Chapter 1

An Eco-Approach to Boost the Sustainability of Carbon Nanotube-Based Composite Products

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I. INTRODUCTION

Historically, the first ecological composite material used in residential construction is known as cob: a composite material reinforced with natural straw fibres imbedded in a clay matrix. Subsequently, this technique of construction progressed to the use of reinforced concrete: an artificial composite material reinforced with long steel bars embedded in a cementitious matrix. Thereafter, this basic technique of reinforcement has evolved towards the use of composite materials reinforced with fibres that are made from glass, carbon, aramid, bore or a mixture of two or more of these fibres; this latter combination is usually called “hybrid reinforcement”.

With this feedback in mind, fibre-reinforced composites are considered, nowadays, to be the main key driver for the development of many structural components and technical devices that have improved and continue to revolutionize the comfort and quality of human life using innovative and modern technologies. The wide-ranging use of these smart materials is believed to be related to the good performance of fibres in terms of stiffness and strength coupled with minimum weight and other physico-chemical properties. In fact, these core objectives are not easily achievable when using isotropic conventional materials [1, 2].

Further to these notable properties, recent advances in nanotechnology have led to the development of a new class of composite materials based on carbon nanotube (CNT) fibres [3]. These CNT-fibres are intended to replace the standard carbon fibres due to their excellent mechanical, electrical and electrochemical properties [4]. In addition to these spectacular properties, it should be noted that the price of CNT fibres remains much higher than that of standard carbon fibres, but the rapid rise of establishment of CNT production plants in several countries (production of a few hundred tons / year / country), will lead probably to a considerable drop in prices within the coming years. Moreover, NTC prices are variable depending on the type, quality and purity of CNTs.

With this great innovation, significant improvements and challenges can be reached within the next generation of fibre-reinforced composites based on CNT nanotechnology. For instance, the strength of these fibres can be several times higher than standard carbon fibres and weigh much less for an equivalent cross-section. In addition to the remarkable inherent properties of these materials, further ecological worries remain, and it is necessary for these to be addressed in order to perform a realistic assessment of the impacts related to environmental and health issues [5-7]. Within this context, the industrial designers, manufacturers and suppliers who work in the field of CNT-based composites have to factor in the impacts of their products on the environment and find new and feasible alternatives. Typically, these alternatives are based on a set of equations, called “sustainability factors” [5]. Further to that point, these factors must guarantee quality assurance, health protection and environment preservation all at the same time, making the product consistent with the sustainable development requirements and consequently more competitive in the worldwide market for polymer nano-composites.

With this approach as an objective, codes and standards for future CNT-based composites and derived products/devices should take into account, at each stage of the design process and life-cycle analysis, three balanced key criteria characterised mainly by quality assurance (Q for short), health protection (H for short) and environmental preservation (E for short). In order to achieve these requirements, we have defined and developed new criteria in the form of three factors; these are called “*quality factor*”, “*health factor*” and “*environmental factor*” that have to be incorporated into the life-cycle analysis (LCA) for better-quality assessment of product sustainability.

In order to develop this idea and provide good estimation of these three important factors, probability approach and optimisation procedures based on the technique of additive colours [8] are applied and well explained in the following sections. And once these factors are determined and then approved by sustainability standards, they can consequently be integrated into the design and analysis formulations, in characterisation tests. Thus, they can also be implemented into future finite-element computer programs and in different stages of LCA process, ranging from raw materials to product end of life and recycling.

This can be done by simply undertaking a comparison of eco-results (which take into account the impact of these factors) with classical results (which do not take into account the impact of these factors), designers and analysts can make better use of sustainability principles to assess environmental and health issues.

With this objective in mind, the purpose of this chapter may be regarded as:

- a stimulation for innovation and research activities towards the sustainability of CNT-based composites and their derived products/devices; and
- an encouragement for designers and engineers involved with CNT-technology to have more motivation towards the integration of *Q-H-E* aspects into the different operations related to the product development process.

On the other hand, this chapter aims to promote the transition from a linear economy to a circular economy through a probabilistic approach characterised by the existent interaction between the three interdependent aspects (i.e., *Q*, *H* and *E*). Indeed, this innovative action will cover all the stages of the product life-cycle analysis from raw material selection, design, manufacturing, production, distribution and use, maintenance and repair, to reuse and recycling; and will focus on measures of various factors related to each stage, aiming at “closing the loop” of the circular economy when taking into consideration extraction and transportation stages, of course.

II. CHIRALITY AND GEOMETRY OF CARBON NANOTUBES

A. *Graphite, Graphene and Carbon Nanotube*

Chemically speaking, CNT materials are based on graphite which is no other than the stable form of carbon at ordinary temperature and pressure (e.g., pencil tip, as shown in Fig. 1), where its molecular structure consists of an intercalated stacking of non-compact hexagonal honeycomb sheets; each sheet is separated by about 0.336 nm along its normal direction (see Fig. 2). An isolated single sheet of graphite is defined as free-standing graphene whose chemical formula is C_n (Fig. 3).

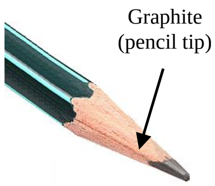


Fig. 1 Stable form of carbon

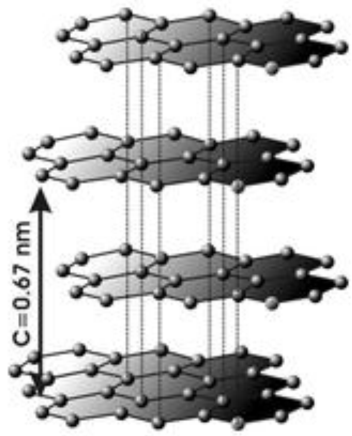


Fig. 2 Graphite molecular structure

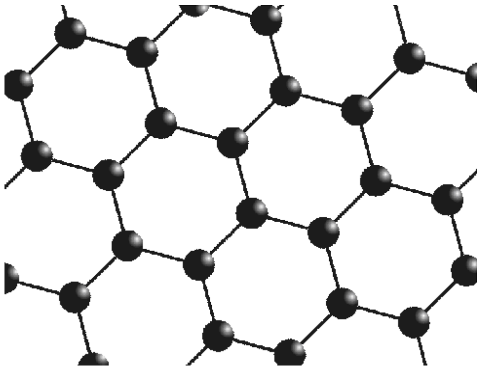


Fig. 3 Chemical formula of graphene (C_n)

In other words, Fig. 4a shows the molecular structure of graphene, i.e., a single flat layer of carbon atoms isolated from the crystal structure of graphite. The CNTs are obtained by rolling graphene sheets on themselves as illustrated in Fig. 4d.

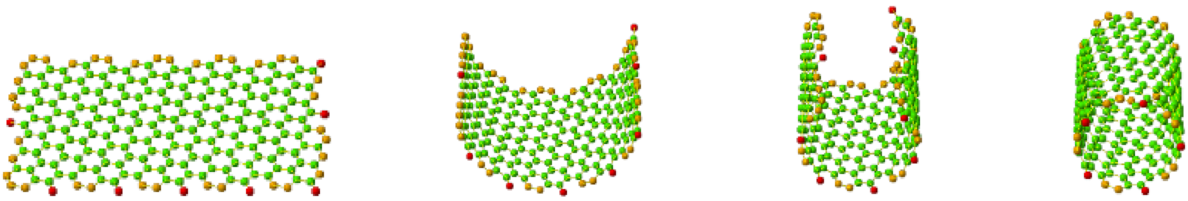

(a) graphene (G) (b) G rolled up at 50% (c) G rolled up at 75% (d) CNT

Fig. 4 Rolling up a graphene sheet into a carbon nanotube [9]

Depending on the cut of the graphene sheet with respect to the referential coordinate system (O; $\vec{a}_1$, $\vec{a}_2$) defined in the hexagonal lattice as illustrated in Fig. 5, several geometries of CNTs can be obtained using the chiral vector

($\vec{C}_k = n \cdot \vec{a}_1 + m \cdot \vec{a}_2$). In general, there are three types of CNTs which are called: (i) armchair (when n=m), (ii) zigzag (when m=0) and (iii) chiral (when $n \neq m$).

On the other hand, the electrical properties of CNTs can be classified either metallic or semiconductor in accordance with the indices (n, m). The armchair CNTs are always metallic. However, the zigzag and chiral CNTs may be either metallic or semi-conductor; they are metallic when the condition (n-m = 3p), where p is an integer ($p \in$ IN). This situation is well explained and presented in Fig. 5, where the red solid circles represent metallic CNTs and yellow solid circles represent semi-conductor CNTs. Moreover, it should be noted that this rule of electrical properties remains applicable only for certain nanotube diameters due to the significant effects generated by small curvature in small diameters.

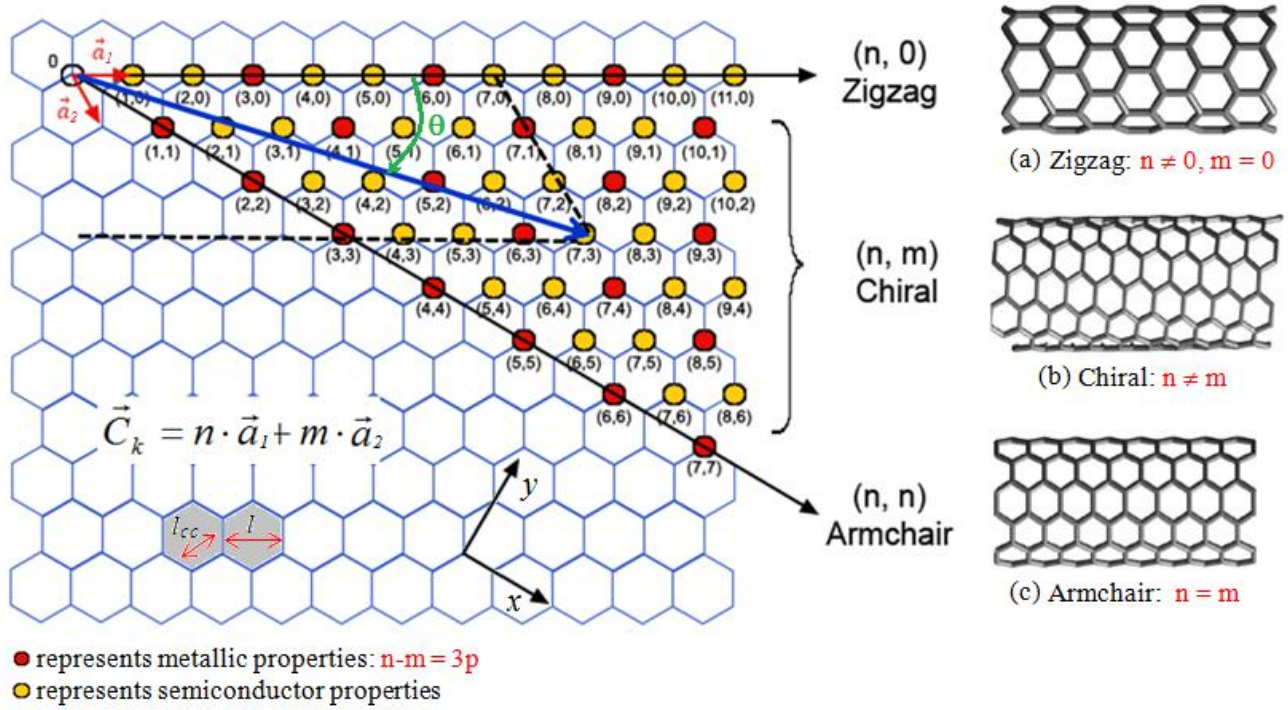


Fig. 5 Chirality and geometry of CNTs and their associated configurations

Structurally speaking, CNTs can be either a single-walled carbon nanotube (SWNT) as shown in Fig. 6a or multi-walled carbon nanotubes (MWNTs) as shown in Fig. 6b. The diameter of CNTs may be ranging from 1-80 nm, whereas the length can reach several micrometres. With these nanometric dimensions, a very high aspect ratio (i.e., length-to-diameter) can be provided. These geometric characteristics can contribute significantly to improving the composite product sustainability.

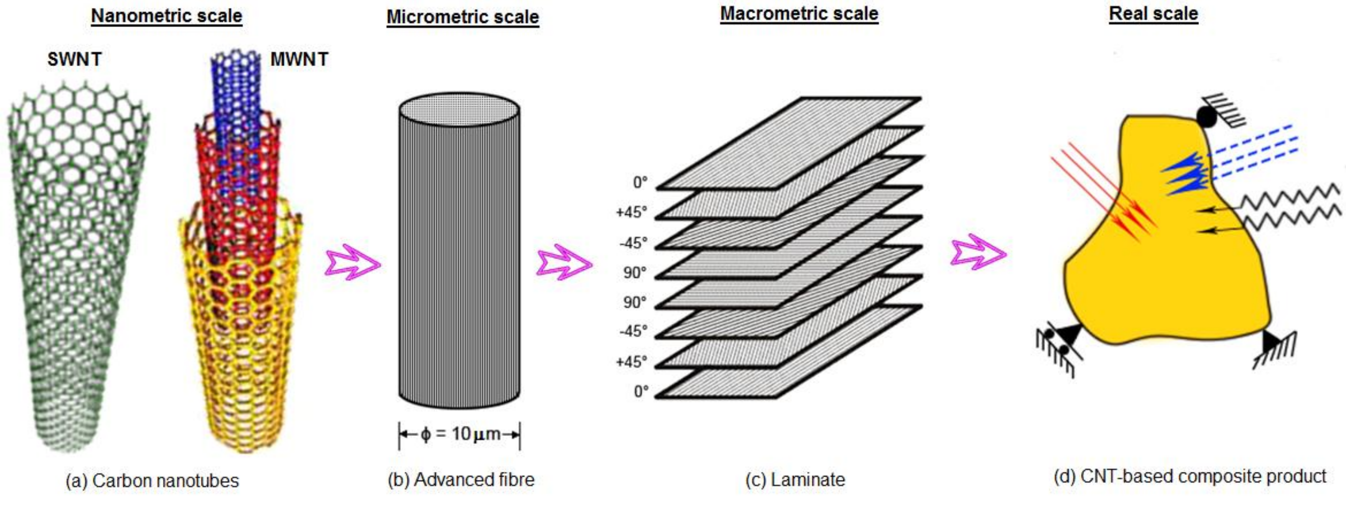


Fig. 6 Design development from carbon nanotubes to CNT-based composite product

B. CNT Geometrical Formulations

Using the referential coordinate system (O; $\vec{a}_1$, $\vec{a}_2$) for the hexagonal lattice, as shown in Fig. 5, the base vectors $\vec{a}_1$ and $\vec{a}_2$ can be expressed as [9, 10]:

$$\vec{a}_1 = \begin{pmatrix} \frac{3}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix} l_{cc} \qquad \vec{a}_2 = \begin{pmatrix} \frac{3}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix} l_{cc} \tag{1a}$$

where l_{cc} is the bond length of atoms, equal to 0.1421 nm for graphite and **0.144 nm** for nanotube due to curvature.

Since the length of both vectors $\|\vec{a}_1\| = \|\vec{a}_2\| = \sqrt{3}\, l_{cc} = l$, Eq. (1a) can be written in the Cartesian coordinate system (x, y) as:

$$\vec{a}_1 = \begin{pmatrix} \frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix} l \qquad \vec{a}_2 = \begin{pmatrix} \frac{\sqrt{3}}{2} \\ -\frac{1}{2} \end{pmatrix} l \tag{1b}$$

where l is the length of unit vector, equal to 0.2494 nm.

With $0 \le \mathrm{m} \le n$, the chiral vector $\vec{C}_k$ and its length (nanotube perimeter) are expressed, respectively, as:

$$\vec{C}_k = n \cdot \vec{a}_1 + m \cdot \vec{a}_2$$
$$\|\vec{C}_k\| = l\sqrt{n^2 + nm + m^2} \tag{2}$$

Consequently, the diameter of the nanotube, d_t, is given by the following equation:

$$d_t = \frac{\|\vec{C}_k\|}{\pi} = \frac{l}{\pi}\sqrt{n^2 + nm + m^2} \tag{3}$$

Whereas, the chiral angle $\theta = (\vec{a}, \vec{C}_k)$ is defined as:

$$\theta = \tan^{-1}\left(\frac{\sqrt{3}m}{m + 2n}\right) \qquad 0 \le |\theta| \le \frac{\pi}{6} \tag{4}$$

Similarly, the translational vector $\vec{T}$ (perpendicular to the chiral vector) and its length are expressed, respectively, as:

$$\vec{T} = \frac{(2m+n)}{d_R}\vec{a}_1 - \frac{(2n+m)}{d_R}\vec{a}_2$$
$$\|\vec{T}\| = \frac{\sqrt{3}\,\|\vec{C}_k\|}{d_R} \tag{5}$$

in which d_R = gcd($2n+m$, $2m+n$); where 'gcd' stands for greatest common divisor.

Finally, the number of hexagons in the nanotube unit cell, N, is expressed as:

$$N = \frac{2(n^2 + m^2 + nm)}{d_R} \tag{6}$$

III. SUSTAINABILITY OF CNT-BASED COMPOSITES

According to the health-quality-environment related issues, these nano-materials have to satisfy sustainability requirements, which are based on new standards for designing environmentally-friendly CNT-composite products.

A. CNT Fibres vs. Asbestos Fibres

Recent findings in medical research have shown that there are several similarities between CNT-fibres and asbestos fibres (see Fig. 7), and revealed that CNTs may act and behave similarly as asbestos on the internal organs of the human body, causing respiratory problems pursued by a mesothelioma: a deadly cancer that affects lungs and may not manifest until 30 to 40 years after exposure to fibres [11-13].

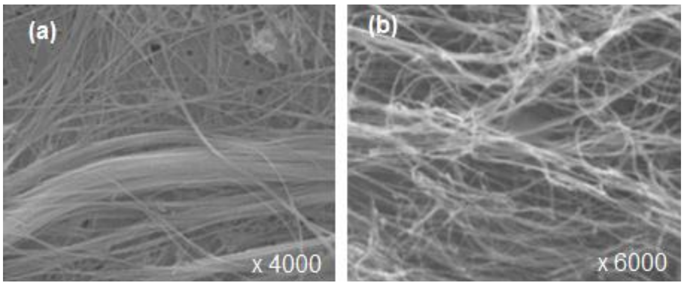


Fig. 7 Microscopic view of fibres: (a) asbestos; (b) CNTs

To answer this question and meet criteria that are fulfilling REACH (Registration, Evaluation, Authorisation and Restriction of Chemicals) regulation [14], a new approach related to sustainability strategy (i.e., eco-approach) was developed using conditional probability theory rules based on the combination of the three principal aspects *Q*, *H* and *E*; all of which taken together will provide healthier, safe, clean and sustainable CNT-based composite products [15]. Hence, the adoption of this contemporary approach aims to respond to these key challenges facing the CNT-technology development.

B. *Sustainability Requirements*

According to most scientific results related to the protection of biodiversity, global warming and climate change may have severe effects on human health and the environment. To improve the well-being and living conditions of present and future generations, it is important that the negative impacts generated from human and industrial activities should be seriously considered in all design stages of a new development. For this purpose, the sustainable development strategy is a strong key solution aiming to address this issue; it is based on three main criteria or "pillars", these are called: (i) environmental sustainability, (ii) economic sustainability and (iii) social sustainability. As sustainability requirements are inseparable from the principles of sustainable development, so they become undissociable parts from it, where quality assurance (*Q*), health protection (*H*) and environmental preservation (*E*) aspects are considered to be important branches belonging to the three main pillars. To better visualize the situation, Fig. 8 illustrates the approach of sustainability in relation to the sustainable development principles.

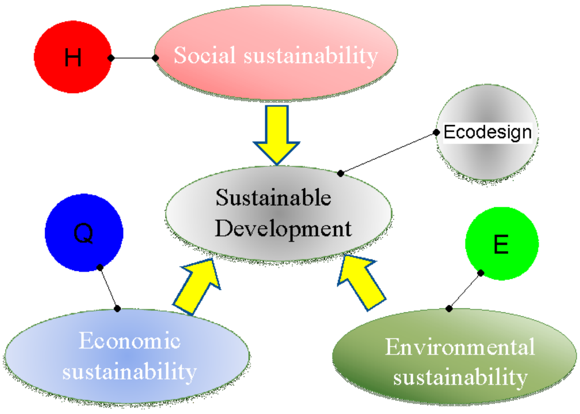
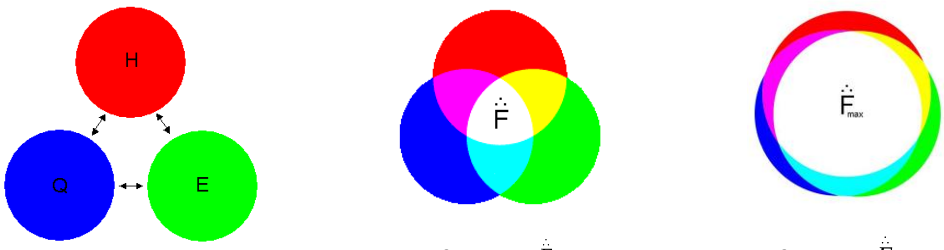


Fig. 8 Relationship between sustainable development and ecodesign requirements

C. *Evolution of the Interaction between Q-H-E*

The condition of sustainability can be considered when the interaction between *Q*, *H*, *E* aspects yields a common area of intersection between these aspects (*i.e.*, $Q \cap H \cap E$). The original diagram (Fig. 9a) shows health, quality and environment as three separate aspects that operate independently from each other. Joining the *Q*, *H*, *E* aspects gives rise to a new diagram fulfilling the sustainability condition [5] that is characterised by the subset $\dot{\ddot{F}}$ as a result of this intersection (see Fig. 9b). The three dots (∴) above the character *'F'* are only a brief description of the diagram illustrated in Fig. 9b, showing interaction between *quality*, *health* and *environment* aspects (*i.e.*, ∴). In other terms, the three dots represent the three pillars that characterise the basic elements of the sustainable development diagram (Fig. 8).

Depending on the size of the proportion represented by the common area of intersection, an optimisation process can be applied to subset $\dot{\ddot{F}}$. If the optimisation is highly improved ($\dot{\ddot{F}} = \dot{\ddot{F}}_{max}$), then the future diagram illustrated in Fig. 9c is achieved and the sought objective is reached!



$Q \cap H \cap E = \varnothing$ | $Q \cap H \cap E = \overset{\therefore}{F}$ | $Q \cap H \cap E = \overset{\therefore}{F}_{max}$

(a) original diagram | (b) actual diagram | (c) future diagram

Fig. 9 Evolution of the interaction between *Q*, *H*, and *E* aspects

IV. ECO-APPROACH TO SUSTAINABILITY OF CNT-BASED COMPOSITES

The present section is directed towards an innovative approach providing a sustainability model which aims to assess and minimize environmental impact and ensure health protection whilst maintaining quality assurance criterion.

A. Sustainability Model and Sample Space

As it was shown in Fig. 9b, the interaction between the three *Q-H-E* related issues yields the apparition of a certain number of events which are illustrated in Fig. 10, noting that each event is assumed to accomplish one or several functions [7]. However, according to Attaf's sustainability model shown in Fig. 10, these events are defined by the following subsets:

- Subset *A* (■): defined by '*an assured quality, a non-protected health and a non-preserved environment*'.
- Subset *B* (■): defined by '*an assured quality, a protected health and a non-preserved environment*'.
- Subset *C* (■): defined by '*a non-assured quality, a protected health and a non-preserved environment*'.
- Subset *D* (■): defined by '*a non-assured quality, a protected health and a preserved environment*'.
- Subset *S* (■): defined by '*an assured quality, a non-protected health and a preserved environment*'.
- Subset $\overset{\therefore}{F}$ (□): defined by '***an assured quality, a protected health*** *and* ***a preserved environment***'.
- Subset *G* (■): defined by '*an assured quality, a non-protected health and a preserved environment*'.

The colour code associated to each subset is shown in Fig. 10.

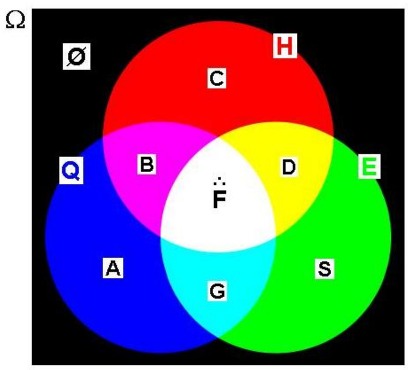


Fig. 10 Attaf's sustainability model and the outcome subsets [5]

The possible outcome subsets can be expressed by the universal sample space [5, 7, 8]:

$$\Omega = \{ A, B, C, D, S, G, \overset{\therefore}{F}, \varnothing \} \tag{7}$$

in which, $A = Q \cap \bar{H} \cap \bar{E}$ $\quad B = Q \cap H \cap \bar{E}$ $\quad C = \bar{Q} \cap H \cap \bar{E}$

$D = \bar{Q} \cap H \cap E$ $\quad S = \bar{Q} \cap \bar{H} \cap E$ $\quad G = Q \cap \bar{H} \cap E$

$\overset{\therefore}{F} = Q \cap H \cap E$ $\quad \varnothing = \bar{Q} \cap \bar{H} \cap \bar{E}$

where, $\cap$ denotes intersection symbol, and $\bar{Q}$, $\bar{H}$, $\bar{E}$ are the complement of *Q*, *H*, *E* and indicate respectively that "*Quality not achievable*", "*Health not achievable*" and "*Environment not achievable*".

By developing this approach, the analysis will concentrate only on the subset $\overset{\therefore}{F}$, a unique sought subset that is defined by the following event: "*intersection between Q, H and E is not an empty set and does exist all the time*".

B. *Application of Probability Theory*

To illustrate the probability set model, let us consider the sample space Ω that contains all the possible subsets (events) expressed by Eq. (7) and illustrated by Attaf's model shown in Fig. 10. Since the three key sets *Q*, *H* and *E* are composed of several variable elements associated to each stage involved in the design process, each key set is assumed to fulfil a specific function. With this conjecture, it can therefore be written that [7, 8]:

$$\begin{aligned} Q &= \{x_1 , x_2 , x_3 , ..., x_m\} \\ H &= \{y_1 , y_2 , y_3 , ..., y_n\} \\ E &= \{z_1 , z_2 , z_3 , ..., z_p\} \end{aligned} \qquad (8)$$

In order to better visualise the different issues and illustrate how the possible outcome probabilities can be calculated, it is convenient to construct the probability tree diagram providing a simple way for probability measure. Fig. 11 illustrates the different branches representing the possible events [7, 8].

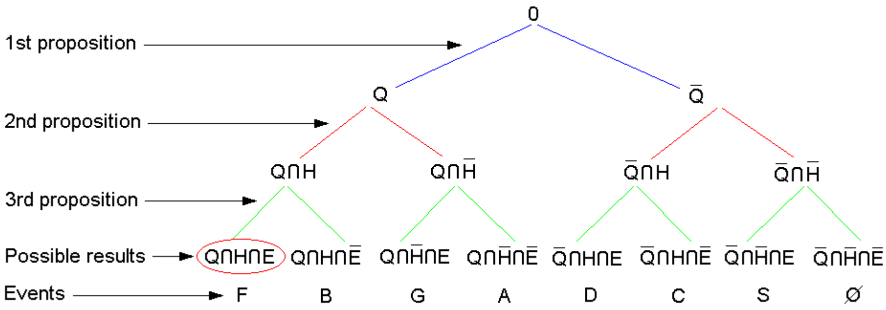


Fig. 11 Probability tree diagram and possible outcome events [7, 8]

Additionally, the number of chances providing the realisation of the event $\overset{\therefore}{F}$ can be calculated using the notion of probability. Consequently, the expressions associated to the event and its probability can, respectively, be written as [7, 8]:

$$\overset{\therefore}{F} = Q \cap H \cap E \qquad (9)$$

$$P(\overset{\therefore}{F}) = P(Q \cap H \cap E) \qquad (10a)$$

where, ∩ denotes intersection symbol.

According to the dependency of sets *Q*, *H* and *E* and the rules of multiplication in the probability theory, Eq. (10a) may be written as follows:

$$P(\overset{\therefore}{F}) = P(Q) \times P_Q(H) \times P_{Q \cap H}(E) \qquad (10b)$$

where, $P(Q)$ represents the probability of an achievable quality;

$P_Q(H)$ represents the probability of an achievable health, knowing that quality has already been achieved;

$P_{Q \cap H}(E)$ represents the probability of an achievable environment, knowing that both quality and health have already been achieved.

C. *Sustainability Factors*

As the sustainability process depends on the probability values expressed by Eq. (10b), it is convenient to assign to each aspect of *Q*, *H* and *E* a specific factor representing the probability of approval [7]. It may therefore be considered that:

- $\alpha = P(Q)$ is a factor representing the probability of approval in terms of quality assurance;
- $\beta = P_Q(H)$ is a factor representing the probability of approval with regard to health protection and known that quality requirement is achieved; and
- $\gamma = P_{Q \cap H}(E)$ is a factor representing the probability of approval with regard to environmental preservation, known that health and quality requirements are achieved.

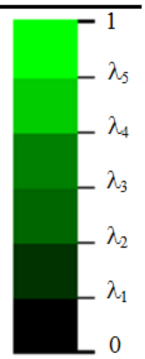
The condition to provide an eco-friendly CNT-based composite product, defined by the subset $\overset{\therefore}{F}$ (Fig. 9), can be performed by considering the mathematical product of the three above-mentioned factors. For notation simplicity, the quantity obtained by the multiplication rule may be represented by a single variable called ‘eco-factor’ and denoted by the Greek letter λ.

With this simplified approach, Eq. (10b) can be written as:

$$\lambda = \alpha \times \beta \times \gamma \tag{10c}$$

This eco-factor is considered to be a key performance indicator (KPI) for sustainability investigation (Attaf, 2011). It is made for the purpose of discussion and analysis and will be used to provide better assessment of *Q-H-E* impacts in relation to each stage involved in the process of life-cycle assessment (LCA). For instance, if the eco-factor λ approaches unity (100%), the stage under consideration fully satisfies the sustainability requirements in the LCA. However, if the eco-factor λ is not close to the target value required by sustainability standards, it is recommended to continue searching for new possible alternatives that provide more advanced factors. Table 1 recapitulates the assessment level for different intervals and shows a rating satisfaction measure in the form of colour gauges, ranging from the lowest level (in black) at the highest level (in green).

TABLE 1 PROBABILITY COLOUR GAUGES FOR DIFFERENT VALUES OF ECO-FACTOR λ [7]

Interval	Assessment	Gauge
$\lambda_5 \le \lambda \le 1$	Excellent	
$\lambda_4 \le \lambda < \lambda_5$	Very good	
$\lambda_3 \le \lambda < \lambda_4$	Good	
$\lambda_2 \le \lambda < \lambda_3$	Fair	
$\lambda_1 \le \lambda < \lambda_2$	Poor	
$0 \le \lambda < \lambda_1$	Very poor	

V. INNOVATIVE ECO-FORMULATIONS FOR CONSTITUTIVE EQUATIONS OF CNT-LAMINATES

The derived eco-factor λ will be inserted into the standard mechanical characterisation formulae of composite materials. Hence, the classical Young’s moduli E_1, E_2, E_3 and shear moduli G_{12}, G_{23}, G_{13} of the unidirectional ply determined initially from experimental tests will be replaced by $\overset{\therefore}{E}_1$, $\overset{\therefore}{E}_2$, $\overset{\therefore}{E}_3$, $\overset{\therefore}{G}_{12}$, $\overset{\therefore}{G}_{23}$, $\overset{\therefore}{G}_{13}$, respectively.

In relation to this innovative eco-approach and for linear-elastic mechanical behaviour of a unidirectional CNT-fibre/matrix ply, the new engineering constants are expressed in the principal coordinate system as [7]:

$$\overset{\therefore}{E}_i = \lambda \times E_i \qquad \overset{\therefore}{G}_{ij} = \lambda \times G_{ij} \qquad \text{with} \quad \frac{\overset{\therefore}{E}_i}{\nu_{ij}} = \frac{\overset{\therefore}{E}_j}{\nu_{ji}} \qquad (i,j=1,2,3 \text{ and } i \neq j) \tag{11}$$

where ν_{ij} is the classical Poisson’s ratio for transverse strain in the *j*-direction when stressed in the *i*-direction. It should be noted that in this study no attempt was made to investigate the new values of Poisson’s ratios when the eco-factor λ is taken into consideration; its impact is beyond the scope of this analysis.

With this approach as an objective, Fig. 12 shows a general illustration of a CNT-based composite component under static structural analysis. The isolated infinitesimal element in the form of cubic parallelepiped shape is assumed to be composed of several plies of CNTs. However, depending on the plate lateral dimensions in comparison with its thickness, the stacking sequence operation results in either thin or thick plate. According to the classical lamination theory for thick plates, the effect of transverse shear deformation will be taken into consideration as shown in Fig. 12.

When the environment and health impacts besides quality are taken into consideration in the analysis, the new constitutive relations for an unsymmetrically *n*-layered laminated composite plate (*k*=1, 2, .. *n*) with transverse shear deformations can, after integration through each ply thickness and summation of forces and moments, be written in compact matrix form as [7, 16, 17]:

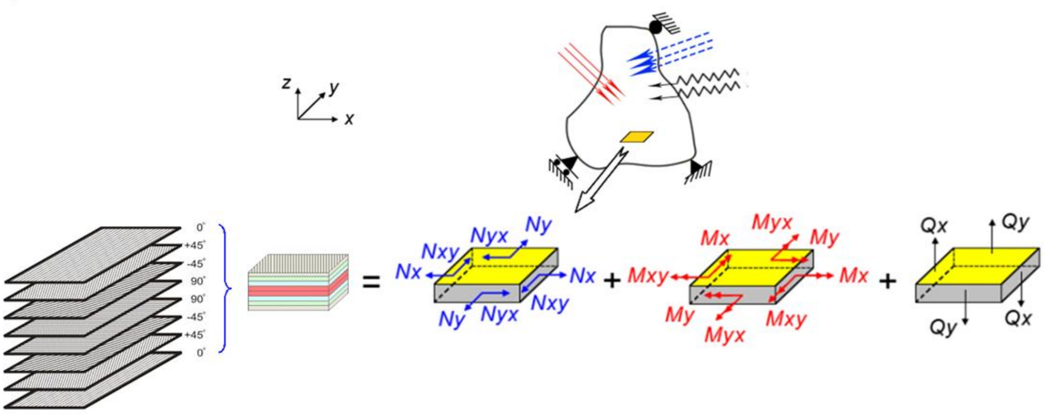


Fig. 12 Internal forces and moments acting on the middle-surface of an infinitesimal laminated plate element reinforced with CNT-based fibres

$$\left\{\begin{matrix} N \\ -- \\ M \end{matrix}\right\}_{xy} = \sum_{k=1}^{n}\int_{z_{k-1}}^{z_k} \left\{\begin{matrix} \{\sigma\}_{xy} \\ ---- \\ z\,\{\sigma\}_{xy} \end{matrix}\right\} dz = \begin{bmatrix} \overset{\therefore}{A} & | & \overset{\therefore}{B} \\ -- & - & --- \\ \overset{\therefore}{B} & | & \overset{\therefore}{D} \end{bmatrix} \left\{\begin{matrix} \varepsilon^0 \\ -- \\ \kappa \end{matrix}\right\}_{xy} \tag{12a}$$

$$\{\,Q\,\}_{xyz} = \left\{\ \overset{\therefore}{F}_{ij}\ \right\}\{\,\gamma\,\}_{xyz} \tag{12b}$$

where, N is the in-plane forces vector;
M is the bending/torsional moments vector;
Q is the out-of-plane forces vector;
ε^0 is the mid-plane strains vector;
κ is the curvatures vector;
γ is the transverse shear strains vector.

The new stiffness components of the matrices $\overset{\therefore}{A}_{ij}$ (extensional matrix), $\overset{\therefore}{B}_{ij}$ (coupling matrix), $\overset{\therefore}{D}_{ij}$ (bending) and $\overset{\therefore}{F}_{ij}$ (transverse shear matrix) are expressed as:

$$(\overset{\therefore}{A}_{ij}\,,\ \overset{\therefore}{B}_{ij}\,,\ \overset{\therefore}{D}_{ij}) = \sum_{k=1}^{n}\int_{z_{k-1}}^{z_k} (\overline{\overset{\therefore}{Q}}_{ij})_k\ (1, z, z^2)\,dz \quad (i, j = 1, 2, 6) \qquad \overset{\therefore}{F}_{ij} = \delta_{ij}\sum_{k=1}^{n}\int_{z_{k-1}}^{z_k} (\overline{\overset{\therefore}{Q}}_{ij})_k\,dz, \quad (i, j = 4, 5)$$

The stiffness matrices $\overline{\overset{\therefore}{Q}}_{ij} = \overline{\overset{\therefore}{Q}}_{ji}$ (i, j = 1, 2, 6 or 4, 5) are functions of the NTC-fibre orientation angle, θ, and the new elastic moduli of each ply when the eco-factor λ is included in the analysis. The coefficient δ_{ij} is a transverse shear correction factor.

With this new approach, it becomes possible by simple comparison between sustainable results (eco-results) and classical results that do not take into account environmental and health impacts, to generate an estimated difference value called "eco-deviation". This latter can be expressed by the following relation:

$$\text{Eco-deviation}\ (\%) = \left|\frac{\overset{\therefore}{V} - V}{V}\right| \times 100 \tag{13}$$

where, $\overset{\therefore}{V}$ is the eco-result corresponding to the result where the eco-factor λ ($0 \le \lambda < 1$) is integrated in the analysis and V is the classical result corresponding to λ=1.

For better discussion and understanding of the sustainability issues, it is suggested that the final results may be presented in the form of graphs with normalized axes. A dimensionless quantity named "eco-efficiency ratio", representing the ratio between eco-results and classical ones, can be chosen for the y-axis and may be denoted for example by the Greek letter $\Lambda = \overset{\therefore}{V}/V$. For instance, when performing stress analysis in design of structural composite elements reinforced with CNT-based continuous fibres, Λ can be equal to $\overset{\therefore}{\sigma}/\sigma$, $\overset{\therefore}{\tau}/\tau$ and so forth. The discrepancy between classical results and eco-results can help designers and analysts to evaluate easily, during stress analysis stage, the environmental and health impacts of their new developed CNT-based composite products. Moreover, this discrepancy can be optimised via further advanced alternatives to reach the target value required by sustainability standards.

VI. OPTIMISATION OF SUSTAINABILITY ECO-FACTORS

A. Flow Chart

The sustainability approach is related to an optimisation of the eco-factor λ, in which the *Q-H-E* issues all interact together (probability of the event $\ddot{F}$). Fig. 13 shows a flow-chart addressing the sustainability issues and the process of optimisation. The analysis of data collected after each loop for the stage $k=1$ will be iterated for the other stages involved in the life-cycle assessment ($k=2, ..., N$). For instance, if the final probability output results are close to unity, then the objective previously outlined in Fig. 9c is fully reached! However, if the output results are not close to the target values required by the sustainability standards, further new alternatives are to be sought.

In this flow-chart, the optimisation process is composed of three steps which are recapitulated by the following points:

- the first step defines the stage involved in the design process (k=1, 2, ...), collects the associated data and specifies the target value of probability to be reached;
- the second step assesses and analyses results on the basis of the three main criteria (*Q*, *H*, *E*);
- the third step applies the optimisation procedure to improve the probability values via alternative solutions for better product sustainability; and
- the forth step reports in the form of a specification sheet the final results of LCA and provides a comparison with classical ones.

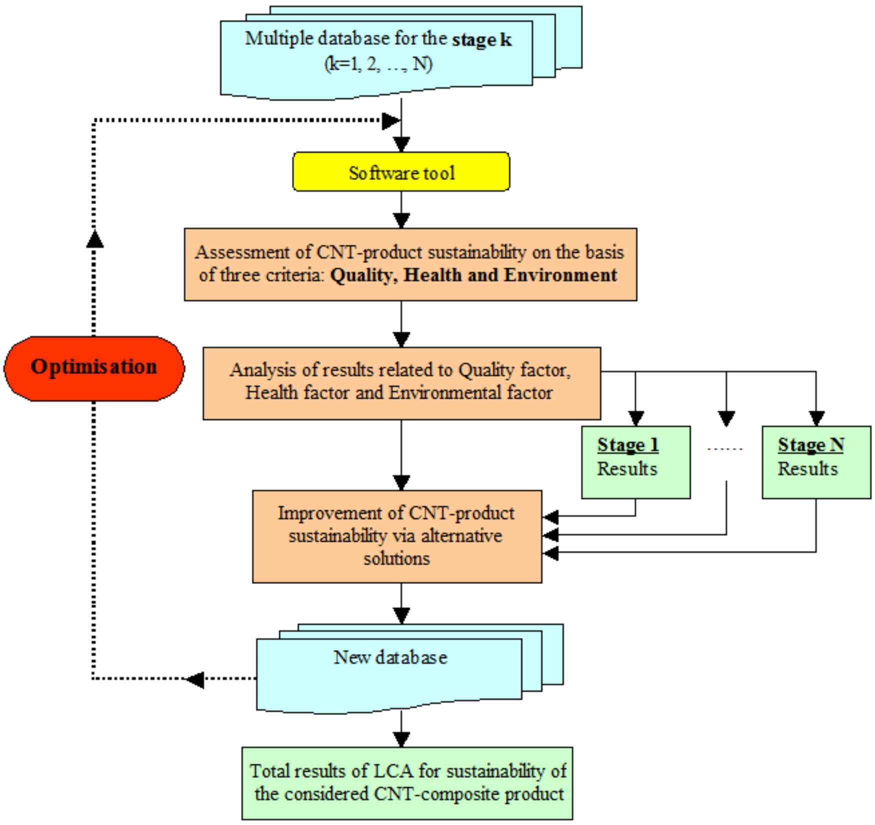


Fig. 13 Process flowchart for sustainability assessment and optimization of CNT-based composite products

B. Software Tool

Given the complexity of the optimisation process, which has to be applied at each stage involved in the life-cycle analysis of a CNT-based composite product whilst taking into account the three key criteria *Q*, *H* & *E*, it is important to develop a software tool capable to solve the probability problem and provide a high technique that can optimise the eco-factors.

The investigation will be made systematically by stage and according to the type of data collected the analysis may be undertaken on the basis of qualitative and/or quantitative approaches. Among the main stages that are likely to be subject to an assessment procedure for the sustainability of CNT-based composite products, we cite the followings:

- Stage 1: Choice of the raw materials and constituents
- Stage 2: Definition of CNT-based composite product materials and design approaches
- Stage 3: Manufacturing and inspection of the first article
- Stage 4: Qualification / certification of the CNT-based composite product
- Stage 5: Launching the production on the Supply Chain
- Stage 6: Distribution and use of the CNT-based composite product
- Stage 7: Repair and maintenance of the CNT-based composite product
- Stage 8: End of life of the CNT-based composite product, reuse, waste management and recycling

The life-cycle analysis will cover all the stages required in the whole value chain, aiming at 'closing the loop' shown in Fig. 14. In addition, the notion of circular economy can be correctly used only if the stage relative to the extraction and transportation of raw materials is included within the loop.

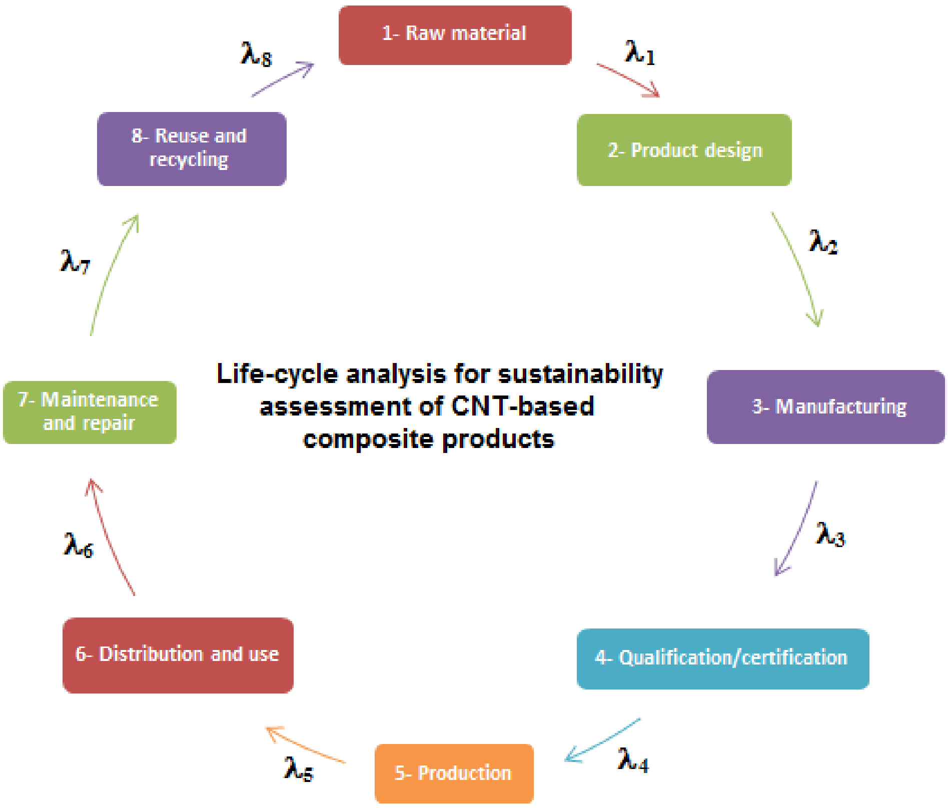


Fig. 14 Life-cycle analysis for sustainability assessment of CNT-based composite products

For better interpretation and visualisation of the output results, the global assessment of CNT-based composite product sustainability may be given in the form of a mathematical matrix of order 3×8 showing the measure of factors associated independently to quality, health and environmental for each stage and the combined resulting eco-factors, as shown in Fig. 15. Nevertheless, it should be noted that a matrix with one or more values equal (or close) to zero does not truly fulfil the LCA condition for sustainability assessment of the CNT-based composite product. Under such circumstances, it is necessary important to carry out an optimization procedure to improve these low values. Likewise, a matrix with all values equal (or close) to one provides the maximum sustainability in the life-cycle assessment.

To obtain an overall and quick view of the CNT-based composite product sustainability, a total eco-factor can be derived using the following formula:

$$\lambda_T = \prod_{i=1}^{i=8} \lambda_i \tag{14}$$

On the other hand, to provide designers with some ideas regarding the magnitude of the sustainability approach, Fig. 16 illustrates an example wherein the results are presented in the form of a spider graph showing the magnitude of each factor with respect to the limiting envelop and the resulting value of the eco-factor.

$$\begin{array}{l} \\ \\ Stage\,1 \rightarrow \\ Stage\,2 \rightarrow \\ Stage\,3 \rightarrow \\ Stage\,4 \rightarrow \\ Stage\,5 \rightarrow \\ Stage\,6 \rightarrow \\ Stage\,7 \rightarrow \\ Stage\,8 \rightarrow \end{array} \begin{array}{c} \begin{array}{ccc} Q & H & E \\ \downarrow & \downarrow & \downarrow \end{array} \\ \begin{bmatrix} \alpha_1 & \beta_1 & \gamma_1 \\ \alpha_2 & \beta_2 & \gamma_2 \\ \alpha_3 & \beta_3 & \gamma_3 \\ \alpha_4 & \beta_4 & \gamma_4 \\ \alpha_5 & \beta_5 & \gamma_5 \\ \alpha_6 & \beta_6 & \gamma_6 \\ \alpha_7 & \beta_7 & \gamma_7 \\ \alpha_8 & \beta_8 & \gamma_8 \end{bmatrix} \end{array} \equiv \begin{array}{c} Ecofactor \\ \downarrow \\ \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \lambda_4 \\ \lambda_5 \\ \lambda_6 \\ \lambda_7 \\ \lambda_8 \end{bmatrix} \end{array}$$

Fig. 15 Typical matrix for sustainability of CNT-based composite product

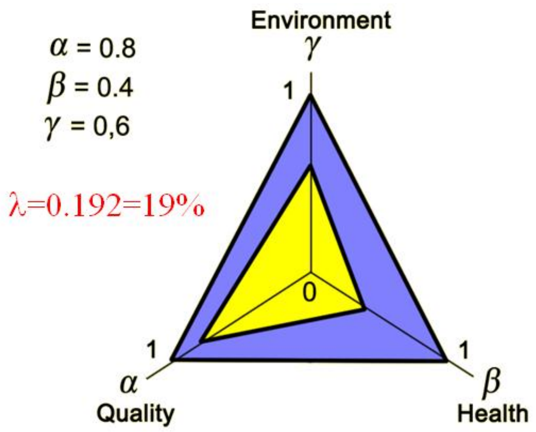


Fig. 16 Example of spider graph showing the magnitude of each factor and the resulting eco-factor

VII. CONCLUSIONS

Based on mathematical formulations, scientific and technological know-how in the field of composite / nano-composite materials and structures, a new and innovative approach was developed with the objective to integrate at each stage of the product life-cycle assessment three balanced key criteria characterised mainly by quality assurance, health protection and environmental preservation. These sustainability requirements were achieved by the development and use of new criteria in the form of factors and eco-factors. However, greater depth of study still required to establish the rating satisfaction measure that yields the appropriate factors required by sustainability standards. Thus, target values of factors remain essential because they constitute an important source of reference for comparison and discussions purposes.

Further to that, probability analysis and some optimisation procedures based on a new technique of additive colours were undertaken in accordance with the three balanced key criteria. It has been shown that the main difficulty in the analysis of sustainability lies in how to maximise in practice the area of intersection between the three main sets (i.e., $\ddot{F}$). This results in a maximisation of the corresponding factors, where each factor is dependent of the two others. Consequently, when these factors are optimised via alternative solutions and approved by sustainability standards, they can then be integrated into the process of product life-cycle assessment.

As a general conclusion, this investigation can be regarded as a contribution to the international standards, codes, guidelines and new orientations towards the design of eco-friendly CNT-based composite products. It may also be regarded as a stimulation of eco-innovation and research activities in the field of sustainability and circular economy and as well as a boosting approach to encouraging designers and engineers to have more motivation towards the integration of health and environment aspects into the life-cycle assessment of CNT-based composites. In addition, new recommendations could be generated from this innovative survey. These recommendations will, however, be taken into account mainly in the design and manufacturing stages to improve the sustainability space of future CNT-based composite products.

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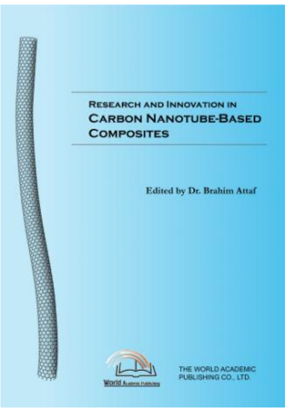
Dr. Attaf has published many scientific papers, edited three books, and successfully trained/supervised many engineers and postgraduate students (Master’s and Ph.D.’s).



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