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NUMERICAL MODELING OF THE MECHANICAL CHARACTERISTICS OF POLYPROPYLENE BIO-LOADED BY THREE NATURAL FIBERS WITH THE FINITE ELEMENT METHOD

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Abstract- The goal of this paper characterizing mechanical characteristics of three biocomposites in terms of traction in order to assess their ability to replace materials in automotive applications. The characterized materials are prepared by the identical matrix (polypropylene-elastomer polyolefine polymer (POE), POE-PP [5%; 95%]) reinforced with 3 different bio-loads. The formulations F_1, F_2 and F_3 are strengthened by 30 % biochar, 30 % miscanthus, and a mixture of 15 wt% of biochar and 15 wt% of miscanthus, respectively. The 3 wt% changed anhydride PP (MAPP) was additional to composites to increase connection between the bio-loads and matrix. Numerical results have shown that the three renforts improve the matrix's Young modulus. In comparison to the other two materials, the formulation (F_2) had the best traction properties. Miscanthus improved the matrix's Young modulus to 107.77% and its traction resistance to 10.54%. These traction characteristics are superior to those of commercially available RTP-132UV material. Hybrid bicomposite F_3 also improved matrix Young modulus to 70.35% while maintaining nearly the same traction resistance as the PP/POE. The biocomposite reinforced with biochar (F_1) increased the rigidity of the matric by 34.68% and decreased its resistance by 8%.

Keywords: Biochar, Miscanthus, Numerical Modeling, Finite Element Method.

1. INTRODUCTION

Composite materials are considered essential in a variety of industries, including automotive, aerospace, aviation, marine, and the sporting goods industry, due to their excellent mechanical properties and light weight. Nonetheless, environmental concerns have led to a reduction in the use of materials derived from fossil fuels [1-5]. Furthermore, the movement toward reducing greenhouse gas emissions and regulations imposed to improve the efficiency of fuel utilization necessitate the use of lighter materials with lower carbon footprints [6-9]. As a result, traditional composite materials are being replaced by materials that are more "green" and lighter, such as bio-composites.

Our research on the incorporation of polypropylene (PP) with various plant reinforcements is being conducted in this light. Due to a good balance of rigidity and impact resistance, this thermoplastic (PP) mixed with talc is widely used in the automotive industry [10, 11]. Polypropylenes (PP) are commonly mixed with elastomers to improve impact resistance. The use of these elastomers reduces the rigidity of polypropylene (PP), which explains the incorporation of this thermoplastic by reinforcements such as talc and glass fibers.

The reinforcements used with this thermos-plastic in the automotive industry are made of mineral or petroleum resources. Several studies have been conducted in order to find renewable resource reinforcements that are both lighter and more environmentally friendly than traditional reinforcements. This study aims to characterize the mechanical properties of polypropylene (PP) mixed with 5% polyolefin elastomers (POE) and reinforced using three forms of random distribution plant reinforcements:

- The first formulation (F_1) uses 30 percent biochar derived from miscanthus fiber pyrolysis;
- The second formulation (F_2) uses 30 percent Miscanthus (ms) fibers;
- The third formulation (F_3) uses 15 percent miscanthus and 15 percent biochar. (Das, Sarmah, & Bhattacharyya, 2015) investigated this hybrid bio-composite technology by combining polypropylene with wood fibers and biochar derived from wood waste [12].

The 3 wt% improved anhydride PP (MAPP) is added to composites to increase connection between matrix and bio-loads. We will characterize mechanical traction properties of 3 formulations in order to determine which of the three forms of renfort is capable of replacing the mineral renfort "talc" in automotive applications.

2. MATERIALS AND METHODS

2.1. Modeling Elasticity of Bio-Composite at Random Distribution with Finite Element Method

The three bio-composite materials to be characterized are described in Table 1. All three materials have the same PP/POE matrix, mixed with a MAPP compatibility agent to increase the connection between matrix and bio-loads. The difference between the materials lies in the reinforcements used. The reinforcements are characterized by a lower density than the density of the mineral reinforcement "talc".

The first formulation is reinforced by biochar, which comes from miscanthus pyrolysis process at 625 °C. The second formulation is loaded with natural miscanthus. The third formulation is a hybrid composite reinforced with natural miscanthus fibers and biochars.

Table 1. Composition of the three formulations

Properties	POE (wt%)	PP (wt%)	MAPP (wt%)	Miscanthus (wt%)	Biochar (wt%)
F_1	5	62	3	0	30
F_2	5	62	3	30	0
F_3	5	62	3	15	15

Miscanthus fibers were used in two formulations. Biochars come from miscanthus pyrolysis process. Compatibility agent used is MAPP known under the trade name FUSABOND 613. Its main role is to increase connection between matrix and fibers. The elastomer used in the formulations is polyolefin elastomer (POE) known under the trade name ENGAGE 7487. Its main role is to improve the impact resistance of the composite. Table 2 presents densities of bio-composites components. The calculation results are shown in Table 3.

Table 2. Density of the components of the three biocomposites

Properties	PP (wt%)	Miscanthus (wt%)	Biochar (wt%)
Density in g/cm^3	0.9 [13]	1.41 [14]	1.34 [15]

Table 3. The densities of the materials studied

Properties	F_1	F_2	F_3
Density in g/cm^3	0.997	1.02	1.005

The calculated densities of the three formulations are lower than the density of the material sold RTP 132 UV, which is equal to 1.14 g/cm^3 [16]. For each formulation, five samples were modeled.

A series of parameters, as shown in Figure 1, must be given before the geometry can be generated. Minimum allowable distance between inclusions, minimum volume of a fiber, periodicity of the geometry, program for generating the geometry, etc. are among those factors.

3. RESULTS AND DISCUSSION

The "conformal" mesh, which contains 10-node tetrahedral components, was used in this investigation. The similar mesh has been utilized in previous related research [1]. The 10-node tetrahedral element is shown in Figure 3.

The mesh utilized with a number of nodes of 174176 and 102387 elements, which yielded good results in terms of convergence, is shown in Figure 4.

We will present and analyze the results of the digital tests. Secondly, it includes a comparison between the results of the three formulations and the marketed material (RTP 132 UV), with a view to investigating which of these three formulations is the most potential to replace the marketed material.

The stress-strain curves recorded during the digital tensile tests for the three formulations appear on Figures 5, 6 and 7.

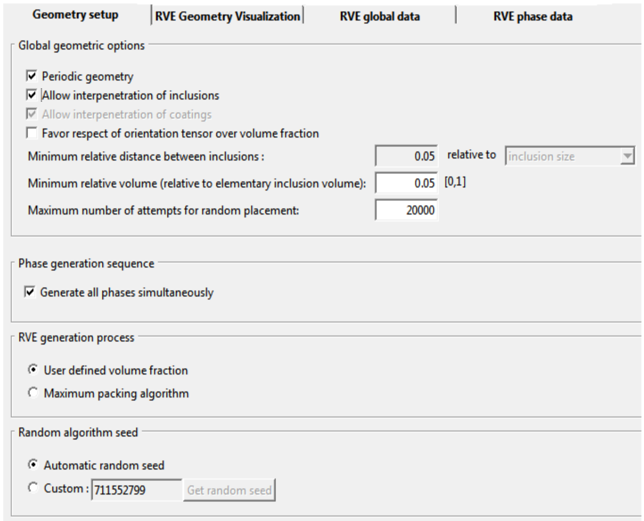

Figure 1. Geometry parameters

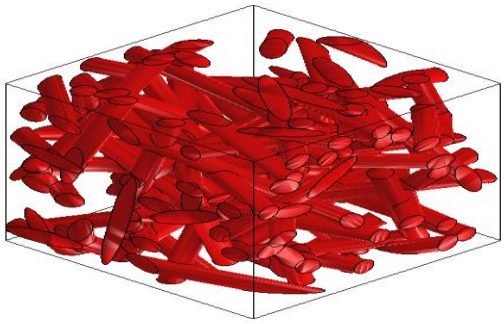

Figure 2. Generated geometry

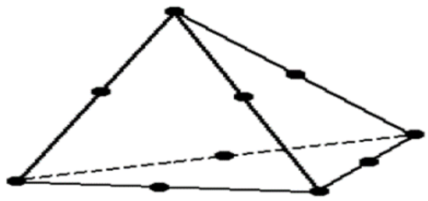

Figure 3. 10-nodes tetrahedral element

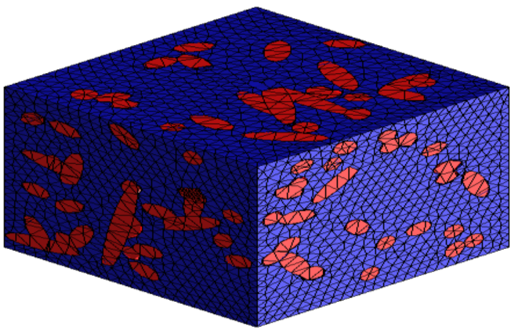

Figure 4. Generated mesh

Table 4. Summary of tensile results

Specimen	F_1: biochar + matrix			F_2: miscanthus + matrix			F_3: biochar + miscanthus + matrix		
	E MPa	σ_m MPa	A (%)	E MPa	σ_m MPa	A (%)	E MPa	σ_m MPa	A (%)
1	2486	31.58	6.73	3891	37.82	2.01	3260	33.99	2.9
2	2421	31.19	6.41	3899	37.04	2.21	3138	34.46	3.7
3	2597	30.94	5.39	3810	36.96	2.32	3145	34.06	3
4	2406	31.14	6.71	3846	37.49	2.71	3101	33.48	2.92
5	2642	30.5	4.58	3918	37.35	1.82	3233	34.13	3.61
Moyenne	2510.4	31.07	5.96	3872.8	37.33	2.21	3175.4	34.02	3.23

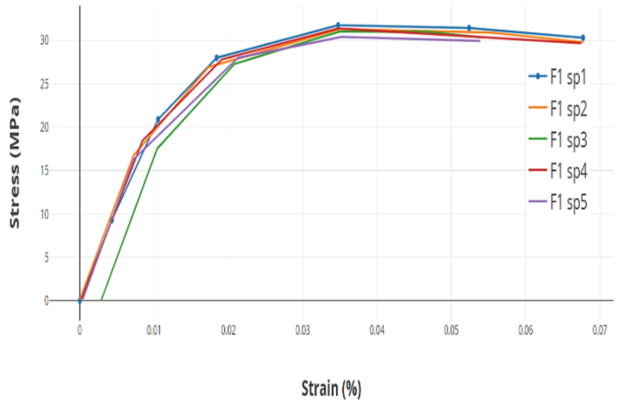

Figure 5. F_1 stress-strain curve

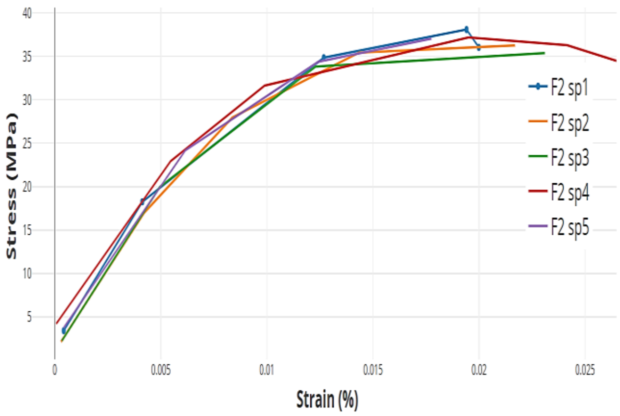

Figure 6. F_2 stress-strain curve

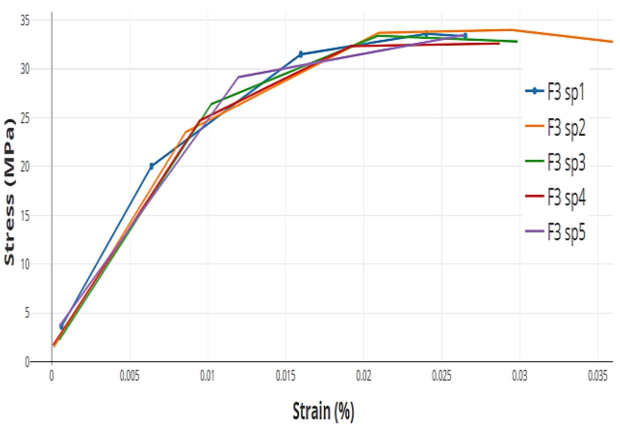

Figure 7. F_3 stress-strain curve

Modulus of elasticity, tensile strength and elongation at break are shown in Table 4. Table 5 illustrates the tensile mechanical properties of the PP/POE mixture (95 wt%, 5 wt%) calculated using double inclusion model.

Table 5. Mechanical characteristics of PP / POE mixture

σ_m (MPa)	Young modulus (MPa)
33.77	1864

3.1. First Formulation

The numerical tensile results show that the addition of biochar to the polypropylene serves to increase the stiffness of the composite, but it decreases the tensile strength somewhat. Indeed, a quantity of 30 wt% of biochar increased the rigidity of (PP/POE) by 34.68%.

The increase in rigidity in the first formulation eliminates the possibility of having the phenomenon of encapsulation of biochars to a great extent, but leaves a possibility of having a partial encapsulation of these fillers. Then from the results found we can conclude that the quantity of MAPP and POE in the composite is suitable to have a better stiffness than that of the matrix. Indeed, if the quantity of POE exceeds a certain threshold, the phenomenon of encapsulation would take place. Therefore, this amount decreases the stiffness of the mixture to values lower than the stiffness of the die.

The decrease in matrix tensile strength after the addition of the biochar can be clarified by poor connection between matrix and biochars.

3.1.1 Interfacial Adhesion

Since biochar particles used in the first formula are considered large in size, one of the problems that can decrease the stiffness of the material is the presence of voids in the structure of the biochar from miscanthus fibers. These voids result from the lumen (void) found in the structure of natural fibers [15]. They can create holes in the structure of the composite. Figure 8 illustrates an example of the lumen present in the structure of biochar.
The decrease in the tensile strength of formulation ($F1$) relative to the tensile strength of PP is noted in the formula reinforced by biochars. Generally, tensile strength depends on connection between matrix and fibers [15]. This shows that the biochar exhibits poor connection with the matrix, and the particles of the biochar are not able to bear the loads.

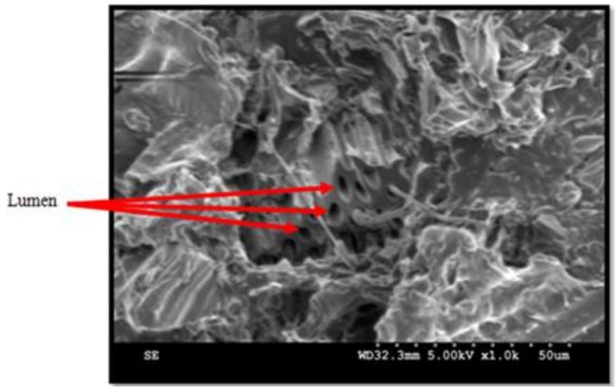

Figure 8. Lumens in the morphology of biochars-SEM [16]

This poor adhesion may be due to:

- The quantity of the MAPP compatibility agent which is not sufficient: In the literature it is known that the MAPP compatibility agent improves the interface between the matrix and the biochars, this has already been proven by several studies in the literature [15-17].
- Particle size: Particle size can also play an important role in improving connection between matrix and fibers. Smaller the size, the more the contact surface increases, which improves the fiber-matrix interface [1]. Behazin et al found that small particle sizes provide a better fiber-matrix interface [15].

3.2. Second Formulation

The numerical results of the tensile test show that the formulation containing hardened polypropylene (by the elastomer) reinforced with miscanthus fibers exhibits the highest E and σ_m compared to those of other formulas. The addition of 30 wt% miscanthus to the matrix serves to increase E of matrix by 107.77%, this may be due to the good dispersion of the fibers. In addition, it increases the strength of the mixture (PP / POE) by 10.54% which gives an impression that the adhesion between the fibers and the matrix is good.

3.3. Third Formulation

The numerical results of the third formula (F_3) (the hybrid composite), are promising. The addition of the reinforcement mixed between biochar and miscanthus increased the stiffness of the material by 70.35% compared to the stiffness of the matrix. It is true that this increase is less than that of the second formulation, but the use of biochar in this matrix helped not only to increase the rigidity, but also to decrease the weight of material. The black color has also been provided which is necessary to increase chances of biochar to replace talc, as a reinforcement of (PP), in automotive applications.

The use of biochar also helps to eliminate the odor given off by miscanthus. In addition, it is expected to be thermally more stable than miscanthus. This prediction comes by analogy with biochar from wood which is thermally more stable than wood fibers (Das et al., 2015). This increase in rigidity may be due to the addition of miscanthus only, because by analogy with biochar from wood, the effect of biochar on polypropylene only appears from a threshold of 24 wt% of biochar [12]. However, reinforcing the polypropylene with biochar and miscanthus at the same time did not help to improve the tensile strength of the matrix too much. Nevertheless, the tensile strength is higher than that of the first formulation which is enhanced by biochar only.

The stability of the tensile strength with respect to the matrix gives the impression that there is good adhesion between the reinforcements and the matrix. On the other hand, microscopic observations show that the adhesion is not perfect. Figure 9 shows pores on the fracture surface of a sample from the third formulation tensile test.

These pores may be due to the problem of tearing the fibers due to the poor adhesion between the matrix and the reinforcements [16]. Figure 10 shows a biochar with poor interfacial adhesion.

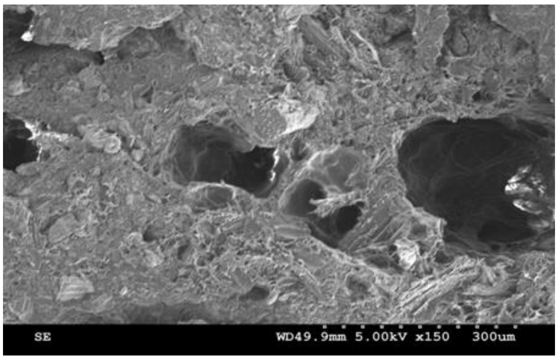

Figure 9. Pores on the fracture surface of an F_3 tensile test sample [16]

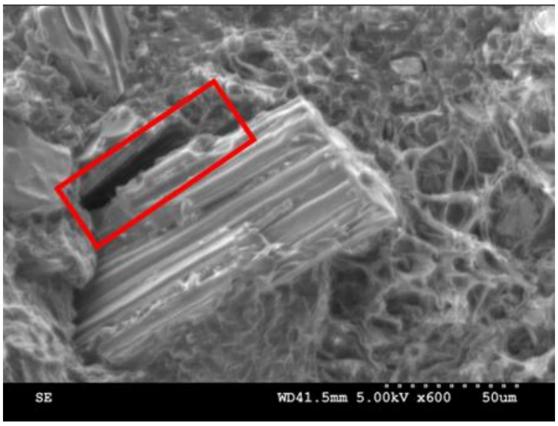

Figure 10. Poor interfacial adhesion [16]

The problem of interfacial adhesion can be solved by adding compatibility agents like MAPP. Although Das et al (2015) used an amount of MAPP in the order of 4 wt% with polypropylene reinforced with 6 wt% of the biochar and 30 wt% of the wood, they found pores on the fracture surfaces of the samples. Indeed, they suspect a formatting problem, which is most likely [12].

Comparison with talc-reinforced polypropylene:

Figure 11 illustrates the results experimentally obtained of the tensile test of 3 formulations, theoretically calculated results of the PP/POE matrix and an example of a commercial material which consists of a PP reinforced with 30 wt% talc. (RTP Company RTP 132 UV).

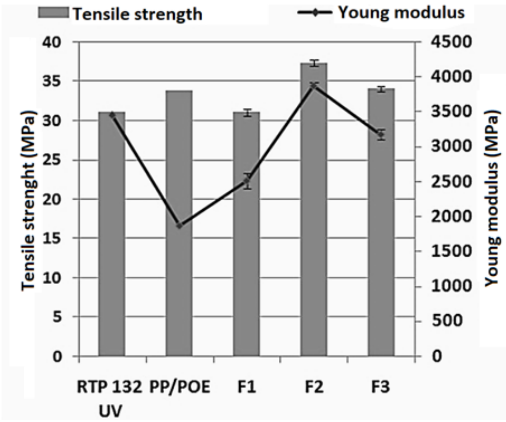

Figure 11. Comparison of tensile properties between the three formulations and RTP 132 UV

The black color is obtained by formulations 1 and 3 as shown in Figure 12 unlike the second formulation which gives us a non-black color.

Figure 12. The three formulations: F_1, F_2 and F_3 [16]

By comparing the mechanical properties in traction of the three formulations with the commercial material, we notice that the second formulation (F_2) containing PP + 30 wt% of miscanthus has tensile properties superior to that of the commercial material. The third formulation (F_3) has a higher tensile strength than that of RTP 132 UV but a lower stiffness of 8% compared to the stiffness of PP + 30 wt% talc [16].

The first formulation (F_1) has a tensile strength similar to that of the commercial material, but a lower rigidity.

4. CONCLUSION

Miscanthus improves matrix stiffness and can achieve values greater than the stiffness provided by mineral reinforcements. The current application of these bio-composites is expected inside automobiles. This application requires meeting two other criteria which are the color black, and the smell.

Unfortunately, the miscanthus reinforced PP does not ensure the black color (Figure 3), moreover it presents an odor which prevents the use of this reinforcement alone with the matrix to replace the PP + talc.

Biochar improves the stiffness of PP only, but not enough to replace talc. Besides, it can maintain higher impact resistance than that maintained by miscanthus. In addition, it ensures the black color and it does not add any odor to the composite. The hybrid composite (F_3) exhibits mechanical properties (rigidity and tensile and flexural strength) inferior to the properties of the second formulation (F_2) and superior to the first formulation (F_1). In addition, it ensures the black color naturally and has no odor despite the presence of miscanthus fibers. So, the hybrid composite is the most promising solution to achieve the targeted mechanical properties.

The following points can be worked on in future work in order to achieve the targeted properties:
• After studying the fracture surfaces of the samples from the various tests, we did not find the phenomenon of agglomeration of the fibers, which means that it is possible to increase the quantity of reinforcements while keeping a lower weight. by the weight of PP + Talc;
• Decrease the size of the biochar: a decrease in the size of the biochar improves the contact surfaces between matrix and bio-loads, that improves tensile strength [15];
• Using natural fibers more rigid than miscanthus such as hemp fibers can improve the stiffness of the composite;
• In order to improve the impact resistance of the composite, an increase in the amount of POE is required. Increasing the amount of POE will decrease the stiffness of the composite. This decrease can be rewarded by increasing the amount of MAPP. This prevents the phenomenon of encapsulation which decreases the rigidity and improves the interfacial connection between matrix and bio-loads. Thus, the mechanical properties of the composite increase. Therefore, a study on the optimal quantity between POE and MAPP must be carried out to ensure a good compromise between rigidity and impact resistance.

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BIOGRAPHIES

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Khalifa Mansouri was born in Azilal, Morocco in 1968. He is now a teacher of computer science and researcher at ENSET Institute, University of Hassan II Casablanca, Morocco. He received Diploma of ENSET Mohammedia, Morocco in 1991, CEA in 1992 and Ph.D. (Calculation and optimization of structures) in 1994 from Mohammed V University of Rabat, Morocco, HDR in 2010 and Ph.D. (Computer Science) in 2016 to Hassan II University of Casablanca, Morocco. His research is focused on real time systems, information systems, e-learning systems, industrial systems (modeling, optimization, and numerical computing).