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Evaluation of Young's Modulus of Single Walled Carbon Nanotube (SWNT) Reinforced Concrete Composite

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Abstract: Carbon nanotubes have excellent mechanical properties that make them ideal reinforcing materials, lab Researches observed crack bridging, bonding and fiber pullout in CNT/cement composites, these results paved the way to analytical and numerical studies based on continuum mechanics, molecular dynamics and the Finite element method. This study is the introduction to multiple modeling approaches and analysis using the finite element method, our first step is to understand the effect of the addition of SWNT in a concrete matrix and its benefits, the next steps will be analyzing the fracture behavior of the composite, which will be discussed in future studies. The FEM is used to estimate the longitudinal elastic modulus of the composite, large-scale models were developed, simulating SWNTs using pipe elements in ABAQUS. With a deflection simulation test in FEM, Results from finite element simulations were compared to the analytical results (rule of mixtures) and validated.

Key words: Concrete, single walled carbon nanotube, fiber reinforced concrete (FRC), nanotechnology, composites, finite element method

INTRODUCTION

Since, the discovery of carbon nanotubes (CNTs) by Iijima (1991) researchers focused on their excellent mechanical properties, exceptional stiffness, high strength-weight ratios and toughness, these outstanding properties set forth the potential of CNTs as ultimate reinforcing materials, for the development of nanocomposites.

One of the methods used to simulate CNT behavior is Molecular dynamics (MD), these simulations are used for small-scale models and this approach at the molecular level requires very powerful computers to solve large-scale problems and therefore not accessible for everyone.

On the other hand Continuum mechanics is a more accessible approach and can be used for large-scale models, modeling and simulations of nanocomposites can be achieved using a desktop personal computer and the computational approaches can play a significant role in characterizing CNT-based composites.

We are going to use the strength of material theory, in this case the Rule of mixture and the finite element method (FEM) and analyze the results.

The main objective of this study is to develop continuum models using FEM to validate and state the fact that FEM has the potential to deliver good estimates in characterizing nano and micro scale composites, in our case SWNT/concrete composites using the commercial finite element software ABAQUS CAE, this approach has achieved very good estimates for overall elastic modulus of the composite and validates the rule of mixture results.

EXPERIMENTAL RESULTS AND APPLICATIONS

Lab researches Makar *et al*. (2005) on carbon nanotubes concrete composite show classical reinforcing behavior, with examples of crack bridging and fiber pullout being easily identified, as well as a strong bond between the concrete and the SWNTs (Fig. 1).

These early researches show very promising results and prove that these new materials are opening the door to new possibilities and will allow existing structural designs to be produced with reduced material volumes and entirely new structural designs and concepts.

Big steps and breakthrough discoveries are being made daily in carbon nanotubes production, wich became more affordable and quality SWNT are more

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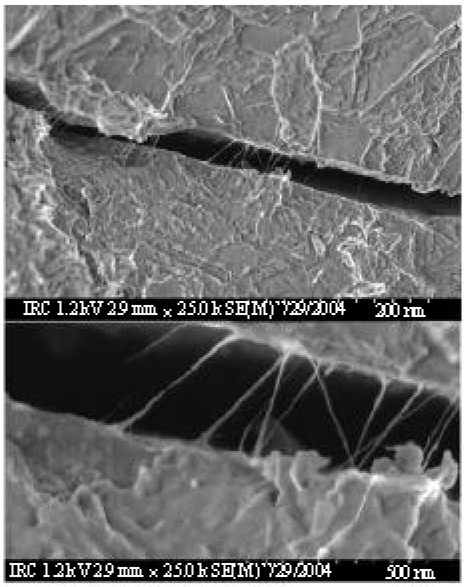


Fig. 1: Multiple SWNT bridging a micro crack in concrete samples

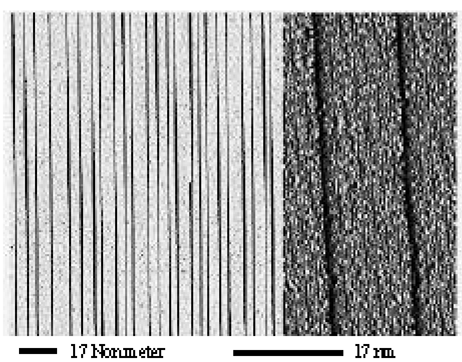


Fig. 2: Multiple SWNT aligned in production sheet

available, especially long SWNT and production process taking the road of mainstream industry we can mention the recent work from Nanocomp Technologies, Inc (Anonmoyus, 2008) that shows a tremendous discovery, a production of a 3-foot by 6-foot sheets of pure carbon nanotube material, where the SWNT are aligned, continuous and 1 millimeter-long (Fig. 2).

This discovery alone opens a big door to future advanced structural composites, this is a proof that creating aligned SWNT with an industrial process is possible, these CNT textil sheets could be easily incorporated into advanced concrete materials as they offer a king of regularity in carbon nanotubes never achieved before, the next step will be aligned SWNT in composites wich is still only theoretical and at the stage of computer simulations, but I'm confident it will be achieved very soon due to the amount of resources mobilized worldwide into carbon nanotubes researches in the present time.

MATERIAL PROPERTIES

Single walled carbon nanotubes (SWNT): CNTs are classified as single-walled carbon nanotubes (SWNT) and multi-walled carbon nanotubes (MWNT) (Fig. 3).

We are focusing our study on SWNT; a hollow structure formed by covalently bonded carbon atoms and can be represented as a thin graphene sheet rolled into a cylindrical shape.

The SWNTs can be sealed at both ends, or open, the focus is on the large aspect ratio of the cylinder (i.e., length to diameter ratio as large as 104-105) which in general called as long/continuous SWNTs.

SWNTs typically have a diameter of 1 nm with thickness of 0.32 nm (Ni *et al.*, 2007), which is the thickness of the graphene sheet

Young's modulus from experimental and theoretical results show that they can reach up to 1 Tera Pascal (Salvetat *et al.*, 1999).

Poisson's ratio is between 0.19 and 0.22 (Jindal and Jindal, 2005) and depends of the chirality of the carbon atoms forming the graphene sheet and do not depend on the tube diameter.

They have a tensile strength of 63 GPa. Low density for a solid of 1.3-1.4 g cm^{-3} (Collins *et al.*, 2000), its specific strength of up to 48,000 kN m kg^{-1} is the best of known materials, Under excessive tensile strain, SWNT undergo plastic deformation that begins at strains of approximately 5% and can increase the maximum strain the tube undergoes before fracture by releasing strain energy.

CNTs are not nearly as strong under compression. Like any tubular structure, they tend to undergo buckling when placed under compressive, torsional or bending stress.

Concrete: Concrete is a construction material that consists of cement (commonly Portland cement) and other cementitious materials, aggregate (sand and water) and chemical admixtures.

Abundance of its ingredients raw materials and a relative ease of production made it the most used man-made material on the planet.

Concrete has relatively high compressive strength, but significantly lower tensile strength (about 10% of the compressive strength). As a result, without reinforcements, concrete would almost always fail from tensile stresses, even when loaded in compression.

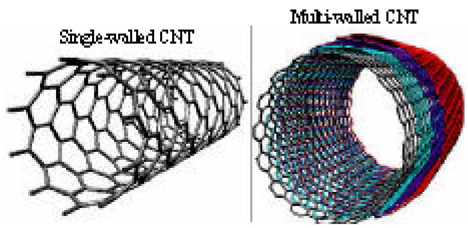


Fig. 3: Single walled, multi walled carbon nanotubes representations

Concrete elements subjected to tensile stresses must be reinforced with materials that are stronger in tension, the addition of steel or fiber reinforcement. The reinforcement can be by bars (rebar), mesh, or fibers, which provide the required tensile strength to concrete producing reinforced concrete.

The modulus of elasticity of concrete is a function of the modulus of elasticity of the aggregates and the cement matrix and their relative proportions. The modulus of elasticity of concrete is relatively linear at low stress levels but becomes increasingly non-linear as matrix cracking develops. The elastic modulus of the hardened paste may be in the order of 10-30 GPa and aggregates about 45-85 GPa. The concrete composite is then in the range of 27-50 GPa.

All concrete structures will crack to some extent, micro cracks become more larger with time, one way to bridge and reinforce micro cracks in concrete is the addition of carbon nanotubes, as demonstrated in Lab researches, CNT fibers bridge the micro fractures and prevent them.

MODELING APPROACH

Analytical approach

Rule of mixture theory for composites: The rule of mixture is an analytical method based on the strength of materials theory, it is used in this research to predict the composite material properties, The effective longitudinal Young's modulus of the CNT-reinforced composite and to validate the numerical results obtained using the FEM.

However, this theory is not accurate when evaluating the interfacial stress but is found to be efficient and accurate in predicting the effective material constants (Young's modulus, Poisson's ratio) in the axial and transverse direction.

We are going to focus our first study on a single long SWNT/ concrete interaction and multiple aligned SWNTs simulating the nanocomp sheets (Anonymous, 2008) a volume element is considered as a hexahedral concrete matrix with the SWNT tube in the middle of the matrix, the

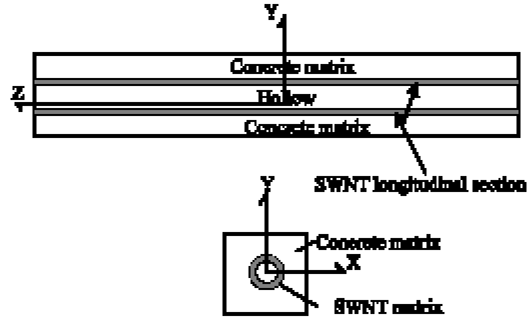


Fig. 4: a) SWNT/concrete volume element longitudinal section, b) SWNT/concrete volume element transverse section

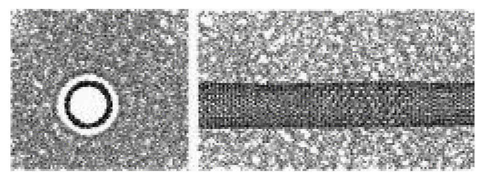


Fig. 5: SWNT in solid matrix

inside of the tube is considered hollow, Fig. 4 and a perfect bond between SWNT and concrete is assumed as observed Lab researches (Makar *et al*., 2005), the SWNT is considered straight and both materials are isotropic, this configuration was observed in lab researches (Fig. 5).

We can calculate the Volume fraction (V s) of SWNT as follow (Fig. 6):

$$V_s = \frac{\text{Volume of SWNT}}{\text{Total volume of the composite material}}$$

$$V_s = \frac{\pi(r_e^2 - r_i^2)}{(a^2 - \pi r_i^2)} \quad (1)$$

Where:

Vs : Volume fraction (V f) of SWNT.
Re : External radius of SWNT.
Ri : Internal radius of SWNT.
A : Hight of the volume element.

Based on the above formula we can easily calculate the Dimensions of the volume element used for a given V s, in our study we are going to use different Volume fractions of SWNT; (1, 1.5, 2, 2.5 and 3%) of SWNT as it approaches the percentage used in Lab researches SWNTs typically have a diameter of 1 nm with a thickness of 0.32 nm (Iijima, 1991; Salvetat *et al*., 1999), Formula 1-1 becomes:

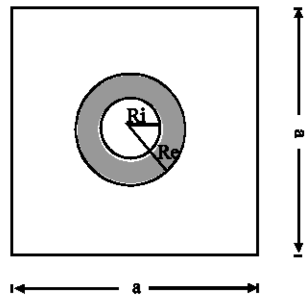


Fig. 6: Volume element transverse section

$$V_s = \frac{\pi(0.82^2 - 0.5^2)}{(a^2 - \pi 0.5^2)} \quad (2)$$

Therefore,

$$a = \sqrt{0.785 + \frac{1.327}{V_s}} \quad (3)$$

For multiple SWNT in the volume element we can introduce "n" as the number of SWNT, formulas 1 and 3 become:

$$V_s = \frac{n\pi(r_e^2 - r_i^2)}{(a^2 - n\pi r_i^2)} \quad (4)$$

And

$$a = \sqrt{n\left(0.785 + \frac{1.327}{V_s}\right)} \quad (5)$$

there are certain assumptions to be made before developing the rule of mixtures expression:

- SWNTs are uniform, straight and continuous.
- Perfect bonding between SWNT and the concrete matrix.
- Longitudinal load produces equal strain in SWNT and concrete.
- The longitudinal deformation resulting from the load are the same in the composite, SWNT and the concrete:

$$\varepsilon_{total} = \varepsilon_{swnt} = \varepsilon_{concrete} \quad (6)$$

The load applied is in the longitudinal direction i.e., the SWNT direction, is shared between SWNT and matrix:

$$F_Z = F_S + F_C \quad (7)$$

Where:

F_Z : Total Load in Z direction
F_S and F_C : SWNT load and concrete load

The stresses depend on the cross-sectional area of the CNT and matrix

$$\sigma_Z A = \sigma_s A_s + \sigma_c A_c \quad (8)$$

Where:

σ_s, σ_c and σ_Z : The stress of SWNT, Concrete and composite.
A_s, A_c and A : The cross-sectional areas of the CNT, matrix and composite.

By applying the Hooke's Law:

$$E_Z\, \varepsilon_z A = E_s \varepsilon_s A_s + E_c \varepsilon_c A_c \quad (9)$$

Where:

EZ, Es and Ec : Young's modulus of the composite, SWNT and concrete.
εz, εs and εc : Composite strain, SWNT strain and concrete strain.
A, As and Ac : Composite section, SWNT section and concrete section.

Poisson's contraction has been ignored and the strain in the SWNT, matrix and composite are the same Eq. (4),

$$E_Z A = E_s A_s + E_c A_c$$

To get the Young modulus of the composite:

$$E_z = E_s\left(\frac{A_s}{A}\right) + E_c\left(\frac{A_c}{A}\right) \quad (10)$$

$$\left(\frac{A_s}{A}\right), \left(\frac{A_c}{A}\right)$$

Equals to Vs and (1-Vs)
Therefore,

$$E_Z = E_s V_s + E_c\,(1 - V_s) \quad (11)$$

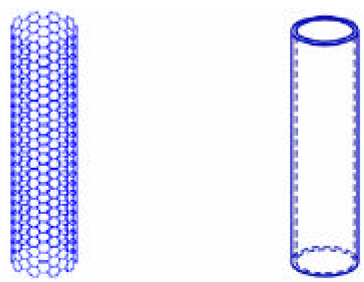
With the linear Eq. (11) we can calculate the young modulus of the composite, for different values of Vs, the results are in Table 1, with Es is 1000 Gpa and Ec is 27 Gpa.

Finite element approach

Single SWNT model: We used the commercial finite elements software ABAQUS (www.simulia.com) to characterize the volume element for a long SWNT reinforced concrete composite, the SWNT is defined as a hollow solid cylinder (Fig. 7) (Sohlberg, 1998) inserted in a matrix from one end to the other (Fig. 8), in the longitudinal direction. Solid elements have been employed

Table 1: Young's modulus results from rule of mixture method

Vs	Es Gpa	Ec Gpa	Ex Gpa
0.01	1000	27	36.73
0.015	1000	27	41.595
0.02	1000	27	46.46
0.025	1000	27	51.325
0.03	1000	27	56.19



(a) (b)

Fig. 7: a) SWNT molecular Dynamics representation, b) Continuum solid model

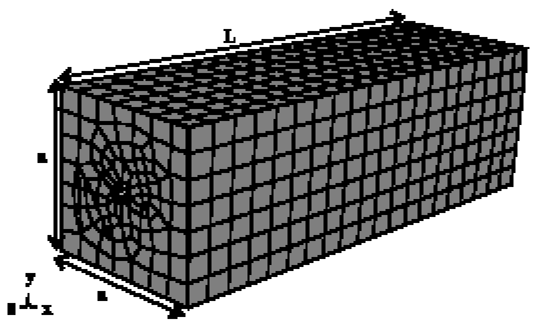


Fig. 8: SWNT/concrete composite volume element

for both the concrete matrix and SWNT and a perfect bond between the SWNT and concrete is assumed (Govindjee and Sackman, 1999).

Mapped meshing using Hexahedral elements has been used as it offers good results compared to the tetrahedral elements (Liu and Quek, 2003) (Fig. 8).

We created 5 finite elements models of the composite beams with the corresponding volume fraction of SWNT (Vs) used in the rule of mixture calculations.

We the formula (1-2) to calculate the concrete section dimensions, the length (l) of the volume element is assumed two times the dimension a, the results are in Table 2, the dimension of the SWNT are constant in all 5 models.

Boundary condition are applied such as one face of the beam is encastred in the three direction and the other is free to move in all directions, a distributed load is applied on the top of the free edge on the model such as it's resultant is equal to 0.1 N (Fig. 9).

Our goal is to simulate a deflection test and knowing the deflection (f) of the cantilever beam we can easily

Table 2: Volume elements dimensions

Vs	a mm	l mm
0.01	11.55	23.10
0.015	9.45	18.90
0.02	8.19	16.38
0.025	7.34	14.68
0.03	6.71	13.42

Table 3: Volume elements dimensions for multi SWNT models

Vs	a mm	b mm	l mm
0.01	8	67	24
0.015	5.4	67	16.2
0.02	4	67	12
0.025	3.2	67	9.6
0.03	2.7	67	8.1

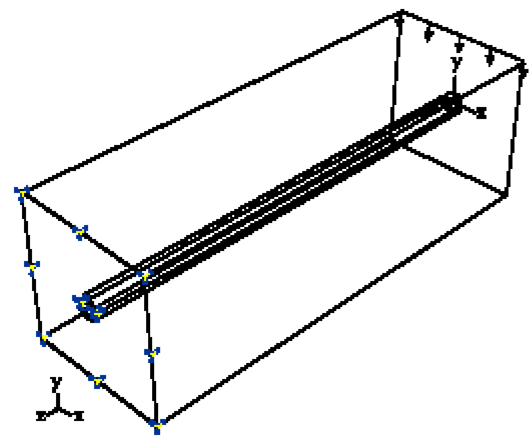


Fig. 9: SWNT/concrete composite volume element deflection method boundary conditions

calculate the effective elastic modulus on the composite using the following formula, the material is assumed identical and isotropic since the volume fraction of SWNT is very small and the section of the material is the section of the composite without the hollow area inside the SWNT.

$$E_x = \frac{F \times L^3}{3f \times I} \qquad (12)$$

Where:

F = Resultant force acting on the tip of the beam.
L = Length of the beam (span).
E = Modulus of elasticity.
I = Area moment of inertia.

The area moment of inertia of the composite section can be calculated as follow:

$$I = \frac{a^4}{12} - \frac{\pi \times r_i^4}{64} \text{ Section with a single SWNT} \qquad (13)$$

$$I=\frac{ba^3}{12}-n\frac{\pi\times r_i^4}{64} \quad \text{Section with n number of SWNTs} \tag{14}$$

Multiple SWNTs model: The same approach has been used for creating the multiple SWNTs volume elements, using the Eq. 5 we can determine the section area of the composite in this case (a×b), since there is a 17 nm distance between the axis of each aligned SWNT (Fig. 10) to simulate the nanocomp SWNT sheets, the volume element can not have equal hight and width.

We created models with 4 SWNT passing through the concrete matrix, (n = 4), we kept the width of the volume element (b) constant for all 5 models because of the position aspect of the aligned SWNT and to keep the number of 4 SWNTs in the model, b is taken equal to 67 nm, three time 17 nm and 8 nm from each edge, we get the following dimensions for the models in Table 3, the length of the module is three times it's hight, same boundary conditions used in the single SWNT models are are applied.

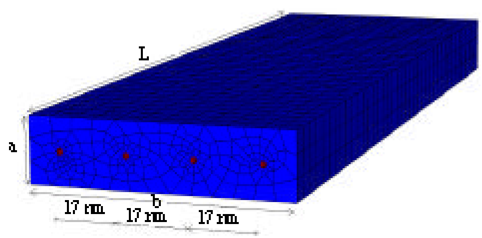


Fig. 10: Multiple SWNTs/concrete composite volume element

DISCUSSION

A mesh convergence study was performed for both methods models and calculations were carried out based on the FEM results, the displacement U2 (Y Direction) and the Young's modulus of each models was calculated, Fig. 11-20, single SWNT FEM results, multiple SWNTs FEM results, we noticed that the FEM results in both single and multi SWNTs configurations up to V s = 2% are pretty close to the rule of mixture results but for 2.5 and 3% of volume fraction there is a significant increase in the young modulus of the composite compared to the rule of mixture.

Table 4 shows the results and comparison plot between both FEM results and the analytical numbers.

Table 4: Comparison of results for single and multiple SWNTs reinforced concrete composite

Vs (%)	Es (Gpa)	Ec (Gpa)	Ex (Gpa) rule of mixture	Ex (Gpa) FEM single SWNT	Ex (Gpa) FEM multiple SWNTs
1	1000	27	36.73	37.17	36.74
1.5	1000	27	41.595	42.93	40.83
2	1000	27	46.46	48.88	46.85
2.5	1000	27	51.325	53.89	52.54
3	1000	27	56.19	60.38	61.34

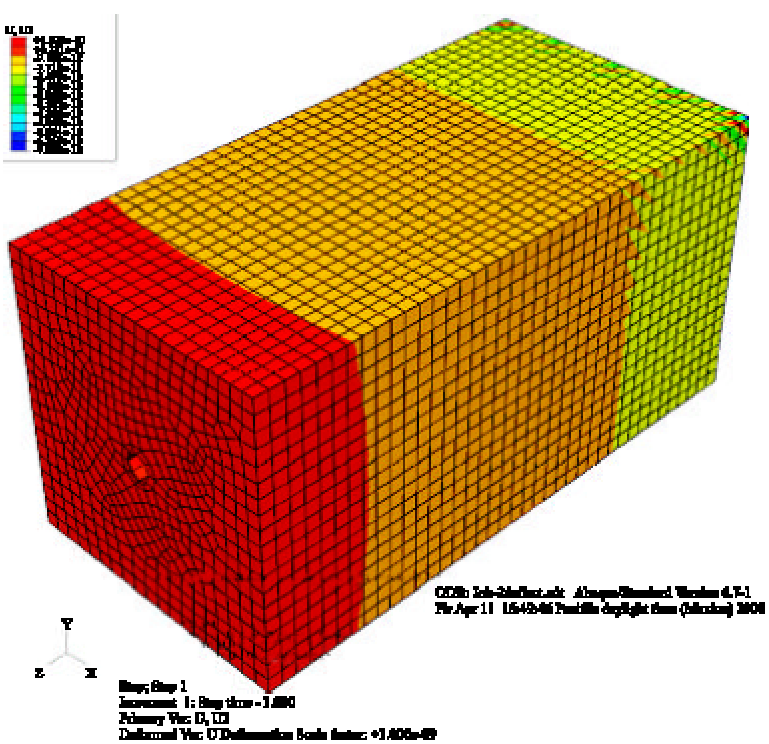


Fig. 11: FEM U2 displacements results in the volume element single SWNT/concrete composite V s = 1%

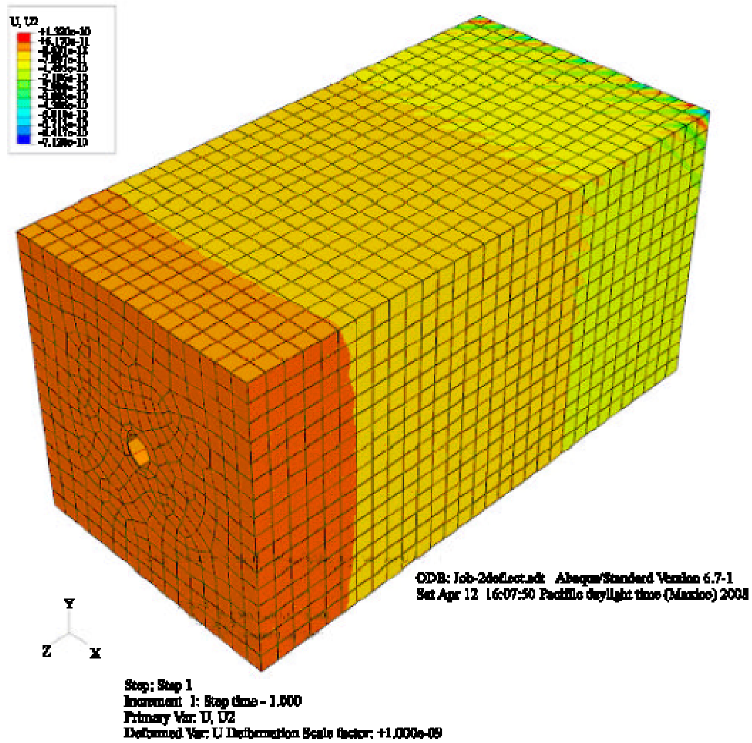


Fig. 12: FEM U2 displacements results in the volume element single SWNT/concrete composite Vs = 1.5%

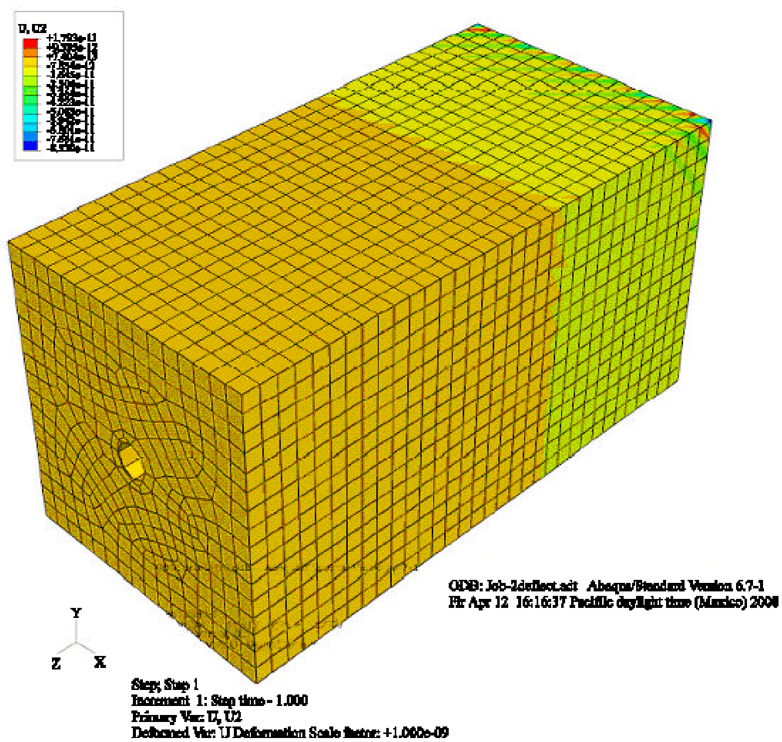


Fig. 13: FEM U2 displacements results in the volume element single SWNT/concrete composite Vs = 2%

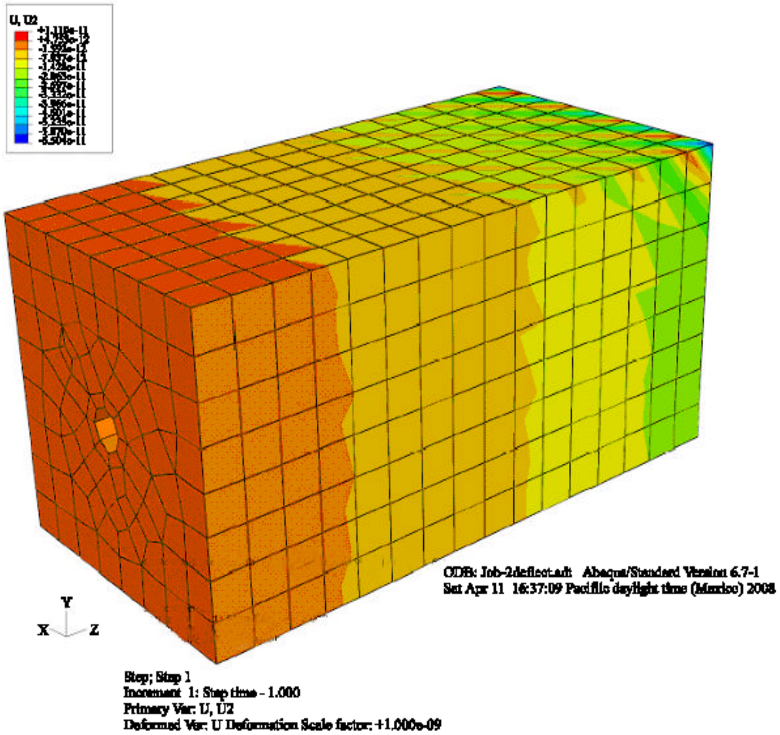


Fig. 14: FEM U2 displacements results in the volume element single SWNT/concrete composite Vs = 2.5%

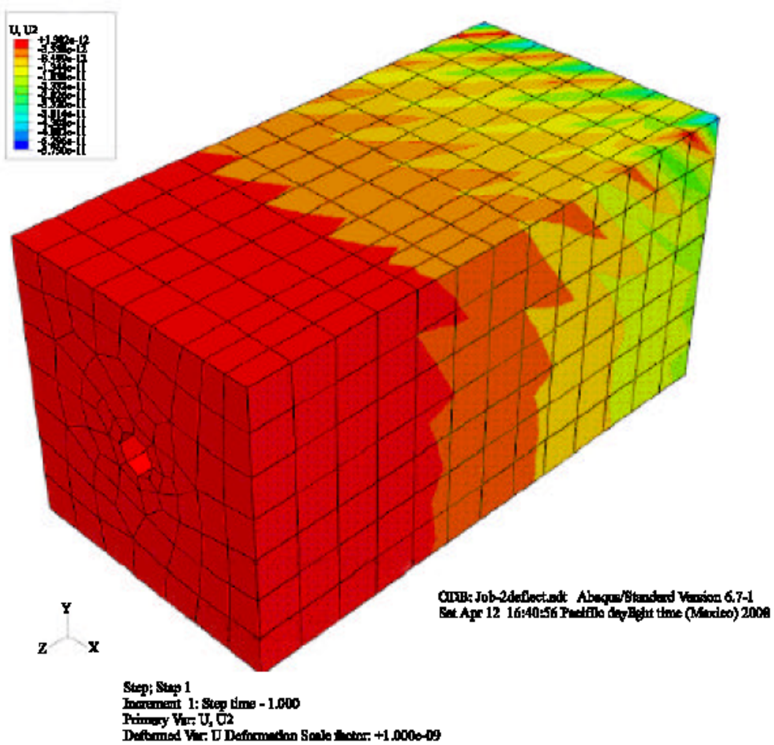


Fig. 15: FEM U2 displacements results in the volume element single SWNT/concrete composite Vs = 3%

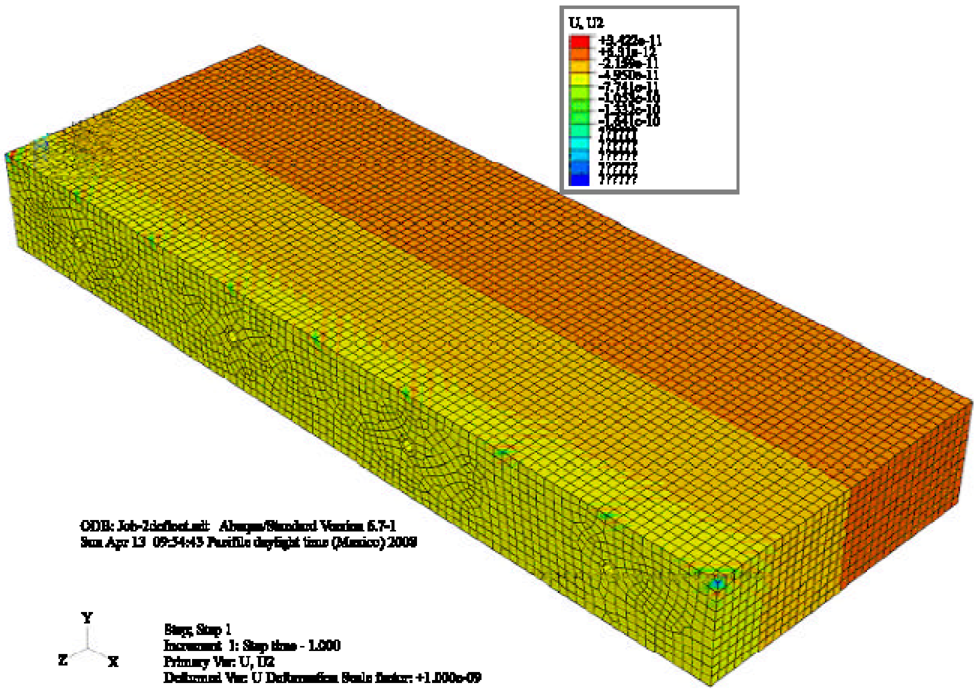


Fig. 16: FEM U2 displacements results in the volume element multiple SWNTs/concrete composite Vs = 1%

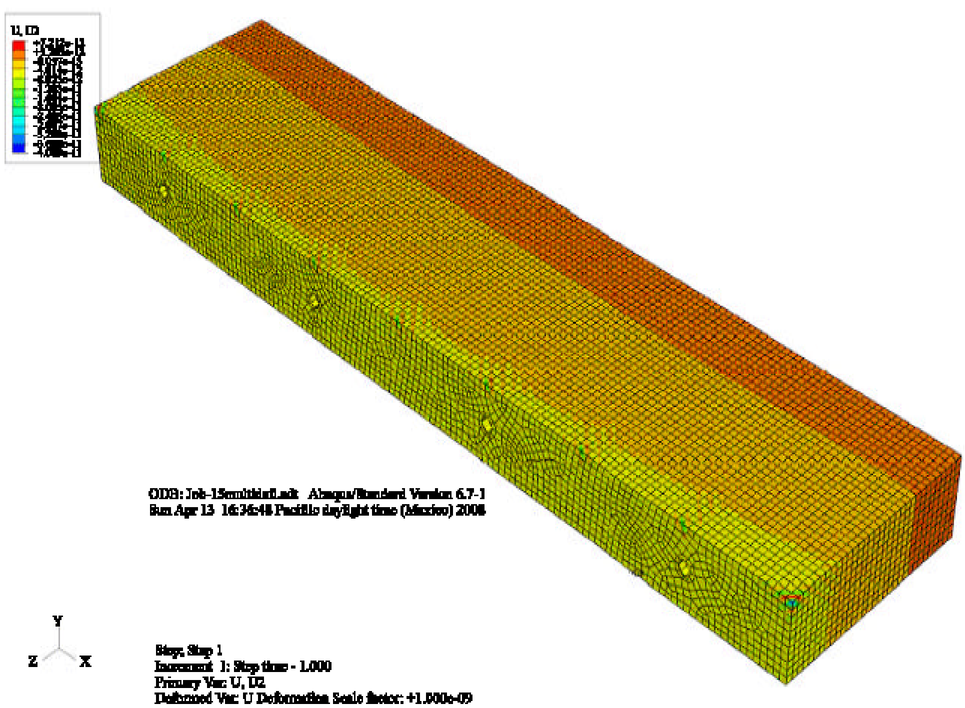


Fig. 17: FEM U2 displacements results in the volume element multiple SWNTs/concrete composite Vs = 1.5%

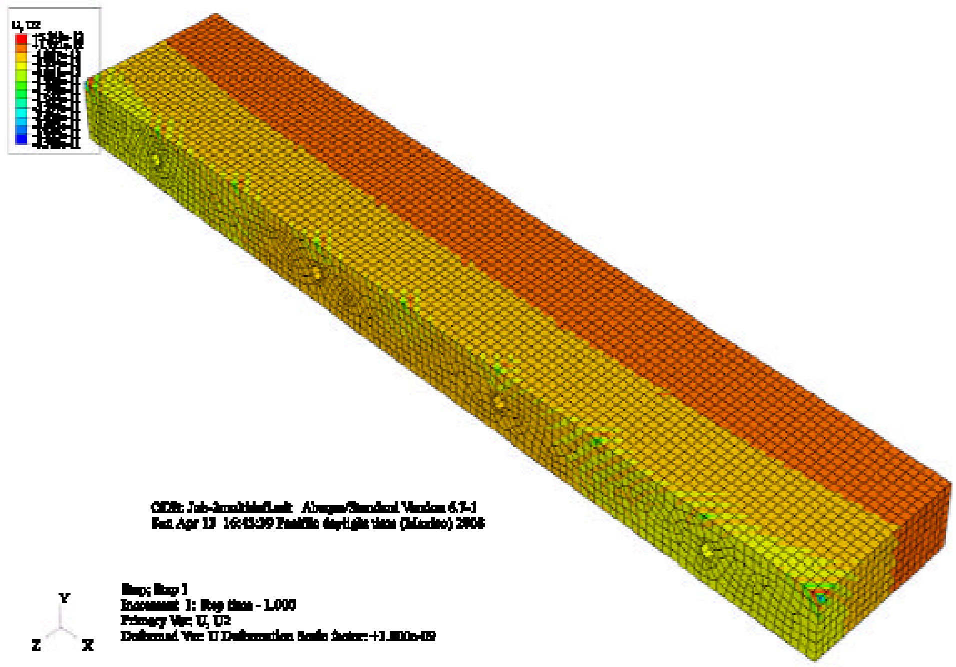


Fig. 18: FEM U2 displacements results in the volume element multiple SWNTs/concrete composite Vs = 2%

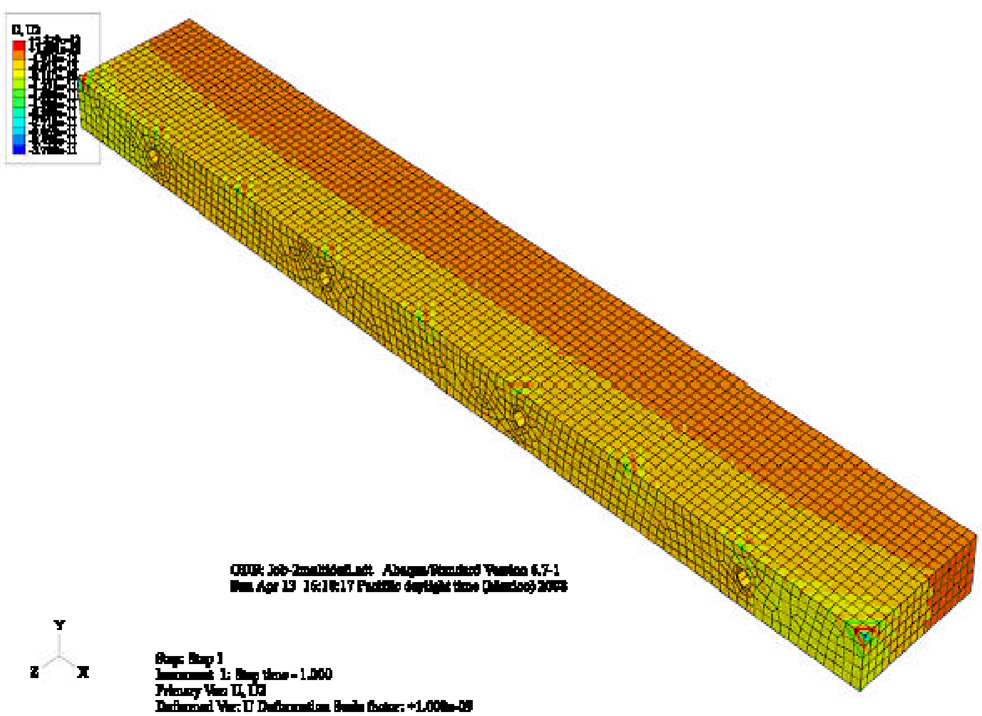


Fig. 19: FEM U2 displacements results in the volume element multiple SWNTs/concrete composite Vs = 2.5%

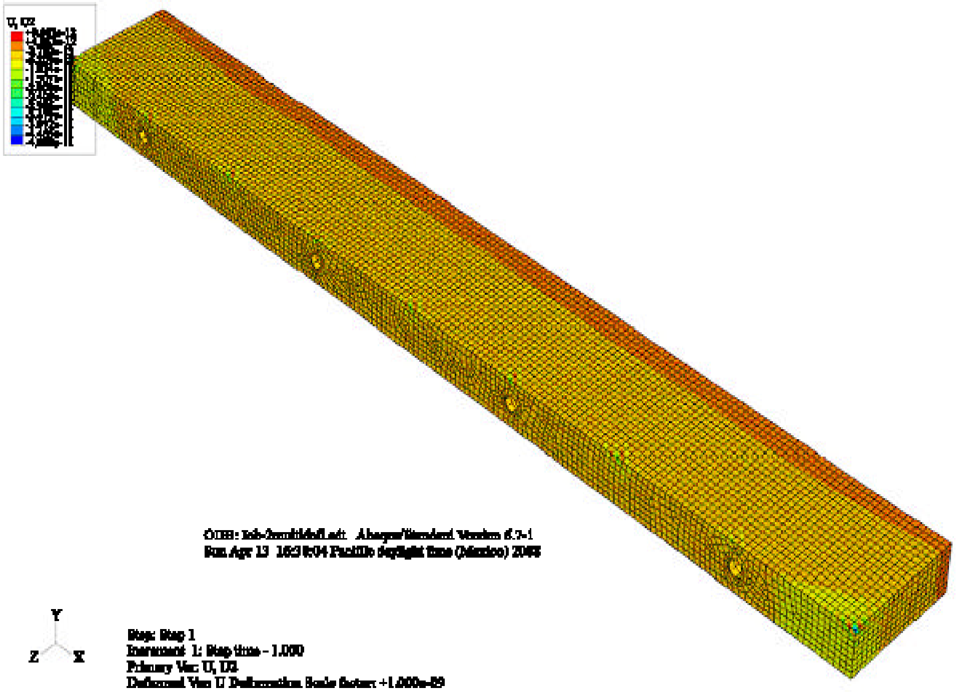


Fig. 20: FEM U2 displacements results in the volume element multiple SWNTs/concrete composite Vs=3%

CONCLUSION AND FUTURE WORK

The results obtained in the FEM simulations validate the use of continuum mechanics and are in complete agreement with the analytical calculations up to 2% of volume fraction of SWNT and they show a significant enhancement of the overall mechanical behaviour of the composite, the SWNT act as micro reinforcement of the concrete matrix and enhance the Young's modulus.

The differences between analytical and FEM results are les than 5.2% for 1% =Vs= 2% and less than 9.1% for 2.5% =Vs= 3%, after the augmentation of the Vs more than 2% the rule of mixture is no longer accurate and the composite has even greater mechanical properties in the longitudinal direction (SWNT direction) based on FEM simulations.

The addition of 1% SWNT in a concrete matrix increased 33% the young's modulus of the concrete composite in both single SWNT and multiple SWNTs, we can even go below the volume fraction of 1% and still have significant young's modulus enhancement of the composite.

The results prove that if we could incorporate successfully long aligned SWNT in the concrete we could tremendously enhance the overall mechanical properties of the concrete composite. A solution is found in the shape of the Nanocomp SWNT textile sheets (Anonymous, 2008), that are ready for industrial production and large enough to be used in construction materials, this will be investigated further in future work and fall into the category of textile reinforced concrete and we intend to investigate the SWNT composite behaviour under fracture by creating a user element subroutine in ABAQUS.

It can be concluded that the continuum mechanics approach can be used as an excellent tool reducing computational time when coupled with multi-scale modelling for micro-scale composites, with nanotubes aligned in uniform fashion and the results show that SWNT addition in the concrete even at a very small and economical volume fractions enhance the mechanical behaviour of the concrete and shows very promising results and opens up the door for more studies especially in fracture and tensile behaviour as we intend to do in future studies.

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