from 40 MPa for normal strength concrete to 60 MPa for high strength concrete and 120 MPa for ultra high strength concrete.

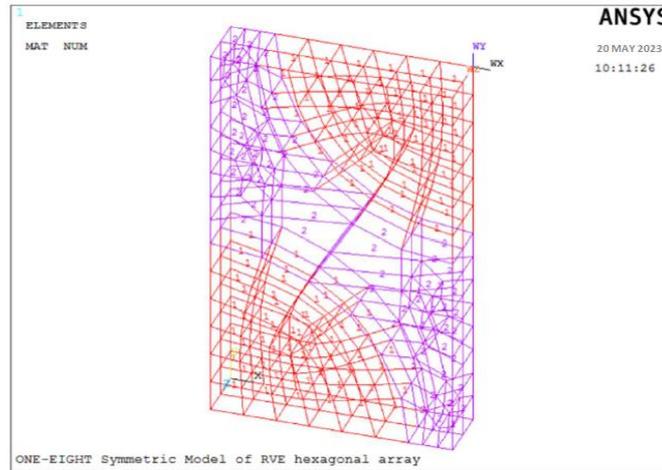


Figure 5 Meshed REV of the concrete matrix

The typical volume after meshing is shown in Figure 5. The boundary conditions were set to $x = y = 0$, then displacement was applied along the z axis to make $z = a_1$. All of the elements and the matrix are macroscopically orthotropic due to the stress boundary conditions used. The analysis produced Young's modulus in both the longitudinal and transverse directions.

DIMENSIONS OF REPRESENTATIVE ELEMENTARY VOLUME METHOD

The diameter of SWNT was chosen as 3nm and for MWNTs, 100 nm was adopted. The dimensions a_2 and a_3 of the RVE, as shown in Figure 6, were chosen to obtain the respective volume fraction (V_f) (in this case it ranges between 0.1 and 0.9 %) with a hexagonal array microstructure. The fiber volume (v_f) and the total volume (v_t) of the RVE are $v_f = 4a_1\pi (df/2)^2$; $v_t = 2a_12a_22a_3$

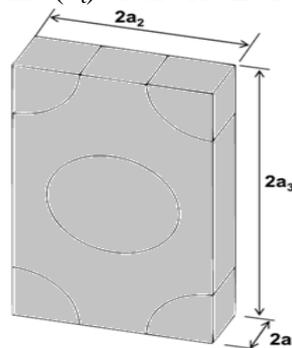


Figure 6 Representative elementary volume method

The ratio between both is the volume fraction. Therefore,

$$V_f = \pi [(df / 2)^2 / 2a_2a_3]$$

Additionally, the relation between a_2 and a_3 is established by the hexagonal array pattern

$$a_3 = a_2 \tan (60^0)$$

Based on the diameter of CNT & the fibre volume fraction V_f , the dimensions of Representative Elementary Volume could be arrived. The dimensions a_2 and a_3 of REV for SWNTs and MWNTs are tabulated in table 1 & 2 respectively

Table 1 Dimensions of a_2 & a_3 for SWNT

Volume Fraction (V_f)	$a_2 \mu_m$	$a_3 \mu_m$
.1	.00453	.00783
.2	.00318	.00554
.3	.00262	.00453

.4	.00225	.00392
.5	.00203	.00351
.6	.00185	.00318
.7	.00172	.00295
.8	.00161	.00276
.9	.00152	.00262

Table 2 Dimensions of a_2 and a_3 for MWNT

V_f %	$a_2 \mu_m$	$a_3 \mu_m$
.1	.1506	.2607
.2	.1062	.1837
.3	.0865	.1502
.4	.0755	.1301
.5	.0672	.1163
.6	.0614	.1062
.7	.0571	.0983
.8	.0533	.0922
.9	.0495	.0865

The above values of a_2 and a_3 are adopted for finiteelement analysis ofCNT reinforced concrete & to derive longitudinal & transverse Young'smodulus (EL and ET).

RESULTS

The SWNTs reinforced concrete was analysedusing REV and FEA software ANSYS. The obtained results of longitudinal &transverse Young'smodulus of SWNT reinforcedconcrete were plotted againstfibre volume fraction of CNT. The figures from 7 to 11 represent the abovediscussed plots. The longitudinal Young's modulus experienced linear variationwhen compared with thetransverse Young's modulus. For all the grades ofconcrete used for study NSC, HSC and UHSC, the same trend was observedand there was no meticulous change observedfor longitudinal Young'smodulusas depicted by the equations arrived in the table 3.

Similarly nonlinear variationwas observed for transverse Young'smodulus of SWNT and MWNT. The arrivedREV converged at 0.9% fibre volume fraction as represented by followingFigure 7.

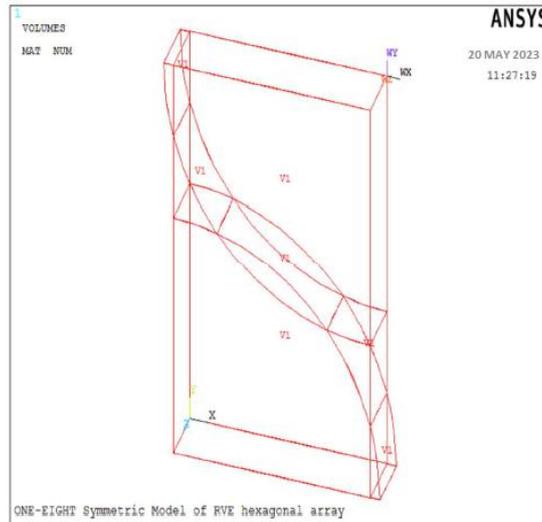


Figure 37 REV hexagonal array

The research was confined to fibre volume fraction from 0.1 to 0.9% of CNTs in the REV generated. Based on the graphical plots of SWNT and MWNT exposing the EL and ET of the CNT reinforced concrete, equations relating Young's modulus and CNT fibre volume fractions $V_f\%$ were arrived. The linear function of longitudinal Young's modulus depicts a line and it is a polynomial with highest exponent being 1 for SWNT. For MWNT, the perfect fit from the graph is exponential. The non-linearity was observed for the relation between transverse Young's modulus ET & fibre volume fraction of SWNT and MWNT. The above facts were observed from figure 8 to Figure 11.

(i) SWNT

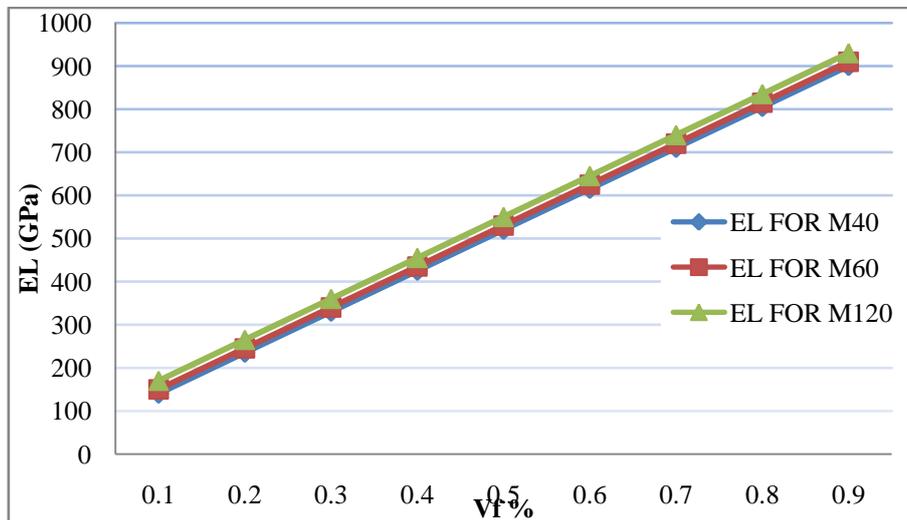


Figure 8 V_f % Vs E_L

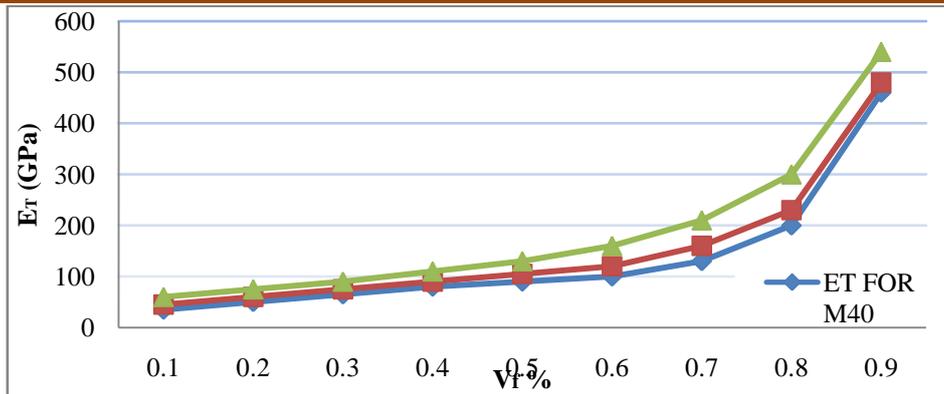


Figure 9 V_f % Vs E_T

(ii) MWCNT

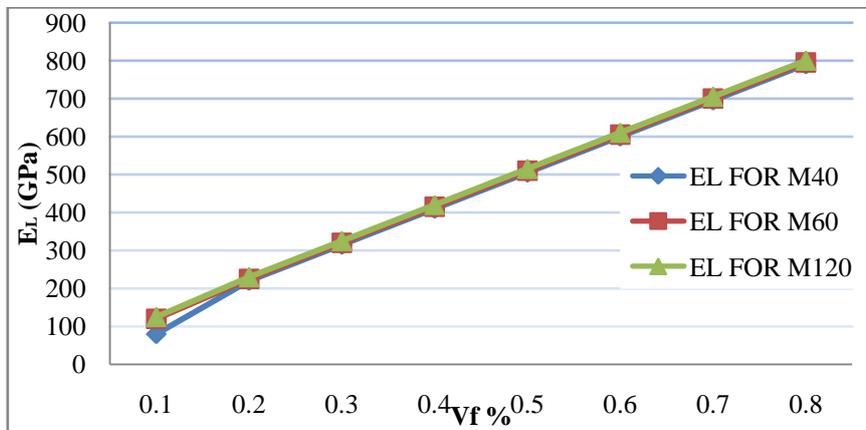


Figure 10 V_f % Vs E_L

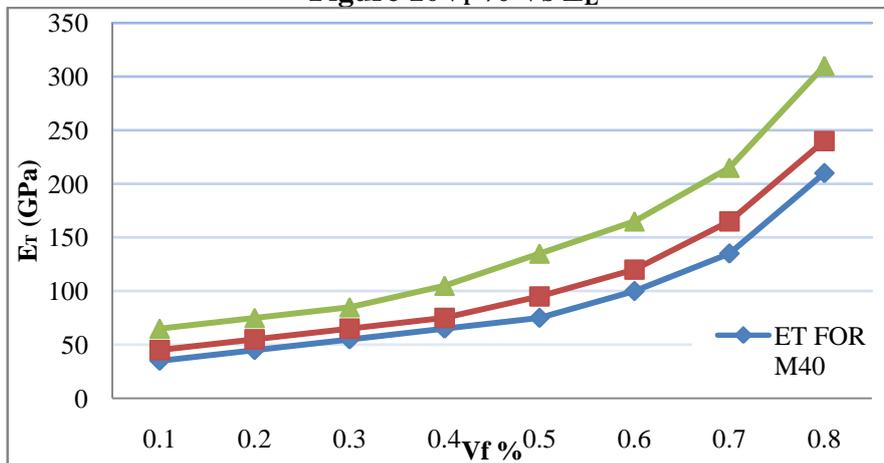


Figure 11 V_f % Vs E_T

Table 3 Equations for young's modulus of CNT reinforced concrete

SWCNT			
GPa	M40	M60	M120
E_L	$934 (V_f) + 33.05$	$946.3 (V_f) + 40.1$	$930.9 (V_f) + 56.1$
E_T	$1015.1 (V_f)^2 - 629.6(V_f) + 122.5$	$1050.8 (V_f)^2 - 629.1(V_f) + 130.1$	$1089.1 (V_f)^2 - 602.2 (V_f) + 144.6$
MWNT			

GPa	M40	M60	M120
E_L	$1073(V_f)^{1.06}$	$948.12(V_f)^{.86}$	$935.34(V_f)^{.83}$
E_T	$417.8(V_f)^2 - 157.8(V_f) + 54.5$	$486.3(V_f)^2 - 186.3(V_f) + 67.6$	$579.2(V_f)^2 - 201.5(V_f) + 87.8$

The above plots and tabulation could be used for any fibre volume of CNTs of range 0.1% to 0.9% and the formula arrived is fit for the same. The E_L and E_T for CNT reinforced concrete could be predicted. As observed from the figures, the convergence was observed for all the grades of concrete and also projects fact that concrete grade does not have a huge impact on the Young's modulus.

The percentile increment on Young's modulus was around 0.125% for SWNT and 0.18% for MWNT as observed from the plots. This impinges that concrete grade does not influence the Young's modulus as stated earlier. Then nonlinear variation as observed from graphical plots was 2.24% for any grade of concrete.

The fibre volume fraction has an appreciable influence on Young's modulus of concrete. The enhancement of 47 percentage was observed in the linear variation of the observed graphical plots on E_L . However exponential variation was observed for the E_T values of SWNT and MWNT due to the drastic changes of the values by fibre orientations.

The table 3 depicts the representation of the equations for predicting Young's modulus of elasticity of CNT reinforced concrete matrix for fibre volume fraction from 0.1 to 0.9% added to the cement matrix. The Equations are meant for evaluating the E_L and E_T for any percentile of fibre volume fraction from 0.1% to 0.9% of CNTs provided the deagglomeration is evicted. The derivations expected linearity for E_L for both SWNT and MWNT, while nonlinear fluctuation for transverse Young's modulus E_T was observed. The analytical analysis might have an influence on the finding that concrete strength had the least impact on CNT reinforcement. Furthermore, the simulations suggest that preventing CNT clumping would result in optimum usage of CNTs as fiber reinforcements.

VERIFICATION OF YOUNG'S MODULUS OF ELASTICITY

The Young's modulus of elasticity of CNT reinforced concrete had been evaluated by FEA program ANSYS. The evaluated values are tabulated in Table 4. The evaluated Young's modulus of SWNT reinforced concrete had been verified with reference to Ghandi Rouainia et al. (2008).

Table 4 Young's modulus of elasticity of SWNT reinforced concrete

V_f (%)	E_L for M40 (GPa)	E_L for M60 (GPa)	E_L for M120 (GPa)	E_T for M40 (GPa)	E_T for M60 (GPa)	E_T for M120 (GPa)
0.1	127.8	133.1	148.3	37.7	46.0	64.3
0.2	223.7	229.4	242.0	44.6	53.1	75.4
0.3	318.8	323.9	334.1	52.6	63.1	88.7
0.4	414.8	418.1	428.9	63.3	76.1	106.8
0.5	510.3	513.8	521.1	78.1	94.9	130.6
0.6	608.2	610.1	617.1	100.1	121.1	164.1
0.7	700.3	702.5	707.1	136.3	162.7	215.1
0.8	795.5	796.1	800.5	203.6	237.9	305.1
0.9	888.9	890.8	892.8	445.0	480.9	543.8

Ghandi Rouainia et al. (2008) proposed the following formula for calculating the Young's modulus of SWNT reinforced concrete:

$$E_z = E_s V_s + E_c (1 - V_s).$$

Where,

E_z , E_s & E_c are Young's modulus of composite, SWNT and concrete. V_s is the volume fraction.

The Young's modulus of elasticity for 0.1 % of SWNT is calculated as follows:

$$\begin{aligned} E_z &= 1000 (0.1) + 5000 \sqrt{f_{ck}} (1 - 0.1) \times 10^{-3} \text{GPa} \\ &= 100 + (5000 \times \sqrt{40}) \times 0.9 \times 10^{-3} \text{GPa} \\ &= 128.46 \text{ GPa as per GhandiRouainia et al. (2008)} \end{aligned}$$

The calculated Young's modulus by ANSYS is 127.35 found in Table 4 for 0.1%. The difference is 0.86%. Similarly the Young's modulus values of other volume fraction of SWNT had been found to be correct. The verified Young's modulus is shown in following Table 5.

Table 5 Percentile difference of calculated Young's modulus

V_f (%)	E_L for M40 (GPa)	GhandiRouainia et al. (2008) (GPa)	Percentile Difference %
0.1	127.7	128.8	0.9
0.2	223.7	225.1	0.8
0.3	318.8	322.3	1.5
0.4	414.8	418.1	1.06
0.5	510.3	515.8	1.08
0.6	608.2	612.1	0.7
0.7	700.3	709.1	1.3
0.8	795.5	806.5	1.4
0.9	888.9	903.7	1.6

The above Table 5 shows calculated Young's modulus as per GhandiRouainia et al. (2008) and percentile difference between ANSYS Young's modulus of SWNT reinforced concrete. Thus the Young's modulus calculated using ANSYS had been verified. However the model proposed by GhandiRouainia et al. (2008) is only meant for SWNT. The researcher had not derived for MWNT. This research had proposed equations for calculating Young's modulus of SWNT & MWNT reinforced concrete.

CONCLUSION

The CNT reinforced cement matrix was modelled using Representative Elementary Volume method (REV) for fibre volume fraction of CNTs from 0.1 to 0.9%. Finite element modelling was carried out using Barbero algorithm. Equations were developed to predict the Young's modulus of a CNT reinforced cement matrix. The longitudinal modulus of the matrix showed linear change, but the transverse Young's modulus showed nonlinear fluctuation. The newer fact that concrete grade does not have much influence in the Young's modulus was arrived based on observation for M40, M60 and M120 grade concrete. The concrete strength has little effect on both the longitudinal and transverse Young's modulus of elasticity. The longitudinal Young's modulus of elasticity for SWNT indicated a 0.125% incremental value for any grade of concrete. This percentile value was roughly 0.18% for the longitudinal Young's modulus of MWNT as the concrete grade increased. When the concrete grade was increased, the transverse Young's modulus increased by approximately 2.24%. Finite element modeling revealed that SWNT outperforms MWNT in terms of strength enhancement. A larger CNT radius results in a lower Young's modulus of elasticity. According to

the research, even 0.1% of the fibre volume percentage of CNTs has a substantial impact on the cement matrix.

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