Computational analysis of the mechanical behavior of carbon nanotubes in a rail-wheel system

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Abstract. Currently, railway systems have presented many problems associated with friction and wear due to movement between the interface of the wheel-rail system, a situation that has been demanding large investments and railway costs in transport companies due to the frequent change of pieces of the system. As a possible solution, the addition of carbon nanotubes (CNTs) has been underway in some modified lubricants to increase the antifriction properties. In this investigation, computational simulations were developed to analyze the behavior of the CNTs as a reducing component of the friction of the material. A constitutive model was considered by Hooke’s law for the wheel-rail system and the CNTs. Numerical lattices were designed to develop the computational simulations. The constitutive equations were solved by the Finite Differences Method (F.D.M.). The computational models were subjected to transverse loads emulating the movement of the system. Simulations were performed for one wheel-rail model with insert of 0.01 percent of CNTs. The results identified in the report of the insertions of the CNTs in the wheel-rail system show a dissipative-absorbent behavior of the deformation energy is detected, combined with rotation effects of the CNTs, a condition that may allow a reduction in friction and wear CNTs can contribute to improve the tribological properties of lubricants in affected railway systems and a longer service life of mechanical elements. The computational developments carried out in this research can facilitate the analysis of behaviors of nanostructured materials under conditions of extreme functionality where the experimental processes are complex.

1. Introduction

Rail systems for years have presented a great difficulty regarding the constant wear experienced by the wheel-rail interface, which leads to multiple maintenance costs, increased energy consumption and decreased useful time for the components involved due to damage caused to rails and wheels. This causes surface irregularities and can lead to potential accidents or increased energy consumption. (see Figure.1 and 2) [2]. The most important function of lubricants is the reduction of friction and wear, in some cases, the relative movement of two surfaces is only possible if a lubricant is present [3]. Modern lubricants are formulated from a wide range of base fluids and chemical additives. The base fluid has several functions, but it is mainly the lubricant that the fluid layer provides to separate moving surfaces. Also, it removes
heat while minimizing friction. Many of the lubricant’s properties are improved or created by adding special chemical agents to the base fluid. For example, the oxidation and degradation stability in a motor oil is improved by the addition of antioxidants, while the anti-wear properties in extreme pressure (EP) lubricants are given by the addition of special additives. The base fluid acts as the carrier for these additives and, therefore, this fluid must be able to remain in solution in all normal working conditions. [5]

![Figure 1. Rail damaged by high friction in the Medellín metro.](image)

![Figure 2. Friction Damage approximation on a)Rail and b)Wheel.](image)

In search of counteracting this problem, multiple tests have been carried out in previous works with modified lubricants with carbon nanotubes to reduce the wear of the wheel-rail systems, specifically for the Medellín Metro (see Figure.3). [7]

CNTs are an allotropic form of carbon, like diamond or graphite. Its structure can be considered as coming from a graphite sheet rolled on itself [5]. Depending on the degree of winding and the way in which the original sheet is formed, the result can lead to nanotubes of different diameters and internal geometries. Nanotubes shaped as if the corners of a sheet were joined at their ends to form a tube, are called single-walled nanotubes, or SWNTs. There are also nanotubes whose structure resembles that of a series of concentric tubes, included one inside the other and logically of increasing thickness from the center to the periphery [3]. The latter are multi-walled nanotubes or MWNTs. Nanotubes usually have a high ratio length /
radius, since the radius is usually less than a couple of nanometers, however, the length can even be centimeters. [1]

![Figure 3. Metro of Medellín city.][12]  

The stability and robustness of the bonds between carbon atoms, of the sp 2 - sp 3 type, which give it the ability to be the strongest fiber that can be manufactured today. On the other hand, in the face of very intense deformation stresses, CNTs are able to deform noticeably and remain in an elastic regime. Young’s modulus could range from 1.3 to 1.8TPa, although to date it has only been possible to obtain experimentally up to 0.8TPa. Furthermore, these mechanical properties could be improved. In this way, even if a nanotube breaks, since they behave as independent units, the fracture would not propagate to the other neighboring units. [2]

In short, they can function as extremely firm springs under small stresses and, under higher loads, can deform drastically and subsequently return to their original shape. Various studies have tried to measure the mechanical properties and the maximum tension supported by a nanotube, with heterogeneous results, although it could be assumed as a guideline that the maximum tension could be around 150GPa [8]. This data implies that a 1cm thick cable made up of CNTs could support a weight of around 1,500 tons. The potential that they have in the tribology area is related to their mechanical properties. [6]

According to what was mentioned in the previous paragraphs, the use of CNTs has been proposed as lubricant additives for sliding wheel rolling systems and it has been verified through a series of computational modeling based on the physical results obtained by J.A Carlos Cornelio et al, verifying that the carbon nanotubes in the lubricant contribute to the reduction of rail wear by studying their behavior at high pressures. [1]

The physical tests to evaluate this lubricant in real systems imply a risk for the structures, because the behavior of the nanotubes can alter the balance of the system and also the cost that these tests would precede would be very high without first being completely certain of the efficiency of this lubricant in the real system, therefore, simulations have been performed to describe the behavior of nanotubes in a real system, to verify the behavior and mechanical properties in a wheel-rail system. For this reason, this work is carried out to verify and describe the behavior of CNTs subjected to high pressures in a rail-wheel system as lubricating agents. [1]

2. Materials and Methods

The simulation was performed in Matlab which is a multi-paradigm numerical computing environment and a proprietary programming language developed by MathWorks, allowing matrix manipulations, the mapping of functions and data which is of total utility for the situation.
performed. The values and data from the literature were taken into account and the variables that adjust to the real conditions that CNTs may have in lubricants were taken into account. [6]

2.1. Mathematical modeling
The constitutive model to describe the mechanical behavior of the CNTs was through the formulation of the hook law [6]. The equation 1 corresponds to that equation expressed in a general way and is [11]:

$$\sigma_{ij} = (C_{ijkl})\varepsilon_{kl}$$ (1)

Where the left side of the equation represents the Cauchy stress tensor. The first term on the right side represents the constitutive tensor that depends on the mechanical properties of the material and the second one the deformation tensor. Matrix formulation can be described as:

$$\begin{pmatrix}
\sigma_{xx} \\
\sigma_{yy} \\
\sigma_{zz} \\
\sigma_{xy} \\
\sigma_{xz} \\
\sigma_{yz}
\end{pmatrix} = \frac{E}{1+v}\begin{pmatrix}
\frac{1-v}{E} & \frac{v}{E} & 0 \\
\frac{v}{E} & \frac{1-v}{E} & 0 \\
0 & 0 & \frac{1-2v}{E}
\end{pmatrix}\begin{pmatrix}
\varepsilon_{xx} \\
\varepsilon_{yy} \\
\varepsilon_{zz} \\
\varepsilon_{xy} \\
\varepsilon_{xz} \\
\varepsilon_{yz}
\end{pmatrix}$$ (2)

The simulation was carried out in the Matlab program. For this simulation, a constitutive model defined by Hooke’s law was established for the analysis of the materials of the Wheel-Lubricant-Rail system subjected to shear forces to model the conditions of the Medellín metro system. The values corresponding to the rheological properties of the lubricant are taken from the literature where the measurement of these properties had been sought through experimental tests [11].

2.2. Design and loads considerations
The geometry of the rail wheel system was designed based on Figure 2 where the carbon nanotube structures were incorporated and a three-dimensional geometry is obtained as illustrated in Figure 4. The concentration of carbon nanotubes in the system is 0.01 because this is the concentration limit where nanotubes exhibit the highest efficiency as possible lubricating agents. Beyond this concentration, the possible lubrication is not increased and therefore CNTs would be wasting unnecessarily. All this is given by the high surface area that these structures have. Loading conditions generated by the shear forces were established at the borders of the CNTs, due to the close interaction of the wheel-nanostructure-rail. Some roughness of the structures were considered. [2]

The mechanical properties of carbon nanotubes were determined and are presented below at Table 1.

| Property               | Value | Unit  |
|------------------------|-------|-------|
| Density                | 2.6   | g/cm³ |
| Young’s modulus        | 1200  | GPa   |
| Tensile strength       | 150   | GPa   |
| Inside diameter        | 5 - 10| nm    |
| External diameter      | 30 - 40| nm    |
2.3. Numerical model

Mathematical equations were solved using the finite difference numerical technique to analyze the mechanical behavior of CNTs. A computational algorithm was built to develop the system of differential equations using the taylor series (see Equation 3). [3]

\[
U_{i+1,j} + U_{i-1,j} + U_{i,j+1} + U_{i,j-1} = 4U_{i,j} + h_x^2 U''_{i,j} |x| + h_y^2 U''_{i,j} |y
\]

(3)

After truncation lead to an F.D.M model, wich was applied to the hooke law as follows(see Equation 4):

\[
-2 \left( \frac{1}{h_x^2} + \frac{1}{h_y^2} \right) U_{i,j} + \frac{U_{i+1,j}}{h_x^2} + \frac{U_{i-1,j}}{h_x^2} + \frac{U_{i,j+1}}{h_y^2} + \frac{U_{i,j-1}}{h_y^2} = -\frac{p}{k}
\]

(4)

The terms hx and hy are the dimensional steps of the mesh, k is the stiffness of the material and is made up of the cross sectional area and young’s modulus. The equations were implemented using an algorithm made in matlab. Numerical lattices were constructed using rectangular elements and node densities equal to 10,000 to be used in the Matlab program. The numerical lattices obtained can see at Figure.5.
3. Results and discussion

The simulations of the behavior of the material were obtained for two different cases, for the conditions of Figure 6, the response of the lubricant was evaluated with the CNTs oriented, thus being able to see the energy absorption that these present and possible rotation; For the conditions in Figure 7, lubricant values were obtained with the unoriented CNTs with a concentration of 0.01, this also presents energy absorption. [1]

![Figure 6](image1)

**Figure 6.** Results of the mechanical behavior of the oriented carbon nanotubes impregnated in the wheel-rail system. Scale 1.

![Figure 7](image2)

**Figure 7.** Results of the mechanical behavior of the unoriented carbon nanotubes impregnated in the wheel-rail system. Scale 1.
Reduced coefficient of friction and high wear resistance may be related to the formation of a carbon film amorphous transferred by carbon nanotubes [4]. The simulation results support this hypothesis, but further studies on the chemistry of worn surfaces are required to reveal the mechanisms real and improve the tribological properties of the tribo-system. Therefore, it is foreseen that the next step is to evaluate the properties in a system with real conditions. [5]

Based on the results of these simulations, it can be verified that the CNTs are fulfilling the function of absorbing as much energy as possible to make the lubrication properties optimal and the shear effects have the least possible wear on the wheel system -rail [7]. The increase in the lubricating properties of the oil occurs because the CNTs absorb a large amount of energy as evidenced in Figures 6 and 7 [9], causing in some cases the breakdown of the CNTs, which leads to the formation of a film of graphene that avoids contact between surfaces and this film continues to absorb energy just like CNTs. [8]

4. Conclusions
In this study the tribological properties of CNTs used as lubricant additives were investigated with the aid of a computational simulations. The best tribological response of the pair evaluated was obtained when CNTs were orientated.

Simulations show that nanotubes improve energy absorption, which contributes to improving the tribological properties of lubricants. The implemented algorithms provide the possibility of analyzing different material properties and working conditions with geometries in 3 dimensions, approaching the real system with higher resolution. The project is in the structural simulation phase in 3 dimensions.

The possible reduced coefficient of friction and high wear resistance may be related to the formation of a carbon film due to the CNTs damage under high pressures. The aspect of the surfaces supports should be studied to disclose the actual mechanisms of enhancing the tribological properties of the system wheel-rail because of the CNTs by using physical experiments.

The results obtained by means of the computer simulation are of great help for future works and allowed us to predict how the behavior of this lubricant would be in real conditions. This allows for greater clarity when making the same assembly in a real environment, in order to be more certain of the results that can be obtained and to reduce the cost of said experiment and its risk factors.

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