Green Design and Multidisciplinary Optimization of Carbon Nanotube Composite Structures

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Summary

This work develops a multi-objective design optimisation method for Carbon Nanotube Composite Structures (CNTCSs) using Genetic Algorithm and Finite Element Analysis (FEA). Two design problems are considered: the first is an optimisation problem to improve the mechanical properties (weight-displacement) of the CNTCSs, minimizing the Not Adherence Green Design Principles (NoAGDP); the second is an optimisation problem to improve the same mechanical properties also minimizing the cost of the CNTCSs. Numerical results show in both cases that a set of optimal CNTCSs can be found, which has similar stiffness, weight and NoAGDP, with sensitive cost increments, compared to common polymer structures.

***Keywords**: multi-objective design optimization, carbon nanotube composite structures, genetic algorithm, finite element analysis, mechanical properties, no adherence to green design principles, cost.*

1. Introduction

The remarkable mechanical properties exhibited by Carbon Nanotubes (CNTs) have stimulated much interest in their use to reinforce advanced composites. So far, hundreds of publications have reported certain aspects of the mechanical enhancement of different polymer system by CNTs. Many of these studies have been discussed in an excellent review[i]. The variation of parameters, such as CNT type, growth method, chemical pre-treatment as well as polymer type and processing strategy has given some encouraging results in fabricating relatively strong CNT-polymer composites. Sustainability, 'cradle-to-grave' design, industrial ecology, eco-efficiency, and 'green' chemistry are not just newly coined buzzwords, but form the principles that are guiding the development of a new generation of 'green' materials[ii]. CNT composite materials are no exception to this new paradigm. In this work, two numerical multidisciplinary problems are presented: in the first, the goal is to apply a multi-objective design optimization methodology in order to study the mechanical performance in terms of weight and stiffness in Carbon Nanotube Composite Structures (CNTCSs), considering additionally the sustainable design quantified through the Not Adherence to Green Design Principles (NoAGDP) of the polymer matrix structure. In the second problem is applied a multi-objective methodology to improve the mechanical properties (weight and stiffness) minimizing the total cost of the composite structures.

2. Methodology

2.1. Multi-Objective Optimization

Engineering design problems often require a simultaneous optimisation of conflicting objectives (multi-objective optimization). Unlike single objective optimisation problems, the solution is a set of points known as the Pareto optimal set. Solutions are compared to other solutions using the concept of Pareto dominance.

2.2. *Robust Multi-Objective Optimization Platform*

Robust Multi-Objective Optimisation Platform (RMOP) is a computational intelligence framework, which is a collection of population based algorithms including Genetic Algorithm (GA) and Particle Swarm Optimisation (PSO)[iii]. RMOP is easily coupled to any analysis tools such as Computation Fluid Dynamic (CFD), Finite Element Analysis (FEA), and/or Computer Aided Design (CAD) systems. In this paper, a GA searching method in RMOP is used under a parallel/distributed optimisation system denoted as RMOGA. RMOGA uses a Pareto tournament selection operator, which ensures that the new individual is not dominated by any other solution in the tournament. Figure 1 shows the overall algorithm for design optimisation problems using RMOGA.

3. Analysis of Laminated Composite Structure

The analysis of composite structures using FEA is based on the classical mixture theory originally develop by Truesdell and Toupin[iv]. The computer program used to solve the mechanical problem is Compack, a FEA based tool able to calculate structural properties. Compack was design to work with composite materials, and has the capability to define different constitutive models for each composite element, as Figure 2 shows.

4. Multidisciplinary Optimization of CNTCSs

There are a variety of studies about the use of CNT as reinforcement in composites [1], however, this work only considers those reinforced composites that improve their mechanical properties with the addition of CNT. This work analyses two multidisciplinary design optimization problems for CNTCS. In the first, we seek to improve the mechanical properties such as weight and stiffness, and the sustainable design considering the NoAGDP definition. In the second test case are improved the same mechanical properties of the case 1 including the total costs of composite structures.

4.1. *Problem Formulation*

In the two problems is use the same model, that consists in a quadrilateral multilayered (11 layers) plate simply supported in two opposite sides, with a constant point force at the central position (L= 1 m). Figure 3 shows the baseline composite structure and boundary conditions for the structural simulation.

4.2. *CNTCS Design Variables*

Thirty one reinforced CNT based polymer composites obtained by different process methods, and eleven layer thicknesses, have been used in the optimization process, as shown Table 1 and 2, respectively.

4.3. *Reference structures*

As a reference for comparison purposes, we have carried out the optimization of the same model using the eight types of polymer matrix constituent of the CNT composites -denoted as Polymer reference Structures PLSs-, namely, a biopolymer: polylactic acid (PLA); and seven polymers from fuel feedstocks: polyethylene terephthalate (PET), high and low density polyethylene (HDPE, LDPE), polypropylene (PP), polycarbonate (PC), polyvinyl chloride (PVC), and polystyrene (PS). Table 1 shows the properties of the polymer matrices.

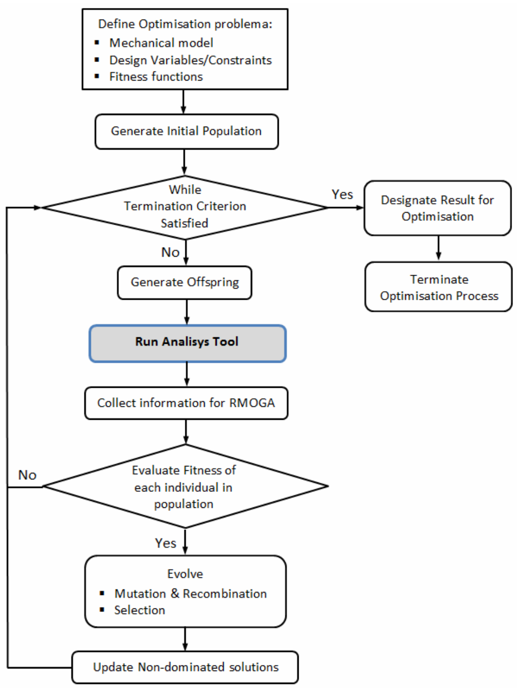


Figure 1: Overall algorithm for design optimization problems using RMOGA

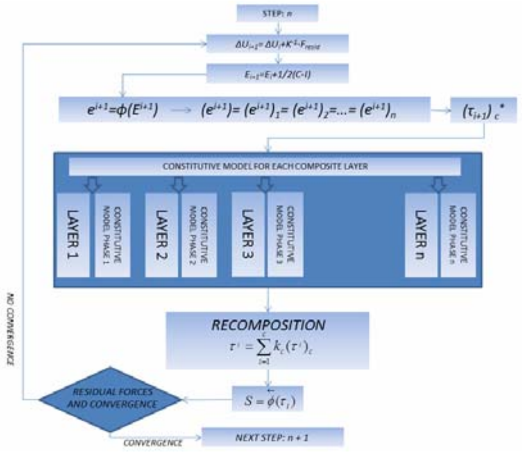


Figure 2: Mechanism of Compack

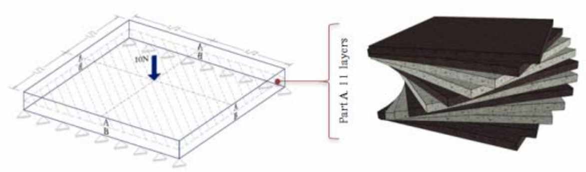
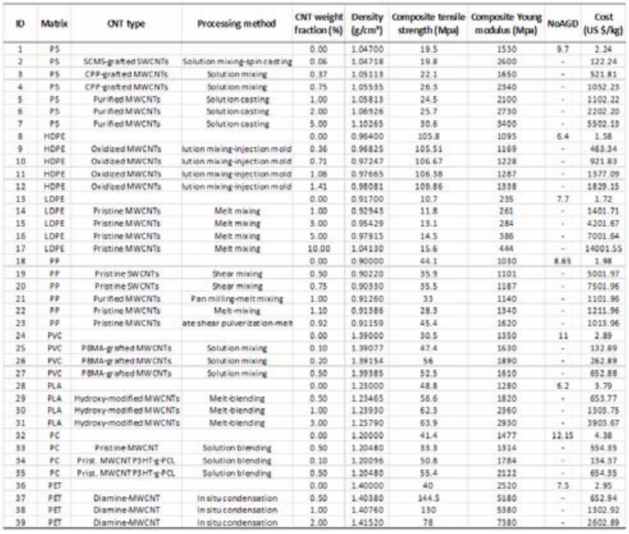


Figure 3: Baseline and boundary conditions for multilayered CNTCS plate

Table 1: Polymer and Carbon Nanotube (CNT) composite material types



ID	Matrix	CNT type	Processing method	CNT weight fraction (%)	Density (g/cm³)	Composite tensile strength (Mpa)	Composite Young modulus (Mpa)	NoAGD	Cost (US $/kg)
1	PS			0.00	1.04700	19.5	1530	9.7	2.24
2	PS	SCMS-grafted SWCNTs	Solution mixing-spin casting	0.06	1.04718	19.8	2600	-	122.24
3	PS	CPP-grafted MWCNTs	Solution mixing	0.37	1.05113	22.1	1650	-	521.81
4	PS	CPP-grafted MWCNTs	Solution mixing	0.75	1.05535	26.3	2340	-	1052.23
5	PS	Purified MWCNTs	Solution casting	1.00	1.05813	24.5	2100	-	1102.22
6	PS	Purified MWCNTs	Solution casting	2.00	1.06926	25.7	2730	-	2202.20
7	PS	Purified MWCNTs	Solution casting	5.00	1.10265	30.6	3400	-	5502.13
8	HDPE			0.00	0.96400	105.8	1095	6.4	1.58
9	HDPE	Oxidized MWCNTs	lution mixing-injection mold	0.36	0.96825	105.51	1169	-	463.34
10	HDPE	Oxidized MWCNTs	lution mixing-injection mold	0.71	0.97247	106.67	1228	-	921.83
11	HDPE	Oxidized MWCNTs	lution mixing-injection mold	1.06	0.97665	106.58	1287	-	1377.09
12	HDPE	Oxidized MWCNTs	lution mixing-injection mold	1.41	0.98081	109.86	1338	-	1829.15
13	LDPE			0.00	0.91700	10.7	235	7.7	1.72
14	LDPE	Pristine MWCNTs	Melt mixing	1.00	0.92943	11.8	261	-	1401.71
15	LDPE	Pristine MWCNTs	Melt mixing	3.00	0.95429	13.1	284	-	4201.67
16	LDPE	Pristine MWCNTs	Melt mixing	5.00	0.97915	14.5	386	-	7001.64
17	LDPE	Pristine MWCNTs	Melt mixing	10.00	1.04130	15.6	444	-	14001.55
18	PP			0.00	0.90000	44.1	1030	8.65	1.98
19	PP	Pristine SWCNTs	Shear mixing	0.50	0.90220	35.9	1101	-	5001.97
20	PP	Pristine SWCNTs	Shear mixing	0.75	0.90330	35.5	1187	-	7501.96
21	PP	Purified MWCNTs	Pan milling-melt mixing	1.00	0.91260	33	1140	-	1101.96
22	PP	Pristine MWCNTs	Melt-mixing	1.10	0.91386	28.3	1340	-	1211.96
23	PP	Pristine MWCNTs	ate shear pulverization-melt	0.92	0.91159	45.4	1620	-	1013.96
24	PVC			0.00	1.39000	30.5	1350	11	2.89
25	PVC	PBMA-grafted MWCNTs	Solution mixing	0.10	1.39077	47.4	1630	-	132.89
26	PVC	PBMA-grafted MWCNTs	Solution mixing	0.20	1.39154	56	1890	-	262.89
27	PVC	PBMA-grafted MWCNTs	Solution mixing	0.50	1.39385	52.5	1610	-	652.88
28	PLA			0.00	1.23000	48.8	1280	6.2	3.79
29	PLA	Hydroxy-modified MWCNTs	Melt-blending	0.50	1.23465	56.6	1820	-	653.77
30	PLA	Hydroxy-modified MWCNTs	Melt-blending	1.00	1.23930	62.3	2360	-	1303.75
31	PLA	Hydroxy-modified MWCNTs	Melt-blending	3.00	1.25790	63.9	2930	-	3903.67
32	PC			0.00	1.20000	41.4	1477	12.15	4.38
33	PC	Pristine MWCNT	Solution blending	0.50	1.20480	33.3	1314	-	554.35
34	PC	Prist. MWCNT P3HT-g-PCL	Solution blending	0.10	1.20096	50.8	1784	-	134.37
35	PC	Prist. MWCNT P3HT-g-PCL	Solution blending	0.50	1.20480	55.4	2122	-	654.35
36	PET			0.00	1.40000	40	2520	7.5	2.95
37	PET	Diamine-MWCNT	In situ condensation	0.50	1.40380	144.5	5180	-	652.94
38	PET	Diamine-MWCNT	In situ condensation	1.00	1.40760	130	5380	-	1302.92
39	PET	Diamine-MWCNT	In situ condensation	2.00	1.41520	78	7380	-	2602.89

Table 2: Layer thicknesses (m)

ID#	1	2	3	4	5	6	7	8	9	10	11
Thickness	1×10^{-4}	2×10^{-4}	4×10^{-4}	6×10^{-4}	8×10^{-4}	1×10^{-3}	1.2×10^{-3}	1.4×10^{-3}	1.6×10^{-3}	1.8×10^{-3}	2×10^{-3}

4.4. *Problem 1. Green Design Optimization*

The fitness functions are to minimize the total weight and maximum displacement of CNTCS while minimizing its NoAGDP, as shown in Equations (1 -3):

$$f_1 = \min(W_{comp}) = \sum_{i=1}^{n} W_i \tag{1}$$

$$f_2 = \min(d_{total}) = \sqrt{(dx^2 + dy^2 + dz^2)} \tag{2}$$

$$f_3 = \min(NoAGDP_{comp}) = \sum_{i=1}^{n}(W_i . NoAGDP_i) \tag{3}$$

where n is the total number of layers (n = 11), W_{comp} and d_{total} represent the total weight and the maximum displacement of CNTCS; W_i and NoAGDPi are the weight and Not Adherence to Green Design Principles for the *ith* layer (*NoAGDP = 9.9 - AGDP).* In this study the estimation of AGDP to polymer materials proposed by Tabone et al.[v] is used.

4.5. *Problem 2. Economic Feasibility Optimization*

In this case we minimize the weight; displacement and the total cost of the composite structures ($Cost_{comp}$), represent for the fitness function define in equation 1, 2 and 4, respectively.

$$f_4 = \min(Cost_{comp}) = \sum_{i=1}^{n}(W_i . Cost_i) \tag{4}$$

5. Results

The CNTCS and PLS (reference structure) Pareto front for the multi-objective green design optimization are shown in Figure 4. The numerical results for CNTCS solutions indicate that the use of reinforced CNT composites layers has not appreciably improved the overall properties of the composite structures in terms of mechanical properties as weight and displacement, nor in terms of NoAGDP, when is compared with the optimized PLS reference solutions. Table 3 presents the comparison of green design solutions of weight, displacement and NoAGDP of some Pareto Members (PMs) for CNTCSs and PLSs, where minimal differences are appreciated.

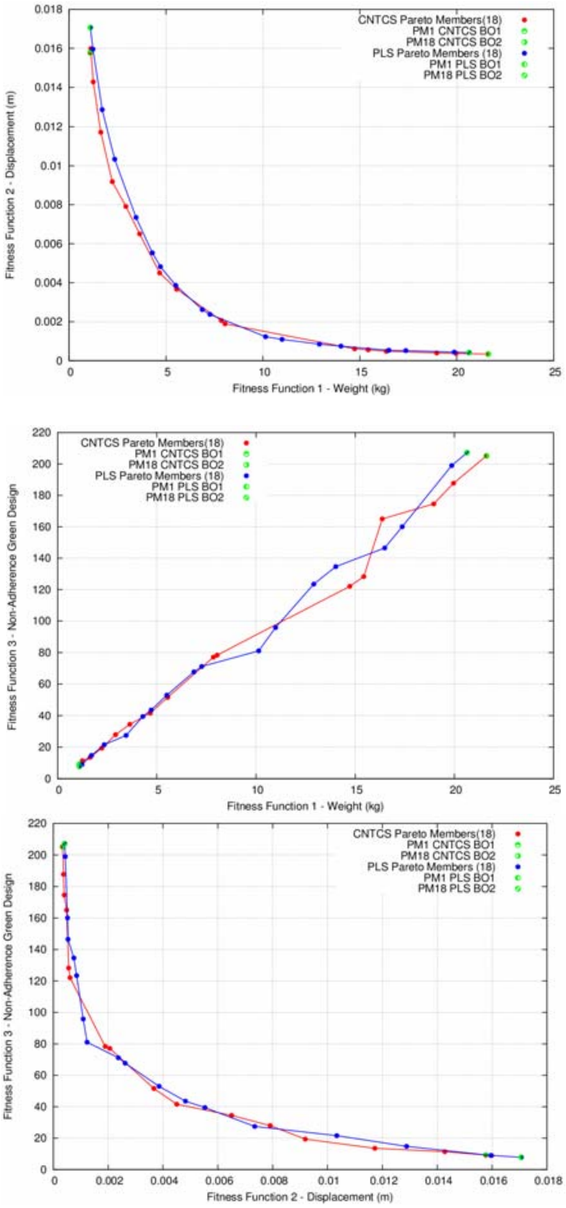


Figure 4: Pareto optimal front for green multi-objective CNTCS and PLS design optimization: top (weight –displacement), center (weight - NoAGDP) and down (displacement – NoAGDP)

Figure 5 shows the Pareto front solutions for mechanical properties (weight-displacement) and total cost of the CNTCSs and PLS reference structures (economic feasibility optimization). Although some minor improvements are achieved with CNTCSs in terms of weight and displacement, the costs are considerably increased compared with PLSs. Table 4 shows the comparison of mechanical properties and costs of some Pareto members for CNTCSs and PLSs.

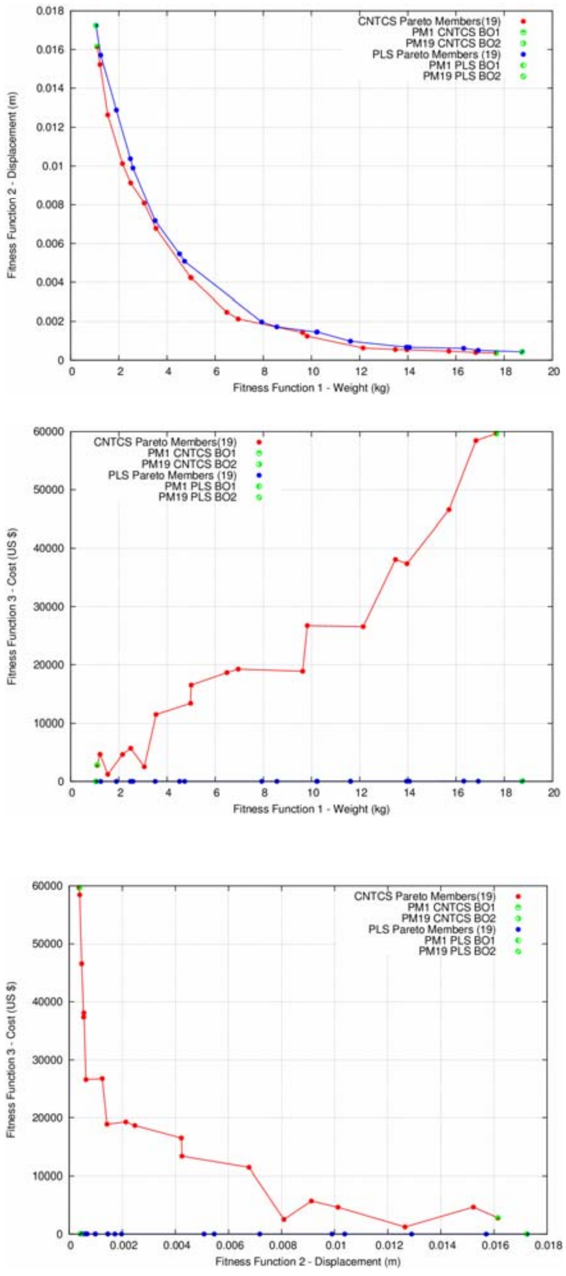


Figure 5: Pareto optimal front for economic feasibility multi-objective CNTCS and PLS design optimization: top (weight – displacement), center (weight - cost) and down (displacement – cost)

Table 3: Comparison of weight, displacement and NoAGDP for CNTCSs and PLSs (green design optimization)

Structure Type	Weight (kg)	Displacement (m)	NoAGPD
PLS PM1 BO1	1.0989	0.017063	7.81859
CNTCS PM1 BO1	***1.09734 (- 0.14 %)***	***0.015775 (- 7.55 %)***	***9.23503 (+ 18.12 %)***
PLS PM8 (Interm. sol.)	5.5083	0.0038587	52.9488
CNTCS PM9 (Interm. Sol)	***5.55056 (+ 0.77 %)***	***0.0036695 (- 4.90%)***	***51.58040 (- 2.58 %)***
PLS PM18 BO2	20.6345	0.00041358	207.153
CNTCS PM18 BO2	***21.62270 (+ 4.79 %)***	***0.00034052 (- 17.67 %)***	***205.188 (- 0.95 %)***

Table 4: Comparison of weight, displacement and Cost for CNTCSs and PLSs (economic feasibility optimization)

Structure Type	Weight (kg)	Displacement (m)	Cost (US $)
PLS PM1 BO1	1.0531	0.017244	1.92294
CNTCS PM1 BO1	***1.1035 (-4.79 %)***	***0.01615 (- 6.36 %)***	***2802.23 (+ 145626 %)***
PLS PM9 (Interm. sol.)	7.9322	0.0019719	16.7306
CNTCS PM11 (Interm. Sol)	***6.9550 (-12.32 %)***	***0.00213 (8.16 %)***	***19241.50 (+ 114907 %***
PLS PM19 BO2	18.7424	0.00043237	52.9253
CNTCS PM19 BO2	***17.6637 (-5.76 %)***	***0.0003757 (- 17.67 %)***	***59690.50 (+112682 %)***

6. Conclusion

A methodology for the stacking sequence design optimisation of multilayered CNTCS has been described and investigated. In the first problem case, it has been implemented to improve the composite structure in terms of weight, stiffness and the NoAGDP; and, for the second problem, to minimize the weight, displacement and cost of composite structures. The methodology couples a robust multi-objective evolutionary algorithm and a finite element analysis based composite structure analysis tool under a parallel optimization system. Results obtained demonstrate that the methodology allows one to get light and stiffness composite structures with low NoAGDP. The results also show that the use of CNT to reinforce polymers structures do not lead to significant improvements in terms of weight, stiffness and NoAGPD. Rather, it does yields a substantial increase in the cost of the composite structures.

7. References

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