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THE RELATIONSHIP BETWEEN MECHANICAL AND PHYSICOCHEMICAL PROPERTIES OF PLANT FIBERS: A STATISTICAL APPROACH

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ABSTRACT

In this work, a statistical study involving, namely, the mechanical properties, physical and chemical content has been conducted on a set of natural fibres. The relationship between these factors has been studied. The Pearson correlation method has been applied to investigate the sensitivity of the chemical content and physical parameters on the mechanical properties of these natural fibres. For this aim, a selected data set, collected from the literature, has been used. It was demonstrated that the mechanical properties are highly sensitive to chemical content and physical parameters more precisely to the MFA which is the key parameters of this study. At the end, statistical models to predict mechanical properties are presented.

INTRODUCTION

Natural fibers are extracted from three sources: animal, plant and mineral. The most suitable and economic fibers for the production of biocompsosite are plant-based fibers (Verma et al. 2016). There are approximately 2000 species of plants used as a source of natural fibers, but only few of these are commercially prominent and constitute around 90% of natural fibers used in the world.

It was demonstrated in the literature that plant fibers have the same morphology and chemical constituent (Pickering, Efendy, and Le 2016; Mochane et al. 2019) .Elsewhere, many works dealt with the physicochemical characterization of natural fibers (Sarikanat et al. 2014; Fiore, Valenza, and Di Bella 2011; Sarikanat et al. 2014).

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Plant based natural fibres are well designed composite in nature and are composed of cellulose, hemicelluloses, lignin, pectin and waxy substances. Cellulose is considered the major framework component of the fibre structure. It provides strength, stiffness and structural stability of the fibre(Kabir 2012). The chemical structure of cellulose consists of three hydroxyl groups (OH). Two of them form hydrogen bonds within the cellulose macromolecules (intramolecular) whilst the rest of the group forms hydrogen bond with other cellulose molecules (intermolecular) (Mathew, Joseph, and Joseph 2007). Hemicellulose occurs mainly in the primary cell wall and has branched polymers containing five and six carbon sugars of varied chemical structures. Lignin is amorphous and has an aromatic structure(Biagiotti, Puglia, and Kenny 2004). Pectin comprises of complex polysaccharides. Their side chains are cross-linked with the calcium ions and arabinose sugars. Additionally, small amounts of organic (extractives) and inorganic (ash) components are present in the fibre structure. Each fibre cell wall consists of primary and secondary layers of cellulose microfibrils. The angle between the fibre axis and cellulose microfibrils constitute the Micro-Fibrillar Angle (MFA). The fibre structure develops in the primary cell wall and is deposited during its growth. The secondary wall consists of three layers and each layer has a long chain of helical cellulose microfibrils(Biagiotti, Puglia, and Kenny 2004). The cellulose content increases steadily from primary to secondary layers and the hemicelluloses amount are similar in each layer. However, lignin content decreases in this sequence. Hemicellulose molecules are hydrogen bonded with cellulose fibrils and they form cementing materials for the fibre structure. Lignin and pectin are coupled with the cellulose– hemicellulose network and provides an adhesive quality to hold the molecules together. Secondary thick layer (s2) determines the mechanical properties of the fibre.

The aim of this work is to provide a measurable relationship between mechanical properties and chemical content and physical properties of Plant fibres.

METHOD

Data of chemical content physical and mechanical properties of 20 fibres were collected from previous study (Tahir et al., n.d.; Kamel 2007; Rakesh et al. 2020; Komuraiah, Kumar, and Prasad 2014).The values of the considered quantities are scattered in interval. For the analysis, the mean value is used.

In the first step, mechanical properties such as -Tensile strength – Young Modulus – Failure Strain- are considered as Variable 2. The chemical content such as – Cellulose (%) – Hemicellulose (%) – Pectin (%) – Lignin (%) – Waxes (%) – and physical properties such as – Density – Micro Fibril Angle (MFA°)-Diameter (µm) – are considered as

Variable 1.

The Pearson Ranks obtained were classified using PARETO technique to determine the most effective variable1. This variables constitute the group A.

In the second step, the interdependency of variable in group A were analyzed using Pearson correlation.

After selecting the independent variables for regression, a statistical model for Tensile Strength, Young Modulus and Failure Strain were elaborated.

The (figure 1) summarized the methodology followed in this present work.

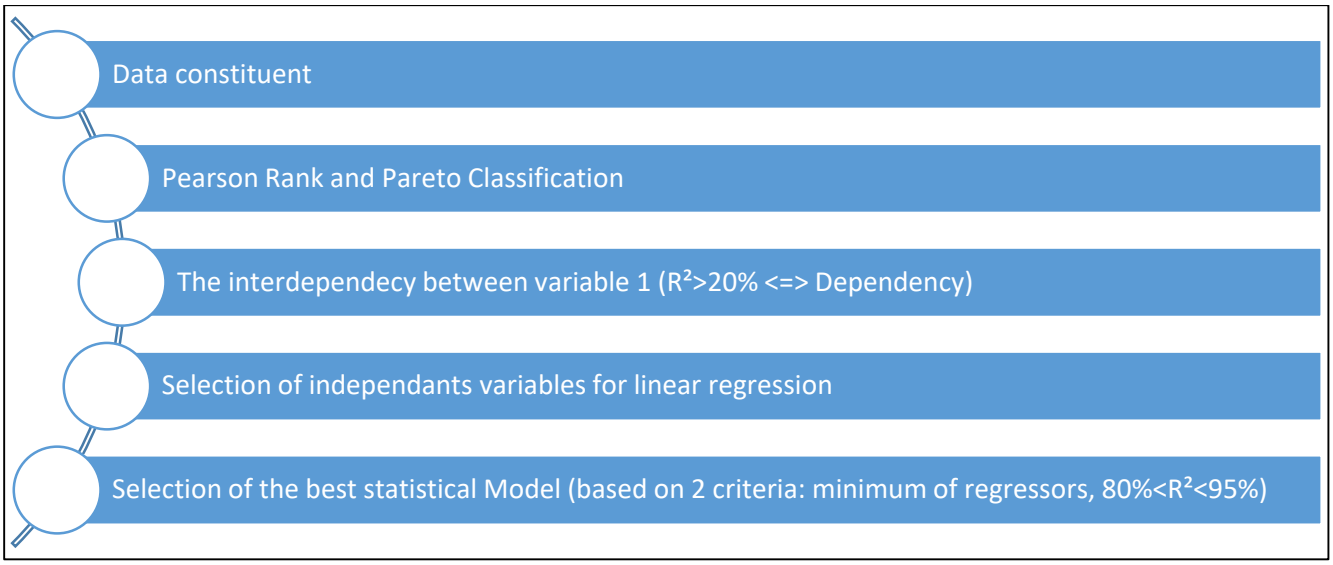

Figure 1: Steps of the Method

RESULTS AND DISCUSSION

The (Table1) shows the results of Pearson Rank and Pareto classification of variables 1. The (Table 2) present the interdependency between them.

Table 1: Pearson Rank and Pareto classification

Variable 2	*Variable 1*	*Pearson Correlation*	*R^2 (%)*	*Ranking*
Tensile Strength	**MFA, (deg)**	-0,621	38,6%	1
	Cellulose (%)	0,596	35,5%	2
	Lignin (%)	-0,555	30,8%	3
	Diameter, µm	0,541	29,3%	4
	Density (Kg/m3)	0,462	21,3%	5
	Waxes (%)	-0,144	2,1%	Excluded
	Hemicelluloses (%)	-0,114	1,3%	Excluded
	Pectin (%)	-0,065	0,4%	Excluded
Young Modulus	**MFA, (deg)**	-0,745	55,5%	1
	Diameter, µm	0,492	24,2%	2
	Cellulose (%)	0,487	23,7%	3
	Lignin (%)	-0,418	17,5%	4
	Waxes (%)	0,417	17,4%	5
	Pectin (%)	-0,411	16,9%	Excluded
	Density (Kg/m3)	0,407	16,6%	Excluded
	Hemicelluloses (%)	0,129	1,7%	Excluded
Failure Strain	**MFA, (deg)**	0,943	88,9%	1
	Lignin (%)	0,626	39,2%	2
	Waxes (%)	-0,457	20,9%	3
	Hemicelluloses (%)	-0,423	17,9%	4
	Diameter, µm	-0,322	10,4%	Excluded
	Pectin (%)	0,318	10,1%	Excluded
	Cellulose (%)	-0,181	3,3%	Excluded
	Density (Kg/m3)	0,011	0,0%	Excluded

Table 2: Relationship between variables of the group A

	Pearson Correlation	***R² (%)***
Hemicelluloses (%) – MFA(°)	-0,94	88%
Lignin (%) – MFA(°)	0,82	67%
Cellulose (%) – MFA(°)	-0,487	24%
Diameter – MFA(°)	-0,288	8%
Waxes (%) – MFA(°)	-0,278	8%
Waxes (%) – Diameter (µm**)**	0,176	3%
Lignin (%) – Diameter (µm**)**	-0,153	2%
Cellulose (%) - Diameter (µm**)**	0,098	1%
Hemicelluloses (%) - Diameter (µm**)**	0,074	1%
Pectin (%) - Diameter (µm**)**	0,03	0%

- ***Results interpretations***

From the results it's has been observed that the MFA (°) is the parameter that highly correlated to mechanical properties.

It's well known in literature that an increase in MFA° induces a decrease in Young Modulus and Tensile strength (Pickering, Efendy, and Le 2016; Djafari Petroudy 2017; Benin et al. 2020; Baillie 2004).

In order to understand and measure the importance of this parameter in predicting the stiffness of NFs, Baley et al.(Baley 2013), suggest to compare two fibers with the same cellulose content or more precisely with the same crystalline volume content. Kulkarni et al.(Kulkarni et al. 1983), have conducted experimental analysis on banana fiber (***MUSA SEPIENTUM).*** Their experimental results show that fibers with an MFA° of 11° have greater Young Modulus compared to fibers with an MFA° of 12°. They have furthermore demonstrated that using the Rule of Mixture (ROM) Eq (1), taking into consideration the mass of crystalline and non-crystalline materials, give a good prediction of the Young Modulus

$$\boldsymbol{E_f = W_c E_c cos^2(MFA°) + W_{nc} E_{nc}} \quad (1)$$

Where E_f is the fiber Young Modulus, W_c, W_{nc} are respectively the mass fraction of crystalline and non-crystalline material. E_c and E_{nc} are the young modulus of crystalline and non-crystalline region and assumed to be 45 GPa and 3 GPa according to Mc Laughlin et al.("Fracture Mechanism of Plant Fibres,"1980).

On the other hand, to estimate the Microfibrilar angle of Hemp from the fiber's young modulus, Mwaikambo et al. (Mwaikambo and Ansell 2006) have used the ROM Eq(1) .The calculated value (6,8°) is close to the experimental one (6.2°).

The work of Kulkarni et al (Kulkarni et al. 1983), and Mwaikambo et al. (Mwaikambo and Ansell 2006) described above, confirm the relationship between the MFA° and Young Modulus for two different fiber plants species with large scattered young Modulus in a controlled experimental environment.

It's important to point out that the MFA° is measured from the stress-strain curve using the formula below Eq (2). This explain the high correlation between the failure strain and the MFA(°)

$$\boldsymbol{\varepsilon = \ln\left(1 + \frac{L_f - L_0}{L_0}\right) = -\ln(\cos(MFA°))} \quad (2)$$

The relative weak apparent relationship between the MFA° and the tensile strength can be explained by the fact that the latter is highly sensitive to structural defects (Bledzki 1999).

A positive correlation between cellulose tensile strength and young modulus and a negative correlation with MFA° has been observed. This confirms the structural role of the cellulose in plant fibers and that fibers with greater cellulose content are more rigid (Sakurada et al. 1962).

A negative correlation between the MFA° and hemicellulose has been recorded. The same observation has been reported by Komuraiah et al. (Komuraiah, Kumar, and Prasad 2014). Elsewhere, Hemicellulose is cementing the cellulose microfibrills(Osorio et al. 2011). In fact, removing Hemicellulose leaves a less rigid inter fibrillar region allowing the micofibrill to rearrange and stretch (Osorio et al. 2011). Therefore, the MFA° increases with decreasing the hemicellulose content.

The decrease in lignin and pectin contents increases the tensile strength and young modulus, this makes the fiber stiffer. The lignin and pectin act as a binder in the plant and contribute to the fiber stability (Walter 2012).

Even if the diameter show great correlation with tensile strength and Young Modulus, this parameter is not reliable. In fact the techniques used to determine the diameter of the natural fibers assumed that the fiber have a circular shape (Monteiro et al. 2011), other works state that the Cross Section Area (CSA) of natural fibers is not circular(Virk, Hall, and Summerscales 2012; “Djafari Petroudy - 2017 - Physical and Mechanical Properties of Natural Fibe.Pdf,”). The CSA calculated with this assumption gives inaccurate results. Using a digital microscopy and image analysis, Almeida et al. (Almeida, Mauricio, and Paciornik 2012) measured the fiber sections and compared them to the calculated sections using geometrical section formula based on diameter. The results show the variation between the measured and calculated sections can reach 400%. The estimation of the CSA with the diameter exaggerates the variations in mechanical properties (Virk, Hall, and Summerscales 2012) which can be naturally considered as a source of biased data.

None significant correlation or tendency has been observed between density and other parameters. This can be explained by the fact that all fiber density ranges are between 1g/cm^3 and 1,6 g/cm^3 which is adjacent to density of all the chemical constituents.

- ***Statistical models to predict mechanical properties***

As mentioned before the MFA (°) is the only reliable independent parameter from all other variable 1 group that can explain the mechanical properties. The (table 3) show the statistical Models and their respective R².

Table 3: Best statistical Models

Mechanical Property	Model	R²
Tensile	**-12.17 * MFA + 723.76**	**0.37**
Young Modulus	**-1.88*MFA + 54.8**	**0.98**
Failure Strain	**0.234 MFA + 1.103**	**0.926**

Conclusion

The variation of the MFA (°) can explain more than 90% of the variation of young Modulus and failure strain.

To improve this work, the capability of the models should be discussed against some others plant fibers that are not considered in the model construction.

In order to enhance the capability of the model proposed for the tensile strength, others independents variables should be take into consideration to run the same analysis.

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