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Numerical Modeling of the Thermo Mechanical Behavior of a Polymer Reinforced by Horn Fibers

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ABSTRACT

The use of bio-loads in the field of composites has become an essential concern for researchers, as opposed to mineral and classical loads that have dangerous effects on the environment. In this work, a tensile test on a virgin material of animal origin was carried out numerically by the finite element method which was able to confirm the experimental tests. The curves from this simulation mainly considered virgin material in a direction parallel to the fiber direction. The results of the numerical modeling have clearly illustrated that the virgin material has a significant Young modulus in the direction parallel to the fiber, which reinforces the assumptions of the anisotropy of the material of animal origin studied and the high rigidity at the direction of the fibers thanks to the keratin that confers this behavior. This bio load has been mixed with polypropylene for different percentages in order to promote the evolution of its thermo mechanical properties. Numerical modeling by the finite elements characterized the studied bio-composite which can find applications in the fields of the automotive, computers, construction and household articles etc.

Key words: Bio composites, Durability, Material modeling, Natural fibers, Recycling.

1. INTRODUCTION

In recent years, the bio-loading of materials has become a major concern for many researchers. Largely neglected by the material actors, our bio-load in question has several advantages such as the integration of the concepts of environment, sustainable development and economy, which pushed the studies of composite materials to widen the field of research in that Sens. The bio-load used is the horn consisting of several keratins: "proteins rich in sulfur, forming fibers. Keratin is present on the surface of the skin in the form of horn or scales. It is also found in hair, wool, feathers, bristles, hooves, claws, horns, nails, bird's beaks, whalebone whales, turtle shells and silk and cobwebs also contain keratin "[1].

This work presents a numerical study based on the finite element method that aims to evaluate tensile tests on a virgin material of animal origin in a direction parallel to the fiber direction [2]. This bio load will be mixed with polypropylene for different percentages to promote the evolution of its thermo mechanical properties. Reinforcement of this thermoplastic is an effective approach to improve its structural, thermal and mechanical properties. PP is widely used as a convenience polymer, but its applications are limited by some constraints that are related to its relatively low properties. It is very interesting to improve the properties of this thermoplastic by the addition of reinforcements, in order to widen its fields of application by taking advantage of its availability in the world market as a virgin polymer.

The bio-composite studied can be modeled numerically and can find applications in the fields of the automotive, computers, construction, household goods, etc. [3]–[5]For this purpose, the finite element method, as opposed to other numerical methods, is the most widely used method and can solve many problems in several applications [6]. It is very robust by combining the largest number of applications and transforming the boundary problem into a variational problem [6]. This method also offers a great ability to deal with non-linear problems as well as complex laws. It is able to give a better approximation of the physical domain by solving several problems in various applications. The resolution is done by dividing the problem into a set of domains (mesh) and then approaching the behavior of the material.

2. MATERIALS AND METHODS

2.1 Materials

The bio load used is the horn. It is therefore a source of animal origin containing keratin which is a protein with an ability to protect the animal against its natural surroundings. As well as a better resistance to chemical actions [7].The keratin used is durable. Organic waste containing this protein can be used as a bio load with no harmful effects [8]. The polymer matrix used in this study is polypropylene. It is a semi crystalline of the class of polyofines. The choice of this polymer is based on its availability, its low cost, its relatively low implementation temperature and its extensive industrial use.

2.2 Methods

2.2.1 Experimental evaluation of virgin material

Figure 1 shows the cutting of the specimens in order to undergo the tensile stress with a parallel cutting in the direction of the fibers (0°) [2]. The air and temperature conditions (≈ 20 ± 2 °C) in Zwick-Roell type machine with a load cell of ± 2.5N. Figure 2 shows the tensile curves obtained by the experimental tests at 0 °.

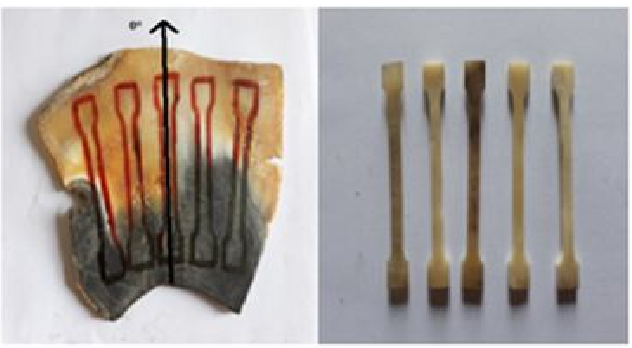

Figure 1: Cutting specimens parallel to the fibers [2]

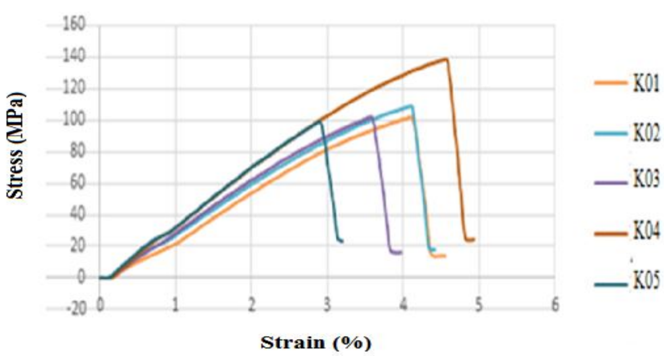

Figure 2: Tensile curves at 0 ° [2]

2.2.2 Numerical modeling of virgin material

Numerical simulation has become an important tool for virtually understanding the behavior of materials. The important thing is that it must be realistic given the complexity of the real environment (nonlinearities, multi physics ...).In order to study the anisotropy of the bio load used and to confirm the results of the experimental tests [2], the present simulation will be focused to the orientation at 0 ° of the direction of the fibers.

The method used is finite elements offering several advantages such as its great ability to deal with nonlinear problems as well as complex laws. It is able to give a better approximation of the physical domain by solving several problems in various applications [9]–[12]. The resolution is done by dividing the problem into a set of domains (mesh) and then approaching the behavior of the material.

A. Geometry

Figure 3 shows the 2D profile and the dimensions of the specimen.

Figure 3: Geometry of the specimen.

B. Mechanical properties

The elastic properties of the virgin material are defined using the experimental data represented and assigned to the geometry presented in figure 3.

C. Incrementation

The direct method for the equation solver and the full Newton method for the technical solution were used. as well as a maximum number of increments of 100. We took a simulation time of 1 ms with a time scale factor for the automatic incrementation of 1. These two parameters play an important role in solving the simulation so as not to have too much elemental distortion and that the calculation can succeed.

D. Boundary conditions and loading

Figure 4 shows the boundary conditions and loading of our model.

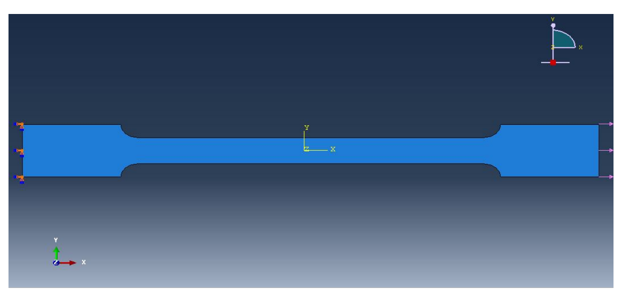

Figure 4: Boundary conditions and loading.

E. Mesh

The mesh used is of the type CPS3 "3 linear nodes" and CPS4R "4 bilinear nodes". Figure 5 shows the mesh obtained. The number of nodes is 835 and of elements is 746, as well as 1670 for the total number of variables in the model.

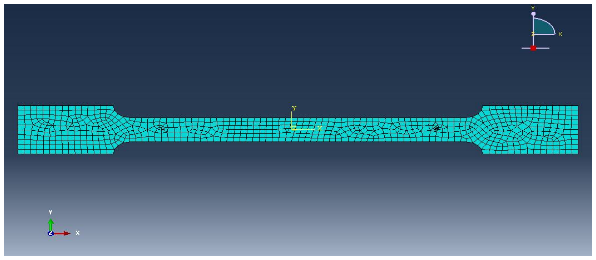

Figure 5: Mesh of the specimen

2.2.3 Modeling polypropylene reinforced with horn fibers

To study the behavior of polypropylene reinforced by horn fibers, several homogenization methods can solve this problem such as asymptotic theory, mathematical theory of homogenization, mean field homogenization, neural network and finite element analysis [13]–[16].. This last method will be chosen for our study because of its efficiency in predicting the thermo mechanical behavior of composites.

The finite element method is used on the Representative Volume Element level to obtain the behavior of the bio composite. It is able to compute the thermo mechanical performances. The model will be built and run to compute the homogenized values. Figure 6 shows the stress-strain curve of the PP without reinforcement and the table 1 shows the horn fibers characteristics.

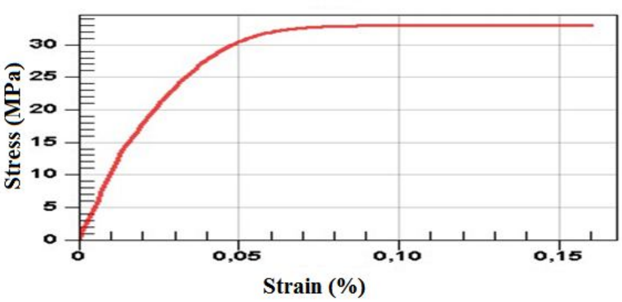

Figure 6: Stress-strain curve of the Polypropylene

Table 1: Characteristics of the horn fibers

Dimensions	Values
Shape	Cylinder
Percentage	15%
Aspect ratio	18
Orientation	Random
Minimum of fibers	30

A. Position

Figure 7 shows the positions according to the different planes.

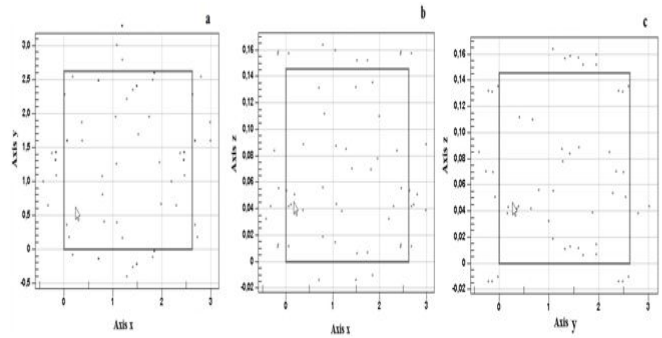

Figure 7: The position in (a) x-y plane,(b) x-z plane, (c) y-z plane

Table 2 shows the statistical values of the position according to the different axes.

Table 2: Horn fibers position in the different axis

Statistical parameters	Mean	Standard deviation	Min	Max
x	1.29	0.968	-0.422	2.99
y	1.29	0.908	-0.405	3.01
z	0.067	0.0536	-0.0141	0.164

B. Nearest neighbor distance

Figure 8 shows the nearest neighbor distance distribution.

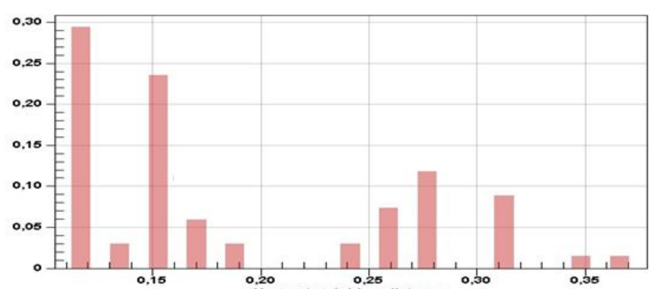

Figure 8: Nearest neighbor distance (between fiber's centers)

Table 3 shows the statistical values of the nearest neighbor distance distribution

Table 3: Statistical values of the nearest neighbor distance distribution.

Statistical parameters	Mean	Standard deviation	Min	Max
Value	0.19	0.079	0.108	0.375

C. Fiber volume distribution

Figure 9 shows the fiber volume distribution.

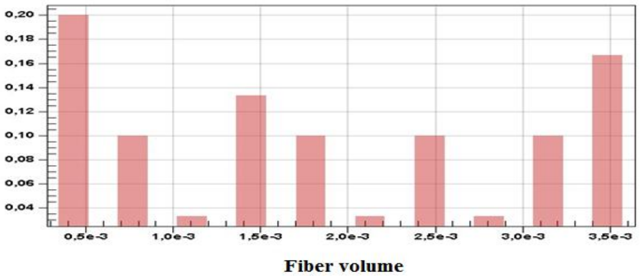

Figure 9: Fiber volume distribution

Table 4 shows the statistical values of the Inclusion volume distribution.

Table 4: Statistical values of the Inclusion volume distribution

Statistical parameters	Mean	Standard deviation	Min	Max
Value	0.0008	0.0013	0.0003	0.0037

Figure 10 shows the fiber distribution with a random orientation and a number of inclusions and an effective volume fraction of 0.109617.

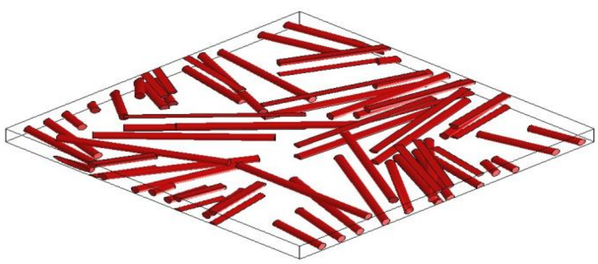

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Figure 10: Distribution of fibers in geometry

D. Incrementation

We used the Casi iterative method for the equation solver with a tolerance of 1 E-8 and the parameters listed in the table 5.

Table 5: Incrementation parameters

	Final time	Maximum time	Minimum time	Initial time
Values	1	0.1	0.01	0.1

E. Mesh

Table 6 shows the parameters of elements and nodes and figure 11 shows the mesh obtained.

Table 6: Mesh parameters

	Element size	Min element size	Elements number	Nodes number
Values	0.032	0.006	199550	329645

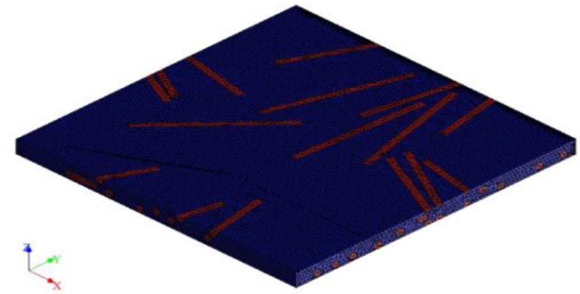

Figure 11: Mesh of the bio composite

Table 7 shows the information for each phase.

Table 7: Number of elements and effective volume fraction in each phase

	Number of elements	Effective volume fraction (on mesh)	Effective volume fraction (on geometry)
Polypropylene	172878	0.891149	0.890397
Horn fibers	26672	0.108851	0.109616

3. RESULTS

3.1 Constitutive law of virgin bio load

Figure 12 shows the results of the tensile tests using finite element numerical modeling on several specimens.

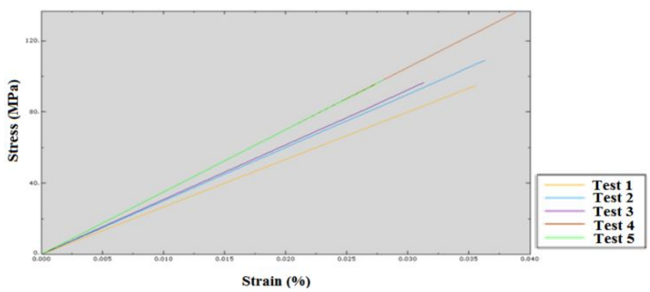

Figure 12: Stress-strain curves at 0 ° of fiber direction

Table 8 shows the mechanical properties obtained using numerical modeling.

Table 8: Parameters obtained using 0° numerical modeling

Specimen	Stress at break (MPa)	% elongation at break	Young modulus (MPa)
1	95	3.57	2666
2	109	3.63	3000
3	96.5	3.14	3076
4	136	3.89	3500
5	98.1	2.8	3500
Mean	106.92	3.41	3148.4

Figure 13 shows the tensile curve obtained numerically for the average behavior of the bio material.

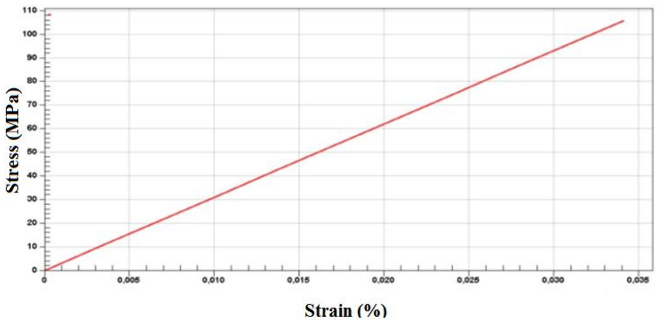

Figure 13: Stress-strain curves at 0 ° of fiber direction

The analysis and interpretation of the results show us that numerical modeling confirms the results obtained experimentally.

- The tensile stress at break is very high;
- The displacement is relatively low and the modulus of elasticity is important characterizing the rigidity of the material;
- The observed behavior is anisotropic since it depends on the orientation of the fibers.

The numerical results confirm the results of the tensile test performed in a direction parallel to the fiber direction of the bio load (0°) .This last one has a high proportion of keratin which forms the fibers [17], [18]. This keratin gives a qualitative hardness to the bio-load in the direction parallel to the fibers.

3.2 Horn fibers reinforced Polypropylene

3.2.1 Mesh quality indicator

The study of the quality of the mesh is important for the analysis of the stability and the convergence of the numerical study. The quality of the mesh may not cause problems of execution time but insufficient quality will minimize the accuracy and efficiency of the solution. Two mesh quality indicators are studied: gamma and rho. The first one is computed as the ratio between the diameter of the inscribed sphere and the diameter of the circumscribed sphere. It is scaled to be equal to 1.

The rho mesh quality indicator is the ratio between the shortest and the longest edge of the element. It is thus also always between 0 and 1. For each indicator, minimum, maximum and mean values are provided as well as an histogram showing the distribution of the full mesh as shown in figures 14 and 15 and table 9.

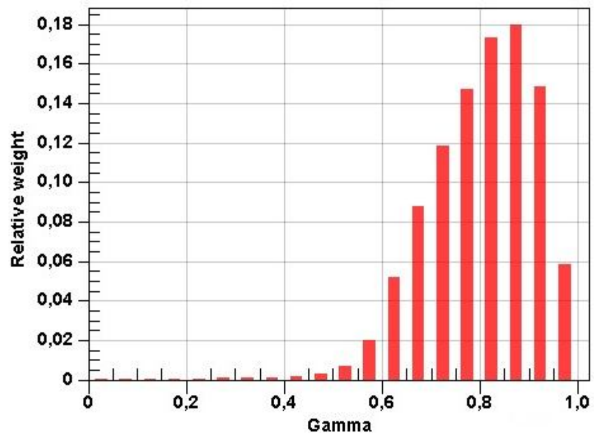

Figure 14: Gamma mesh quality indicator

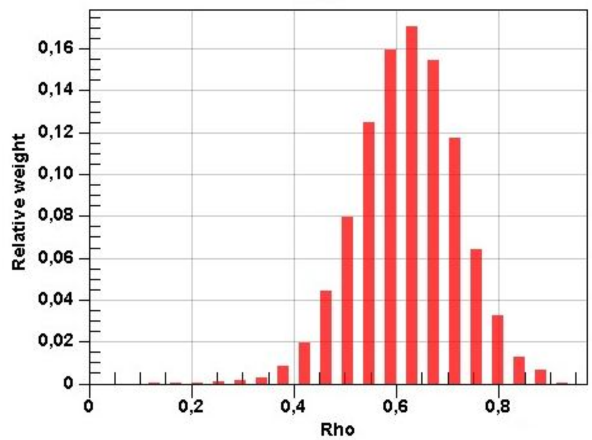

Figure 15: Rho mesh quality indicator

Table 9: Minimum, maximum and mean values for each indicator

Values	Gamma	Rho
Minimum value	0.0025	0.1066
Maximum value	0.9975	0.9452
Mean value	0.8024	0.6226

The analysis of the results shows us that the average values of the two mesh quality indicators are far from zero, which confirms the good quality of our mesh and the good convergence obtained during the numerical computation.

Figure 16 shows the curves of PP reinforced by horn fibers for different percentages.

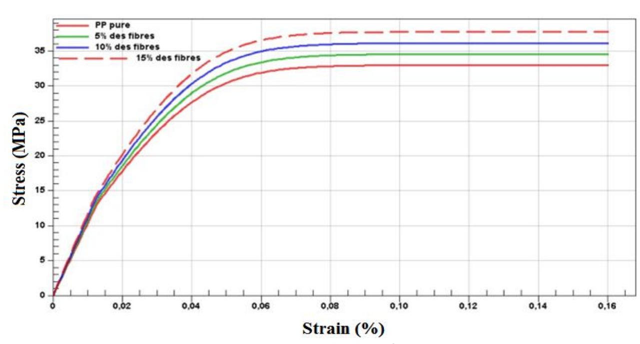

Figure 16: Stress-strain curves of the bio composite

Table 10 shows the elastic properties obtained for different percentages of fibers. The Young's modulus of the bio composites increases by adding the percentage of fibers to the pure PP from 1034 to 1171 MPa for 15% of mixture. The stress at the break increases slightly from 32.7 MPa for pure PP to 37.5 for the same percentage of mixing.

Table 10: Elastic properties for different percentages of fibers

Percentage of fibers	Stress at break (MPa)	Young modulus (MPa)
0%	32.7	1034
5%	34.5	1077
10%	36	1122.6
15%	37.5	1171

3.2.2 Criterion of Von Mises and displacement

In the case of uniaxial tensile test, the Von Mises criterion is written as follows: $\sigma eq = \sigma 11$ (1)
Figure 17 shows the values of the Von Mises stresses obtained during the tensile test and the figure 18 shows the displacement obtained numerically. A reading of these constraints shows us that they are greater than the elastic limit (15 MPa) which confirms that the deformations are made plastically.

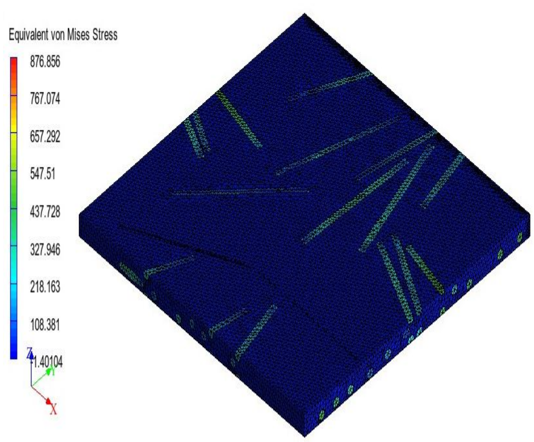

Figure 17: Equivalent Von Mises Stress

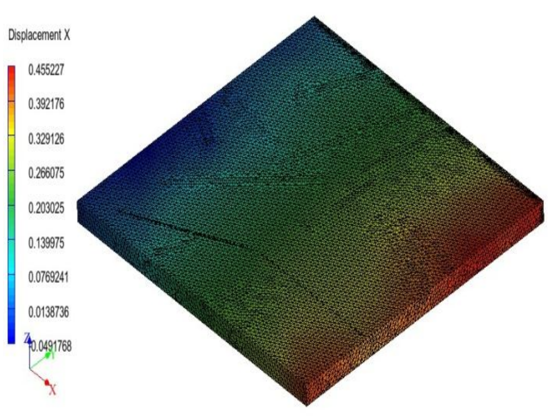

Figure 18: Displacement of the bio composite

3.2.3 Thermal analysis

The total deformation is given by the following relation:

$$\epsilon=\epsilon^{e}+\epsilon^{P}+\epsilon^{th} \quad (2)$$

$$\dot{\epsilon}^{p} = \dot{p}\frac{\partial f}{\partial \sigma}\,;\ \epsilon^{e}=\sigma_{11} \quad (3)$$

$$\epsilon^{th}(T)=\{\alpha(T)[T-T_{ref}]-\alpha(T_{ini})[T_{ini}-T_{ref}]\} \quad (4)$$

$\dot{p}$: a hardening parameter ; $\alpha(T)$: thermal expansion coefficient ($5.18*10^{-3}$ K^{-1} for the horn fibers and 10^{-4} K^{-1} for the PP) The temperature of the bio reinforcement is 130°C. The matrix of the thermal expansion obtained at 15% of the horn fibers is given by:

$$\alpha = \begin{bmatrix} 14.21^{-5} & 0 & 0 \\ 0 & 14.751^{-5} & 0 \\ 0 & 0 & 14.751^{-5} \end{bmatrix} \quad (5)$$

3.2.4 Thermal conductivity: Fourier model

The first law of thermodynamics states that in a closed system, energy is conserved in time. This statement translates into the following equation

$$p c \frac{dT}{dt} = -div(q) + r \quad (6)$$

With, p, c, T, t, q et r respectively density, specific heat, temperature, time, heat flow and volume heat input. The thermal flow according to Fourier's law is:

$$q=-K^{th} grad\,(T) \quad (7)$$

With K^{th} is the matrix of thermal conductivity:

$$K^{th} = \begin{bmatrix} K_1 & 0 & 0 \\ 0 & K_2 & 0 \\ 0 & 0 & K_3 \end{bmatrix} \quad (8)$$

Table 11 shows the resistivity and conductivity tensor matrices and the heat capacity obtained for different percentages of the horn fibers..

Table 11: Thermal properties of the composite for different percentages of horn fibers

% of fibers	Resistivity tensor (K/W)	Conductivity of fibers (W/m.K)	Thermal capacity (J/kg.K)
5 %	$\begin{bmatrix} 6.37 & 0 & 0 \\ 0 & 6.83 & 0 \\ 0 & 0 & 6.83 \end{bmatrix}$	$\begin{bmatrix} 0.16 & 0 & 0 \\ 0 & 0.15 & 0 \\ 0 & 0 & 0.15 \end{bmatrix}$	1881.5
10 %	$\begin{bmatrix} 5.74 & 0 & 0 \\ 0 & 6.52 & 0 \\ 0 & 0 & 6.52 \end{bmatrix}$	$\begin{bmatrix} 0.17 & 0 & 0 \\ 0 & 0.15 & 0 \\ 0 & 0 & 0.15 \end{bmatrix}$	1863
15 %	$\begin{bmatrix} 5.19 & 0 & 0 \\ 0 & 6.21 & 0 \\ 0 & 0 & 6.21 \end{bmatrix}$	$\begin{bmatrix} 0.19 & 0 & 0 \\ 0 & 0.16 & 0 \\ 0 & 0 & 0.16 \end{bmatrix}$	1844.5

According to the table above, we have high thermal capacities and resistivity's at 5% of the fibers and we note a decrease in these two quantities as the percentage of fibers increases. For thermal conductivity, increasing the percentage of fibers increases this conductivity by up to 15%. Figure 19 shows the increase in thermal flux with increasing percentage of fibers.

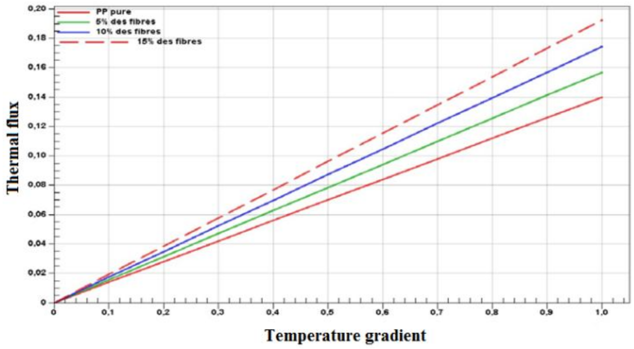

Figure 19: Thermal flux for different percentages of fibers

5. CONCLUSION

A tensile test on a bio material was carried out numerically by the finite element method which was used in the microscopic level to obtain an approximation of the thermo mechanical behavior of the bio composite studied by the direct investigation of Representative Volume Elements (RVEs). It was able to predict the elasto plastic behavior of horn fibers reinforced polypropylene by dividing the problem into a set of domains (mesh) and then approaching the behavior of the material.

This method helped us to define the elasto plastic properties as well as in terms of thermal behavior of the studied bio composite. The Young's modulus of bio composites increases by adding the content of the horn fibers from1034 for the pure PP to 1171 MPa for 15% of mixture. The stress at break increases slightly from 32.7 MPa for pure PP to 37.5 for the same content of mixing.

Using Fourier's law, it was possible to determine the thermal flux of the bio composite (the thermal capacity, the tensors of resistivity and conductivity).

The values of the Von Mises stresses obtained during the tensile test showed us that they are greater than the elastic limit (15MPa) which confirms that the deformations are made plastically. We can also notice, through the different results of recorded elastic behaviors, that the bio composite has a great stress at break and an important Young modulus due to the keratin fibers offering several advantages thanks to their biodegradability, biocompatibility and sustainable development.

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