



**T.R.
İSTANBUL UNIVERSITY
INSTITUTE OF SCIENCES**



[MASTER'S THESIS]

**[DEVELOPING A MODEL WITH MACHINE LEARNING FOR THE
PREDICTION OF FLAX-BASED BIOCOMPOSITE BEHAVIOR**

]

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PREFACE

[There are turning points in our lives when we finally realize the enormous influence others have had on our path. This introduction is a meek way for me to express my gratitude to everyone who has helped me throughout this important stage by advising, supporting, and encouraging me.

My instructors, Çiğdem Erol, Sofiane Guessasma ,Johnny Beaugrand, have my deepest appreciation and admiration. They have trusted me and made themselves available to me despite their hectic schedules whenever I needed their advice. My personal and professional development has been greatly influenced by their priceless counsel, thorough explanations, and steadfast support. Their advice and support have ignited a fire inside of me, pushing me over my comfort zone and motivating me to work for bigger successes.

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To my beloved family, I am eternally thankful for being my constant pillars of strength and love. Your unwavering faith in my abilities, unconditional support, and endless encouragement have formed the foundation of my journey. Your presence has provided me with a sanctuary, a place where I can always find comfort and rejuvenation. Your love and support have given me the courage to confront challenges head-on and persevere in the pursuit of my dreams. Even when I doubted myself, you never wavered in your belief in me, and for that, I am forever indebted to you.

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With immense gratitude]

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LIST OF SYMBOLS AND ABBREVIATIONS

Symbols	Explanations
E	: Elasticity modulus / Young's modulus
σ	: the reaction force per unit surface
F	: Reaction force
ε	: Strain/deformation
EM	: Mean Young's modulus

Abbreviations	Explanations
ANN	: Artificial neural networks
CNN	: Convolutional neural networks
FE	: Finite element
FEA	: Finite element analyses
FEM	: Finite element methode
GPa	: Gega pascal
MSE	: Mean square error
RVE	: Representative volume element

]

ÖZET

[KETEN BAZLI BIYOKOMPOZIT DAVRANIŞIN TAHMINİ İÇİN MAKİNE ÖĞRENMESİ İLE MODEL GELİŞTİRİLMESİ]

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Biyo-kompozit maddeler, birçok endüstride sentetik maddelerin yerine kullanılır. Güçlendirici olarak, son yıllarda cam fiberinin yerine geçmek üzere giderek daha fazla kullanılmaktadır. Bu çalışma, keten fiberi biyo-kompozitlerinin mikroyapısal özelliklerini incelemeyi, genç modülünü (esneklik davranışı) ve anizotropiyi tahmin etmeyi, ayrıca mikroyapıların temsilci hacim elemanının özelliklerini sergileyip sergilemediğini belirlemeyi amaçlamaktadır. Bu özelliği tahmin etmek ve hesaplamaların maliyetlerini önemli ölçüde azaltmak için bir yapay sinir ağı tabanlı modelin geliştirilmesinde kullanılmak üzere bir yapılar ve elastiklik modülü veritabanı oluşturuldu. Sonlu elemanlar modeline ve yapay sinir ağları modellerine dayalı sayısal simülasyon yaklaşımları ile, ANN modelinden elde edilen sonuçların FE modelinden elde edilenlerle uyumlu olduğu gösterilmiş ve ANN uygulamasıyla maliyet etkin hesaplama yaklaşımımızın başarısı kanıtlanmıştır. Mikroyapısal özellikler ile mekanik özellikler arasındaki ilişkiler de tartışılmış ve bu çalışmanın, sentetik fiber maddelerin yerine keten bazlı

kompozitlerin elastikiyet ve mikroyapısal performansları açısından ekolojik tasarımın uyarlanmasına katkı sağlayabileceđi vurgulanmıřtır.

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Anahtar Kelimeler: Sonlu Elemanlar, Sonlu Eleman Analizi, YSA, Keten lifi, Young's modulus, Biyokompozit.



ABSTRACT

[DEVELOPMENT OF COMPUTER MODELS FOR THE PREDICTION OF BIOSOURCED FLAX-BASED COMPOSITE BEHAVIOUR]

[THESIS OF MASTER]

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[Biocomposite materials are usually used to replace synthetic materials in many industries. As reinforcements, they are increasingly used as a substitute for glass fibers during the last years. This work aims to study the microstructural properties of the flax fiber biocomposites, to predict their young modulus (elasticity behavior) and anisotropy and to determine if the microstructures display the properties of a representative volume element (RVE). A database of structures and their elasticity modulus was built to be used in the development of a neural network based model to predict this property and significantly reduce the costs of computations. With numerical simulation approaches based on the finite element (FE) and the artificial neural networks (ANN) models, it has been showed that the results obtained from the ANN model align well with those from the finite element model, demonstrating the success of our cost-effective computational approach through the application of ANN. The correlations between microstructural properties and mechanical properties are also discussed and

highlighting that this study can contribute in adapting the eco-design of flax based composites in terms of elasticity and microstructural performances for the substitution of the synthetic fiber materials..]

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Keywords: [Finite element, FEA, ANN, flax fibers, Young's modulus, biocomposites]



1. INTRODUCTION

[Commercial interest in plant fibers has increased in recent years due to the increasing pressure to find environmentally friendly methods of producing and consuming food and energy while also reducing our reliance on nonrenewable fossil fuels. In this light, biocomposites made from plant fibers have gained attention since they are considered as a promising step toward a more sustainable economy and the eventual elimination of their synthetic counterparts [1-5]. According to the Nova Institute, European production of biocomposites reached 480000 tonnes [6] in 2020. Glass fibers might theoretically be replaced by a wide variety of plant fibers.

Reinforcing composite materials, plant fibers are increasingly employed as an alternative to glass fibers. The environmental and mechanical benefits of these alternatives are undeniable [7]. As mentioned in [8], flax fibers are more environmentally advantageous than glass fibers, and this makes them the material of choice for use in composite applications. In 2012, flax accounted for more than 51% of the total fiber mass used in European applications. Several factors, such as the difficulty in predicting quality and making sure that the mechanical performances can be reproduced correctly, still pose challenges to its usage as a larger-scale replacement for glass fibers in semi-structural goods. This thesis is suggested as part of the European Interreg Trans-Manche FLOWER project (<http://flower-project.eu/>) devoted to the research and development of innovative flax preforms for the composites industry. FLOWER stands for Flax composites, LOW weight, End of life, and Recycling. INRAE BIA-Nantes, University of South Brittany, Cambridge University, University of Portsmouth, and industrial partners Ecotechnilin, Depestele, Karos, and Howa-Tramico are the eight partners working on the project since its 2018 inception.

Accurate forecasts of the mechanical behaviors of flax fiber reinforced composites and flax fiber fabrics are necessary due to the rising demand in a variety of engineering applications. However, in order to scale up production, many unknowns must be resolved. One such unknown is the extent to which defects in plant fibers reduce their mechanical properties. To address this issue, researchers must gain a deeper understanding of defect nature, origin, and consequences at the fiber scale. As a result, finite element analysis (FEA) and other

computational approaches are becoming increasingly popular as supplements to time-consuming experimental characterization. When dealing with complex issues or ones that demand a high degree of accuracy, the finite elements technique (FEM) can be very resource intensive. Discrete elements are used to break down the issue domain and solve the corresponding equations one at a time. The computational work needed grows with the number of elements. However, advancements in computing technology have made FEM more accessible and efficient. High-performance computing systems do reduce the overall time required for computation. It's also important to note that the expense of FEM should be weighed against the advantages it offers. Better outcomes results from the accurate modelling and analysis of complex structures and systems is made possible by FEM [9]. On the other hand FEM may not be a suitable approach on time sensitive cases [10]. Another popular computational approach in material science to predict the mechanical behavior of biocomposites is ANNs. With the use of this approach, scientists may more precisely regulate the parameters that govern all laboratory activities, from fabrication to testing. For instance, numerous research projects have been carried out on ANNs to forecast experimental data like mechanical characteristics, thermal conductivity, or even viscosity [11].

Building upon the limitations of the finite element method (FEM) in time-sensitive cases and the potential offered by artificial neural networks (ANNs) in accurately predicting mechanical behavior, this thesis aims to:

- Investigate the microstructural properties of the flax fiber biocomposites with a numerical simulation approach based on the finite element method and predict the young modulus of the biocomposites.
- Determine if the microstructures display the proprieties of a representative volume element (RVE).
- Build a database of structures and their elasticity modulus to and use it in the development of a neural network based model to predict this propriety and significantly reduce the costs of computations.

Through the pursuit of these objectives, this research endeavors to offer significant understandings regarding the computational methods employed in material science to forecast the mechanical characteristics of biocomposites.

In the GENERAL PARTS section of thesis a bibliographical review about the finite elements method, plant fibers and the artificial neural networks is presented. Followed by a MATERIAL AND METHODS section where the work done is displayed in detail, this section includes 3 main parts and starts with a porosity analyses of flax fibers biocomposites which contains information about the data used and how it was processed and analysed followed by a numerical simulation based mechanical study on the Anisotropic Properties and Elasticity of flax fibers biocomposites where FEM is applied and explained and many deeper insights on the data are done to build a dataset that is used to develop an ANN model to predict the those proprieties. The findings of the various analyses are presented in results section and they are discussed in discussion and conclusion's section.]



2. GENERAL PARTS

[This section is a bibliographical review that covers plant fibers, the finite elements method, and artificial neural networks.

2.1 PLANT FIBER

The fibrous material known as "plant fiber" comes from the cellular walls of plant tissues [12]. Because of its versatility, durability, and eco-friendliness, this natural fiber is increasingly being employed in commercial and industrial fields [13].

One of the most popular plant fibers is flax. Extracted flax fibers were among the earliest fibers to be woven into textiles [14].

France produces 68% of the world's flax and has an area of 122,000 hectares dedicated to growing the crop. The European preference for composite materials—from automobile dashboards to boat hulls—often includes flax fiber, a plant fiber. Despite its widespread textile application, flax is more expensive (\$1700-2600/ton) than shorter-staple plant fibers like sisal (\$700-1800/ton) or bamboo (\$250-500/ton) [15]. The following Figure 2.1 displays the major flax producers in Europe [16] where the green color scaling represents the production contribution of each country:

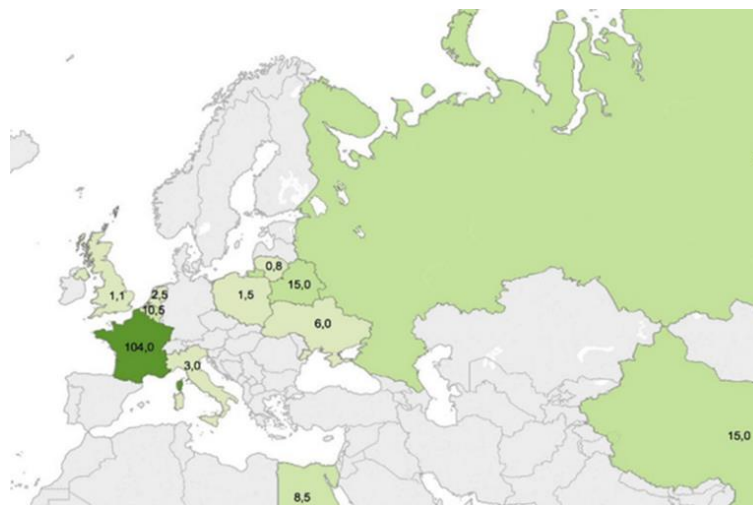


Figure 2.1: Flax production in Europe [16].

According to the origin of the plant, a classification is represented in Figure 2.2:

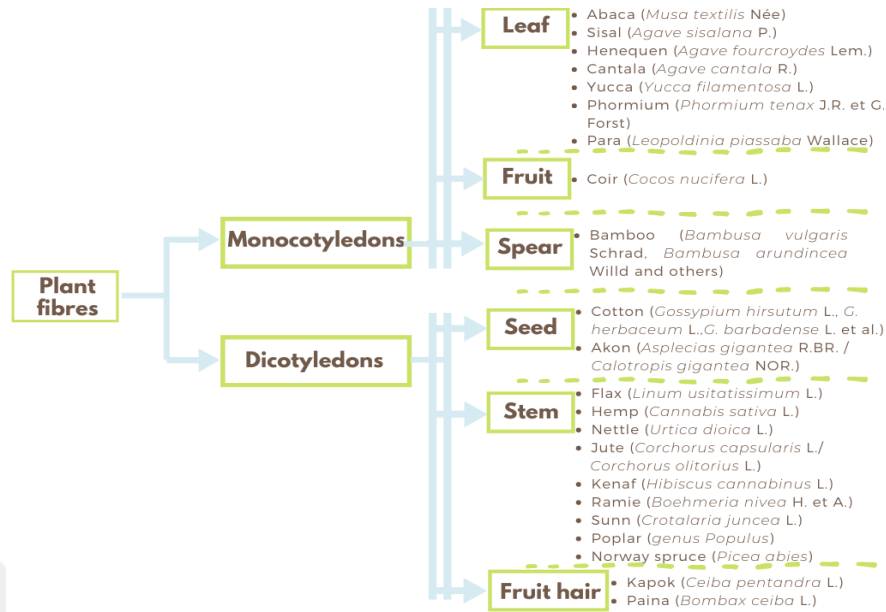


Figure 2.2: Classification of plant fibers, adapted from [17].

As displayed in Figure 2.2 plant fibers are classified into 2 main groups Monocotyledons and Dicotyledons where each one is divided into 3 sub-classes.

In the context of this thesis, flax is studied with other stem fibers. One of the earliest plants grown by humans, flax has long been used in the textile industry and now also appears to be a popular choice for composite uses.

The performances vary according to the fiber and it should therefore be noted that each type of fiber has very variable characteristics, due to the natural character [7], sample has been provided in Table 2.1.

Table 2.1: The mechanical characteristics of some natural fibers [18].

Fibre	Technical fibre length (mm)	Diameter (um)	Young's modulus (Gpa)	Maximal strain (%)
Cotton	25	12-25	6-10	6-8
Flax	4-8,5	12 -30	50 -70	1,3 -3,3
Hemp	5,0 -40	16 -50	30 -60	1,7-2,7

As displayed in Table 2.1 flax fibers shows outstanding mechanical properties which explain its utility in textiles and biocomposites applications.

2.1.1 Flax Fibers Bibliographic Review

Structure of Flax Fibers:

Understanding the mechanical properties of plant fibers requires an appreciation of their underlying physicochemical structures. Structure of flax fiber from the stem to the micro fibril, including the position of flax fibers within the stem.

By separating the fiber bundles from the stem mechanically, technical fibers are produced. . Figure 2.3 [17] depicts the structure of a flax fiber, showing that the technical fiber consists of anywhere from 10 to 40 primary fibers in cross section.

The diameter of the individual fibers ranges from 5 to 35 μm , while their lengths range from 2 to 5 cm. Pectins and hemicelluloses, a variety of low-molecular-weight branching polysaccharides, make up the bulk of the adhesive interphase that holds them together. As shown Figure 2.3 [19], a unit fiber has three parts: a primary cell wall, a secondary cell wall, and a lumen. The diameter of the fiber is concentrated in the secondary cell wall.

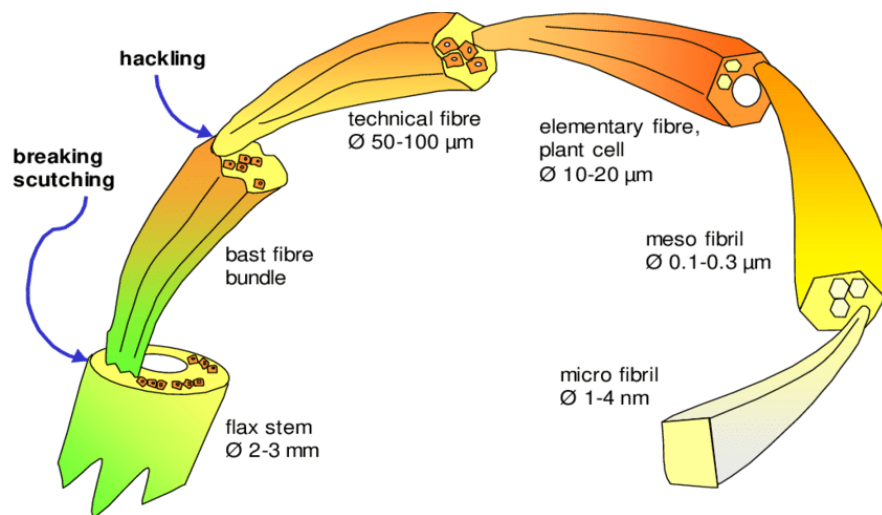


Figure 2.3: Schematic representation of flax fiber from stalk to micro fibril [19].

2.1.2 Flax Fibers Mechanical Behavior

Flax fibers offer the highest capacity for absorbing vibrations and mechanical qualities similar to glass fibers [20]

The cellulose micro fibrils in flax fibers are what give them their mechanical strength. Their rigidity is predicted to be between 120 GPa and 140 GPa, indicating that they possess impressive mechanical qualities.

Tensile strength was reported to be 945 200 MPa by Baley and Bourmaud [15] [21], and strain at break was 2.1 0.5%. In addition, the density of flax fibers is only about 1.45-1.50 g.cm³ [15], which is significantly less than the density of glass fibers (2.55 g.cm³).

The matrix in a composite material holds the reinforcements in place, transmits mechanical loads, and gives the material its definitive form. According on the composition of the matrix, composites can be broken down into several distinct categories [22]:

Composites made of metal matrices, ceramic matrices, and polymer or organic matrices.

As part of this thesis, we focus on the family of composites based on BioSource thermoplastic polymers (resin).

2.1.3 The Interface In A Composite Material Reinforced With Flax Fibers Notion Of Adhesion

Fiber strength and stiffness, chemical resistance and stability of the matrix, and the nature of the link between the fibers and the matrix are the primary determinants of the mechanical performance and longevity of composite materials. [23].

Composites consist of (at least) two different materials fused together. When put together in this way, the adhesive and substrate have a very tiny contact area, which limits the amount of stress that may be transferred from the backing to the matrix. This region can be either very thick (interphase) or very thin (interface) [15]. It penetrates not only the substrate but also the adhesive. Adhesion is produced through physical-chemical interactions, and its thickness is predicted to be between 5 and 500 nm [24], as shown in Figure 2.4.

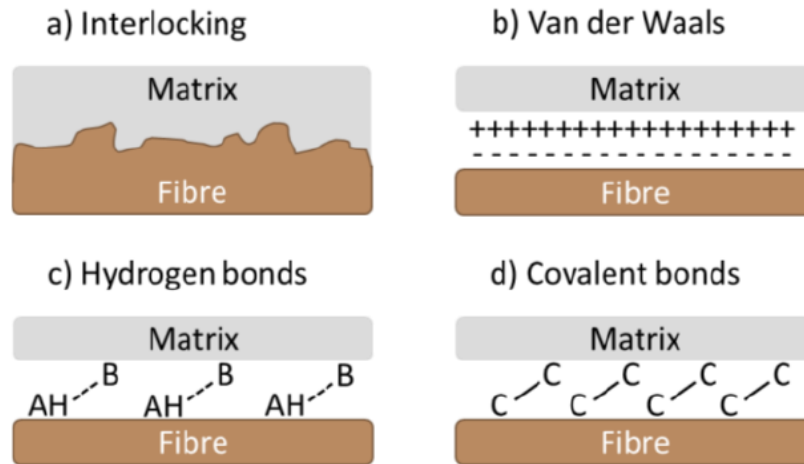


Figure 2.4: Diagram of interfacial mechanism between fiber and matrix [25].

The various interfacial bonding methods at fiber-matrix interfaces are depicted in Figure 2.4. Bonding can occur in a variety of ways at the same interface and at the same time [26].

Assessment of the adhesion between flax fibers and resin [24]:

There is penetration of the flax fiber by the resin. The roughness and chemical quality of the flax fiber surface directly affects the quality of adhesion.

The interface is also crucial in the load transmission between the fiber and the matrix, and thus the overall performance of the structure [28], as well as in the mechanical behavior, fatigue resistance, and durability of composite materials [27].

2.2 FINITE ELEMENT METHOD

The definition of finite element method (FEM) is based on the distribution of the entire computational domain into several sub-domains. The more these subdomains are numerous and small, the more this method makes it possible to approach fairly quickly the exact solution of the partial differential equations. Each subdomain contains discrete elements. On each side of an element, two nodes make it possible to connect this element to one or more other elements present in the whole of the computational domain. The finite element method considers each sub-domain as an independent geometric domain. The resolution of the partial differential equations of the physical model of interest makes it possible to obtain all the unknown variables of the given problem. This method gives high accuracy of calculations compared to other numerical calculation methods [1]. Each unknown variable (for example

the speed) is calculated at the nodes, then its value is represented in a finite element by a basis function. The linear combination of the values of the nodes of the variables and the basic functions of the element makes it possible to find the approximate solution of the physical equation in the element and thus in the studied system. More information about the FEM are provided through the next sections.

History

Finite element methods (FEM) have been enabled by many developments to become an ideal numerical method for many problems that are based on solid mechanics [29] .

The finite element method development started in the 1940s in structural engineering field in the work done by Hrennikoff [30] in 1941 and and McHenry [31] in 1943 ,in a later time a setting up solution of stresses in a variational form was proposed by Courant [32] where he introduced the shape functions over triangular subdivisions which made the whole region as a method to obtain approximate numerical solutions ,in 1947 a flexibility method was developed by Levy [33] and was used in his work [34] where he suggested another method that may be a promising potential alternative to analyzing statically redundant aircraft structures which carried the name of stiffness-displacement method, his equations were too heavy to be handled manually , consequently only with the development of the High-speed digital computer this method gained more popularity .

Matrix structural analysis methods using energy principles. were developed later In 1954 by Argyris and Kelsey [35] and it showed its importance in the FEM , in a later time a matrix notation expressed the finite element stiffness equations were more developed in the work of Turner et al [36].

in 1960 when both triangular and rectangular elements were used for plane stress analysis the term finite element were introduced by Clough [37], in this period the work related to FE concerned only the small strains and small displacements, elastic material behavior , the text by Belytschko, Liu, and Moran [38] can be consulted For more on these topics.

APPLICATIONS OF FEM:

Many subfields of mechanical engineering (including the aerospace, biomechanical, and automotive industries, to name a few) routinely include FEM into the design and development of their products. Many modern FEM systems take into account the thermal, electromagnetic, hydrodynamic, and structural aspects of the workplace. Stiffness and strength can be visualized, as well as weight, materials, and prices cut, with the use of finite element modeling (FEM) in a structural simulation. [39].

By displaying stress and displacement distributions, FEM provides a clear picture of where structural deformations occur. The complexity of system modeling and analysis can be handled by the many simulation tools available in FEM software.

FEM allows for the building, enhancing, and optimizing of an entire design before it is manufactured.

The mesh is an integral part of the model and must be maintained correctly for optimal results. The higher the number of elements in a mesh, the more precise the solution to the discretized issue. After a certain threshold, further mesh refinement does not lead to an increase in accuracy, and the results have converged [29].

The finite element method has recently been applied to the field of bioengineering [40, 41]. Nonlinear materials, geometric nonlinearities, and other complications are still obstacles in this sector.

In conclusion, FEM's benefits include higher quality designs, shorter and cheaper design cycles, greater understanding of key design parameters, virtual prototyping, fewer hardware prototypes, and higher levels of productivity.

2.2.1 THE ROLE OF COMPUTERS IN FEM DEVELOPMENT

As we've already established, matrix methods and the accompanying finite element approach had a hard time dealing with complexity before the early 1950s. Complex structures were previously described using the finite element method (FEM) of structural analysis; however, this approach was extremely challenging and impractical due to the large number of algebraic equations that produced. However, with the advent of computers, it is now possible to efficiently and rapidly solve hundreds of equations.

Due to the advancement of integrated circuit-based technology between the years of 1969 and the late 1970s, it was possible to solve finite element problems that were more complicated and had more degrees of freedom.

The Internet and the World Wide Web were two innovations that came forth during the era of networked computing.

When the Windows operating system was introduced in the 1990s, it improved the usability of IBM and IBM compatible PCs by incorporating a graphical user interface.

The development of the computer resulted in the writing of computational programs. Numerous special-purpose and general-purpose programs have been written to handle various complicated structural (and non-structural) problems. Programs such as [42, 43] illustrate the elegance of the finite element method and reinforced understanding of it.

Computational programs were written as a result of computer progress. Numerous general-purpose and specialized programs have been created to address a wide range of challenging structural (and non-structural) issues. The elegance of the finite element method is illustrated and further understood in programs [43, 44].

The analyst enters the data into the computer to use it after defining the finite element model. These details could include the location of the element's nodal coordinates, how the elements are connected, the materials the elements are made of, the loads that have been applied, any boundary conditions or constraints, and the type of analysis that will be carried out. The equations required to do the analysis are then generated and solved by the computer using the information provided.

2.2.2 GENERAL STEPS OF THE FINITE ELEMENT METHOD

Two general direct approaches are generally associated with FEM when its related to structural mechanical problems, the first one uses the internal forces as the unknowns of the problem to get the equations and it's called flexibility method. The second approaches the displacement it assumes the displacements of the nodes as the unknowns of the problem then equations are expressed in term of nodal stiffness or displacements.

These two direct methods produce various forces or displacements in the analysis, as well as various matrices that are connected to their formulations (flexibilities or stiffnesses).

The displacement (or stiffness) technique is preferable for computational purposes as most structural analysis problems can be formulated using its formulation as it has been shown in [45].

The FEM uses tiny, interconnected elements called finite elements to simulate the structure. Each finite element possesses a displacement function. Every member in a network is connected to every other element, either directly or indirectly, by means of shared or common interfaces, such as nodes, boundary lines, surfaces, or other interfaces. One may predict the behavior of a specific node in terms of the characteristics of every other element in the structure by using known stress/strain values for the material making up the structure. A series of algebraic equations that are best described in matrix notation make up the entire set of equations that describe the behavior of each node.

A short descriptions of the steps goes as follow [29]:

Step 1: Discretize and Select the Element Types.

In step 1, the body is divided into an equivalent system of finite elements with connected nodes, and the element type that best represent the real physical behaviour is selected.

Step 2: Select a Displacement Function

It includes selecting a displacement function within each element. The function is defined within the element using the nodal values of the element.

Step 3: Define the Strain-Displacement and Stress-Strain Relationships.

Strain/displacement & stress/strain relationships are mandatory for getting the equations for each FE.

Step 4: Derive the element stiffness matrix and equations

The development of element stiffness matrices and element equations was based on the concept of stiffness influence coefficients or by an alternative such as direct equilibrium method, work or energy methods, and methods of weighted residual.

Step 5: Assemble the element equations to obtain the global or total equations and introduce the boundary conditions.

In this step the individual element nodal equilibrium equations generated in step 4 are assembled into the global nodal equilibrium equations.

Step 6: Solve for the Unknown Degrees of Freedom (or Generalized Displacements) .

Step 7: Solve for the Element Strains and Stresses.

For the structural stress-analysis problem, important secondary quantities of strain

And stress (or moment and shear force) can be obtained because they can be directly expressed in terms of the displacements determined in step 6

Step 8: Interpret the Results

The outcomes interpretation and analysis are the final objectives to be used in the design and analysis process. Making design and analysis decisions often involve knowing where in the structure large deformations and large stresses occur. Utilizing graphical displays, postprocessor computer programs assist the user in understanding the results.

There are many softwares developed to use the finite element approach to solve problems. Before using any software, interested users should carefully examine one of the many providers who support finite element programs. However, we present a small list of current programs to give you an idea of the numerous commercial personal computer programs currently offered for using the finite element approach to solve issues:

Algor [42],Abaqus [46],ANSYS [47],COSMOS/M [48],GT-STRUDL [49],MARC [50],MSC/NASTRAN [51].

2.3 ARTIFICIAL NEURAL NETWORK

The development of artificial neural networks uses a model of the human brain. It is a method that can be successfully applied in many fields (Pattern recognition, Recommendation systems, Medical diagnosis, Material science ... ect) [52]. It is an advantageous method in terms of its features such as working with high-dimensional data, being resistant to noise, multitasking without loss of productivity Figure 2.5 depicts a sample of artificial neural network model.

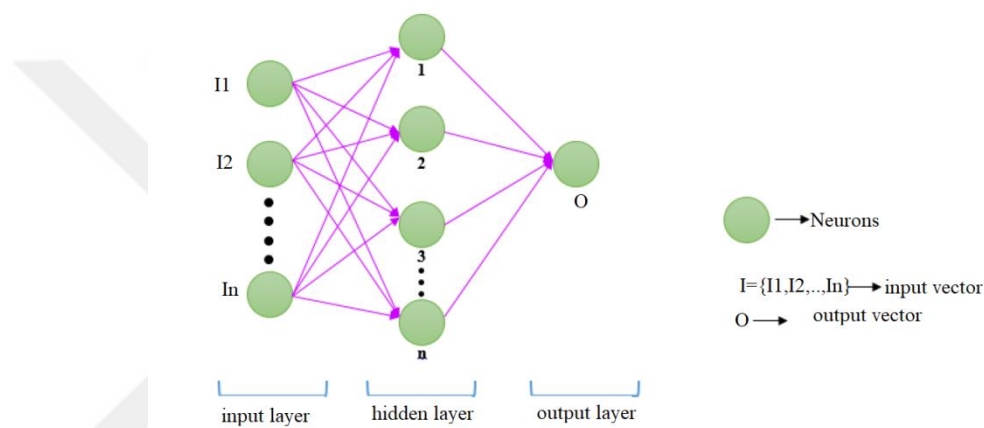


Figure 2.5: an example of an artificial neural network model [53].

Basically, a neural network model is made up of three layers: input, hidden (intermediate), and output. Each layer contains neurons, which are synthetic nerve cells (process elements). There is a procedure in artificial neural networks (ANN) that converts input data into output data. The input layer of the network is sent samples of the data collection. The class values of the unknown samples are then identified by creating multiple connections between neurons. The input values must be expressed numerically.

Each neuron has five components: inputs, weights, summation function, activation function and output. The way the process works in nerve cells and its similarity to biological neurons is as shown in Figure 2.6. In-depth discussions of the neural network concept can be found elsewhere [54, 55].

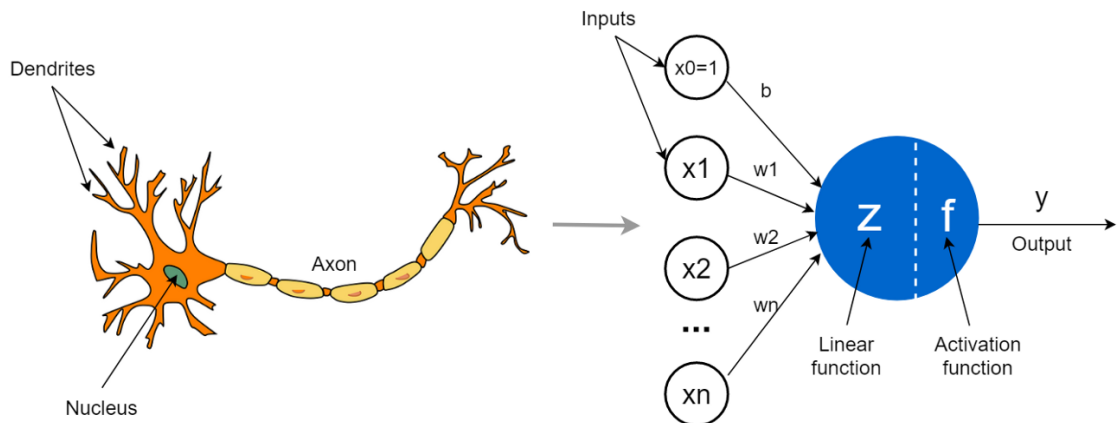


Figure 2.6: Biological and artificial neurons [56].

2.3.1 Biological Neurons

Numerous neurophysiologists have researched the composition and operation of the human brain.

But right now, all that is available is an overview. The brain basically runs on an extremely thick network of neurons. A typical biological neuron is seen in Figure 2.6. Up to 10^{11} interconnections between each of the brain's 10^{15} neurons connect them to one another. The following components mainly make up a neuron:

- The cell body.
- The axon.
- The dendrite.

In order for the neuron of which it is a component to receive messages from different other neurons, the dendrite is necessary. To transmit complicated electro-chemical information, these dendrites are diffused in a branching shape. On the other hand, an axon relays the signal to numerous additional neurons from the cell body. Signals are effectively aggregated in the cell body when multiple dendrites send them there. When enough time has passed, the cell body produces a signal, and if the accumulation rises above a certain point, the axon sends the same signal down. The artificial neural network's neural units are created as a very rough representation of biological neurons as a result. The biological neural network also exhibits a

number of additional behaviors that are exceedingly challenging to replicate with the hardware and software that is currently on the market [56].

2.3.2 Artificial Neurons

The function of an artificial neuron can be described in a simple mathematical operation (an\or\>...), as described in Figure 2.6 an artificial neuron gets input directly from the environment or by other neurons. The synaptic strength of the connection between two neurons is represented by a specific variable weight attached to their path. The output of the connected neuron is multiplied by the synaptic strength of the connection between them to determine the input to a neuron from another neuron. The synthetic neuron then adds up all of the weighted inputs that are being sent to it. By changing the neuron's synaptic strengths and threshold values, the output of the neuron for a particular input can be made to correspond to a desired value. A variety of connections between several neurons can be made in an artificial neural network (ANN). Neural nets have already been built in a wide variety of forms, The current issue must be taken into consideration when choosing the network architecture [57].

2.3.3 ANNs In Material Science

In this work a combined methodology between finite element analysis (FEA) and artificial neural network (ANN) is used to predict the behavior of flax bio-composites. FEA have been utilized more and more recently to replicate different mechanical testing as well as impact tests [58, 59], FE model must have the ability to get the experimentally observed behavior of the material, The results of FE studies have to be generalized to develop a model for predicting the behavior of the composites because making an FE solution for each new situation becomes computationally expensive.

The behavior of such composite materials under various mechanical characterization tests can also be predicted using machine learning approaches. These contemporary, data-driven, theoretical, and computational methods have made it possible to precisely solve engineering issues for a wide range of materials under certain circumstances [60] and many researchers have successfully employed ANNs to study mechanical behaviors of composites. Birecikli et al [61] used ANN to predict the failure in glass fiber composites when subjected to tensile loads. Galatas et al [62] used ANN to predict the mechanical properties of composite

structures, in the same way Artero-Guerrero et al.[63] to predict the effect of fiber orientation & stacking sequence.

The distinctiveness of ANN rests in its capacity to learn from past mistakes and successfully extract significant outputs from a set of input data that has been fed into it [64]. ANNs can be very helpful to get the material behavior directly, which reduces the necessity of developing analytical expressions. ANNs can generalize on their own. As a result, they can accurately forecast how a new material will behave even before the material is created in a lab. This could lower the cost of pricey trials, also as one of the main advantages of ANNs is that They don't need any kind of external parametric relationship presentation. Therefore, the network automatically maps complex correlations between multiple parameters.

In our work we use the data collected from FEA results as input data to train and validate the algorithm to produce accurate results.

2.3.4 Development Of ANN Model

The main aim of this work is to use ANNs for the development of a mechanical model for flax biocomposites behavior, ANNs can use given patterns during the training to learn a physical phenomenon this can be exploited for the development of our mechanical model that involves complex correlations of various parameters. The process of the model's development is presented as the following [65]:

- Generation of training examples
- Selection of a network type
- Selection of the input and the output for the network
- Arriving at a suitable network configuration
- Selection of a suitable training strategy
- Training and validation of the resulting network

2.4 LITERATURE REVIEW

Using finite element analysis (FEM) and artificial neural networks (ANNs), this thesis examines and expands upon comparable studies into the construction of computer models for the prediction of biocomposites' behavior. Using Google Scholar and Web of Science to look

for terms like "finite element" and "material science" and "biocomposites" and "artificial neural networks." The easiest way to do the work is outlined below.

Finite element analysis using the ANSYS software predicted the effective Young's modulus as a function of the phase ratio for the studied microstructures [66], which was proposed by Guessasma et al. (2009) as a numerical method to evaluate the impact of random microstructure on the effective Young's modulus of a two-phase biopolymer composite material. based on the work of Guessasma et al. (2014) [67], which entails performing experiments to examine the material's microstructural features and conducting mechanical testing. Damage kinetics leading to failure attributes are simulated using a finite element model. The findings provide experimental evidence for the phenomenon of failure due to interfacial damage. Using an abrupt damage criteria, the finite element model accurately represents this behavior. Comparing the experimental reaction to the numerical simulation verifies the observed behavior and permits fine-tuning of the mechanical parameters. Through this process of optimization, accurate mechanical parameters are determined, allowing the observed ultimate qualities to be quantified.

Some studies, such as "Application of artificial neural networks to predict Young's moduli of cartilage scaffolds: An in-vitro and micromechanical study" by Khalvandi et al. (2022), used a combined approach, with the authors fabricating and analyzing four-phase Gelatin-Polypyrrole-Akermanite-Magnetite scaffolds via in-vitro tests and numerical simulations. Young's moduli of the scaffolds were predicted using artificial neural networks trained on data from finite element analysis. The micromechanical models' results for the samples matched those of the simulations and the experimental testing quite closely.

To predict Young's modulus from pore size and shape, a neural network learning approach called Liebenberg-Marquardt was chosen for this study. The FEA findings served as input to the feedforward neural network, and the hyperbolic tangent function was chosen as the activation function. The optimal architecture for predicting the Young's modulus was found to have one input layer, a hidden layer of 3,4 neurons, and an output layer. During the training phase, 70% of the data were used for training, while the remaining 30% were split evenly between validation and test data. Good agreement was found between the ANNs' predictions and the FEA findings, as well as between the FEA results and the experimental data.

The absolute discrepancy between the ANNs' predictions and the FEA model was on the order of [0.004-0.007], with a mean squared error of around $10(-6)$ on average.

Ayender (2017) [68] has produced an equally impressive piece of work titled "a numerical study for prediction of forming load and experimental verification of bimetallic disc upsetting," which utilizes a hybrid of the finite element method model and a neural network model to predict and simulate the deformation load in bimetallic materials. Using forming load as a criterion, DEFORM-3D's FEM results were compared and validated with those from actual experiments. The forming load was analyzed and predicted for various process factors using the ANN model as well. It has been observed that the suggested ANN and FEM are excellent tools for predicting the forming load without the need for any tests, and that they provide important insight into the parameters impacting forming load.

Trial and error were an expensive strategy because a large number of tests are required to construct realistic models. In addition, there are drawbacks to using FEM techniques, such as the fact that they are computationally intensive and have mathematical restrictions.

The output parameter was forming load, and the input parameters were the height to diameter ratio, the percentage of formed specimens, and the punch displacement.

The ANN model was developed and trained in MATLAB; the highest absolute relative error for projected values was 2.83 percent; employing ANN values allowed for good results to be reached; as a result, the testing process required less time and money. One ANN architecture with 10 neurons in a single hidden layer and tanh as the activation function performed the best.

Finally, we found that the forming load curves generated using ANN, FEM, and experimental data all agreed well with one another. In a related study, Stephen et al. (2022) [69] used finite element analysis and an artificial neural network to predict the impact resistance of fiber-reinforced polymer composites. The purpose of this research is to use an artificial neural network (ANN) and finite element analysis (FEA) to forecast how fabric reinforced polymer (FRP) composites would react to an impact. The study's technique involves simulating impact testing on digital models of composites made of Kevlar, carbon, and glass fabric. The ANN prediction was trained using the FEA residual velocity results. The methodology employed in the study successfully predicted the impact behavior of FRP composites with high accuracy.

Based on this research into the subject of predicting projectile residual velocity after impact with various hybrid and non-hybrid composite laminates, the following conclusions can be drawn: Accuracy of 98.45% was achieved by the ANN network trained using FEA data. To accurately predict the residual velocity (V_r) values and, by extension, the impact behavior of different hybrid and non-hybrid composites, the proposed methodology combines FEA with ANN. The maximum dissimilarity between the predicted output values and the FEA data was only 6.6%. The best outcomes were achieved by an MLP architecture network consisting of a single hidden layer and 10 neurons. Using FEA and ANN data, it was found that the impact resistance of FRP composites can be affected by the stacking sequence. Penetration resistance was best demonstrated by K/K/K specimens, followed by those with Kevlar in both the front and rear layers.]

3. MATERIAL AND METHODS

[In order to study and predict the mechanical behavior of flax based biocomposites a finite element model and an artificial neural network model are developed according to the workflow presented in the following Figure 3.1 provides a systematic and logical progression of the research to achieve the objectives of the thesis.

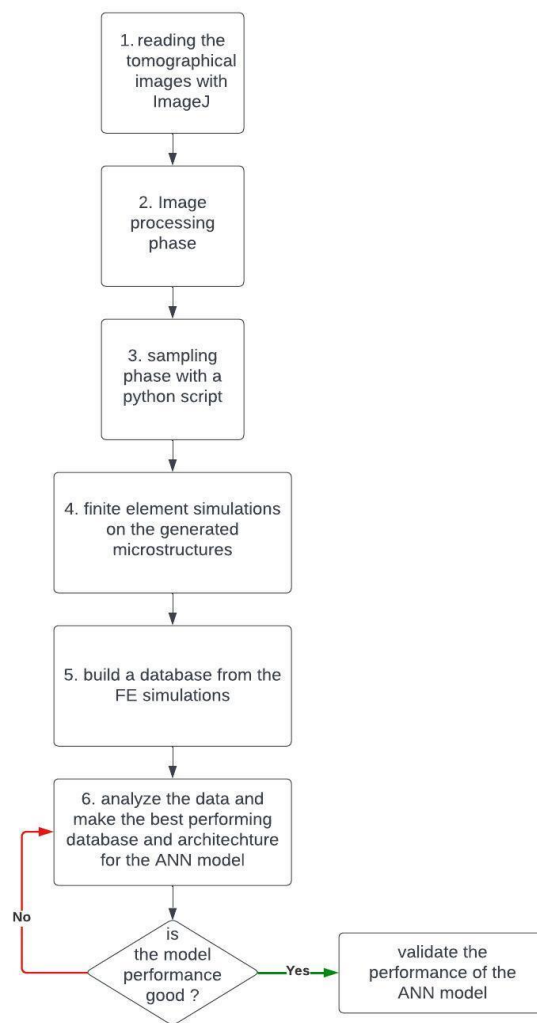


Figure 3.1: the workflow diagram of the research.

3.1 DATA

The samples used at this study are flax mats biocomposites (Figure 3.3 c) provided by EchoTechlin company and flax based biocomposites (Figure 3.3 a and b) (sandwiches)

provided by howa-tramico (an automobile company). The data used in this work are tomographical images of the previously mentioned samples provided by Laboratory's tomograph (Xradia 510 Versa, Zeiss) from the University of Portsmouth as shown in Figure 3.2.



Figure 3.2: Xradia 510 Versa, Zeiss.

real images of the samples can be seen at Figure 3.3. A summary of sample's information is displayed in Table 3.1:

Table 3.1: Samples description.

Sample name	Weight [g/m ²]	Voxel size[um]	Width [px]	Height [px]	Density [px]	Observation [px]	anotation
Flax Mat 1	100	10	2859	2853	701	clear	FM100C
Flax Mat 2	100	7.5	2814	2811	617	stained	FM100N
Flat Mat 3	150	7.5	2835	2835	351	clear	FM150C
Flax Mat 4	150	7.5	2487	2499	901	stained	FM150N
FL1	X	10	1194	1431	1931	X	FL1
FL3	X	10	1503	1446	1932	X	FL3



a. FL1

b. FL2

c. Flax mats

Figure 3.3: biocomposites samples.

3.2 DATA PROCESSING & METHODOLOGY

The samples have been processed by ImageJ software which is a widely used open-sourced program for scientific image analysis and also offers a user-friendly interface and a comprehensive set of built-in functions, making it accessible to both non-programmers and professional developers [70], it has been utilized in various scientific disciplines, including biology and material science [71]. The following protocol has been used to process the images:

Image Segmentation

For each sample, we adjusted the brightness of the image and selected a threshold to separate the materials clearly as a binary image.

Eliminating Noise

After setting the threshold and turned the images into binary some noise appeared and it has been eliminated by applying erode method followed by a dilate, after that we have removed the unnecessary slices to reduce the sample size. Figure 3.4 displays a 3d visualization of this process on the flax mat samples.

Sampling Phase

- In order to study the samples we have manually taken many crops of different sizes and in different levels inside the core of the sample, after that we have generated a large number of sub-crops of different sizes by using a python script and it works in the following way:
- It takes the width and height of the image and generates 2 lists with increasing values by a step of 25px for both of the width and height.
- We generate all the possible combination of width and height that we have got in the lists by doing the Cartesian product of both lists and we inverse it and delete the duplications.
- Now we have got all the new crop sizes so by iterating on each crop we generate our new sub-crops and of course the width and height of the original crop is respected.
- After generating the new crops we calculate the percentage of black pixels in that's image and store that data
- With the same way we have also tested the porosity on the other surfaces by making a 90° rotation on the x-axis of the images
- Output the results as a scatter.

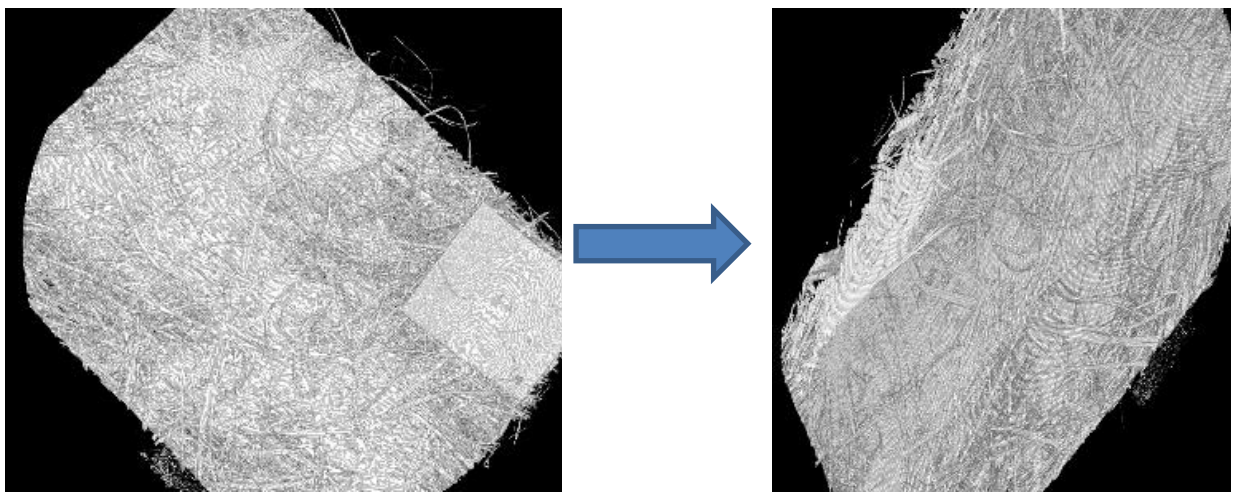


Figure 3.4: flax mat's 3D visualisation.

The following figures (Figure 3.5 & Figure 3.6) represents the tomographical image of FL1 sample and explains its composition: The following figures (Figure 3.5 & Figure 3.6) represents the tomographical image of FL1 sample and explains its composition:

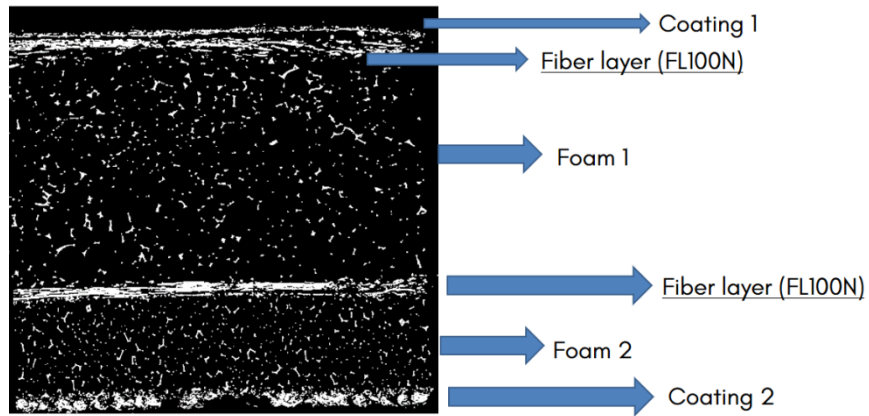


Figure 3.5: FL1 tomographical image.

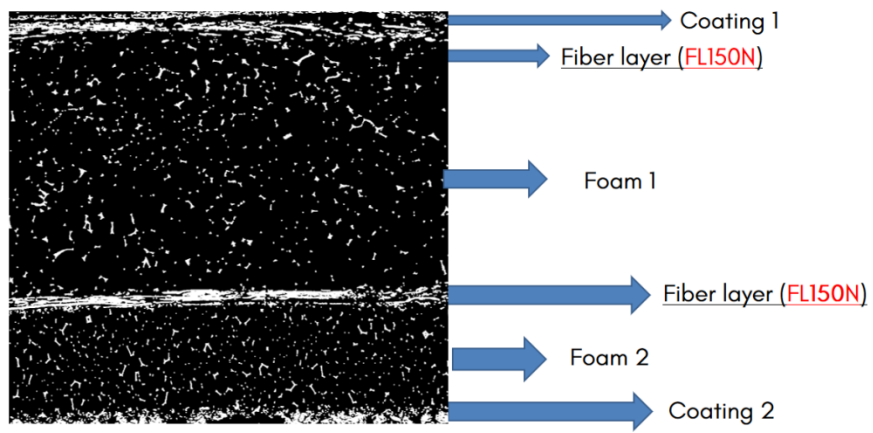


Figure 3.6: FL3 tomographical image.

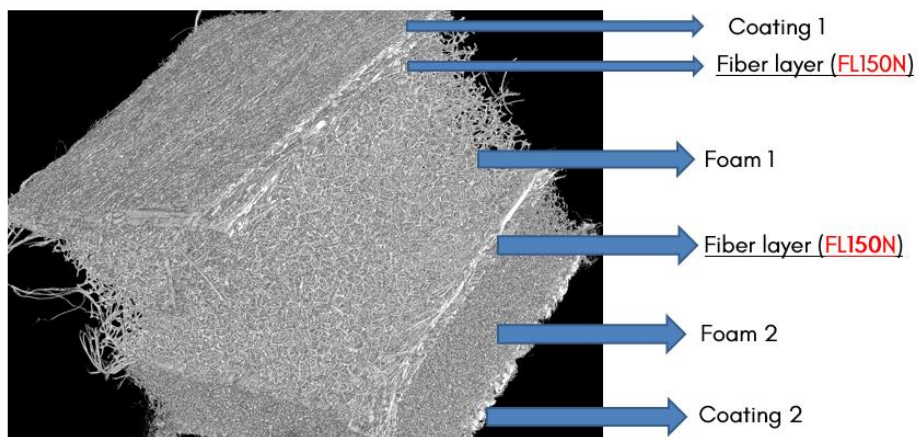


Figure 3.7: A 3D visualization of FL3 sample tomographical image.

In order to analyze the images of another angel a rotation of 90° with ImageJ was applied on the mat samples as displayed in Figure 3.8.

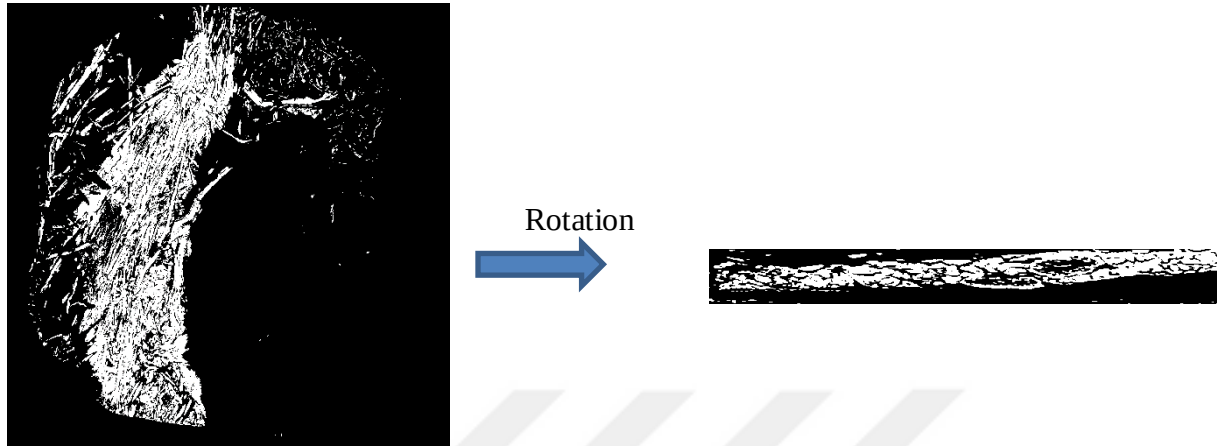


Figure 3.8: The tomographical image after 90° rotation on x-axis.

3.3 POROSITY ANALYSES

Characterizing a material's porosity is referred to as porosity analysis. Porosity is a measurement of the vacant space or empty gaps within a material and is often given as a percentage [72]. It impacts the characteristics and behaviors of materials, including their stiffness, strength, and Young modulus, making it a crucial element in studying a material's properties. Figure 3.9 gives a clear idea about the composition of a flax mat.

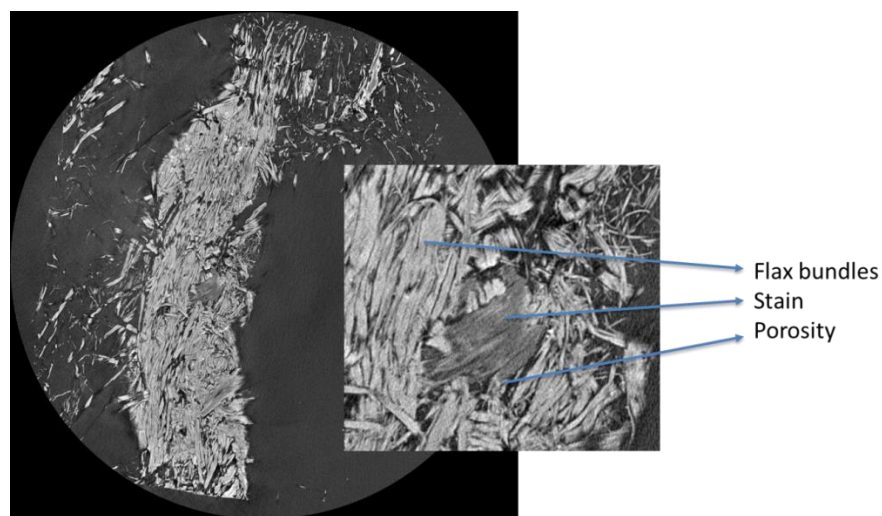


Figure 3.9: Flax fibre mat tomographical image.

After processing the data of flax mats samples and generated a set of microstructures as mentioned in the Sampling Phase a porosity analyses is performed by calculating the porosity of each microstructure (the black pixels ratio) , this process is displayed in Figure 3.10. The findings of this analyses are presented in the RESULTS section.

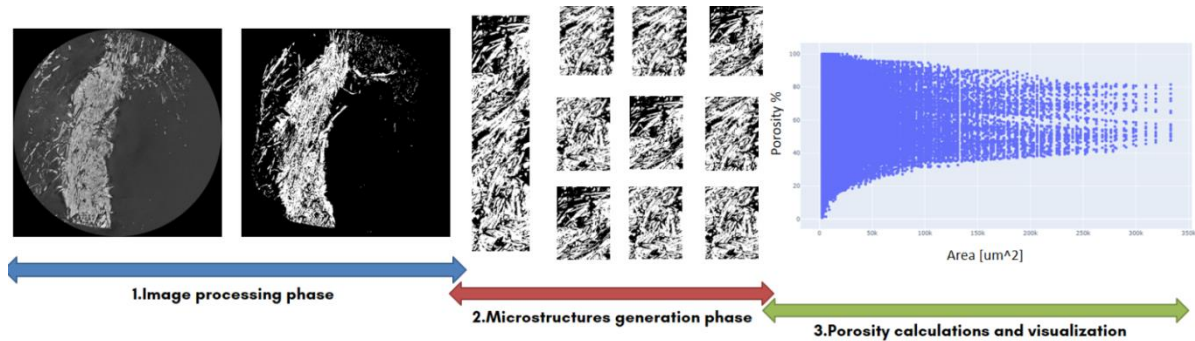


Figure 3.10: An example of the applied process for the porosity analyses on FM150N sample.

3.4 A MECHANICAL CHARACTERIZATION FLAX BASED BIOCOMPOSITES SAMPLES

The process of mechanical characterization involves identifying a material or structure's mechanical characteristics, including how it reacts to different pressures, stresses, and strains. These characteristics may include elements like ductility, toughness, stiffness, strength, and fatigue resistance, among others.

The process of mechanical characterization includes a variety of methods and tests, including tensile, compression, flexural, impact, hardness, and fatigue tests. In order to measure and assess the mechanical behavior of materials and structures under various situations, these tests are often carried out using specialized equipment.

For a better understanding of how materials and structures functions in various applications and conditions, mechanical characterization data are crucial. Designing new materials and structures, streamlining production methods, and ensuring the dependability of products can all be done with the use of this information.

In our experiment we have applied tensile testing to our FL1 and FL3 samples which are displayed in Figure 3.5 & Figure 3.6, tensile testing is a type of mechanical testing used to find

out how materials react when they are under tension. A sample of the material is tested by being put under controlled, progressively increasing tensile force until it fails or breaks.

The sample has a particular cross-sectional area and is shaped like a rectangle. It is put the tensile which exerts a tensile force along the length of the sample.

Throughout the test, the load and deformation data are collected and used to compute the material's ultimate tensile strength (UTS), yield strength, elastic modulus, elongation, and area reduction. The yield strength, on the other hand, is the amount of stress that causes a material to permanently deform or yield. The UTS is the maximum load that a sample can bear before it breaks.

In the following section we show the experiment we have run.

As shown in Figure 3.11 we attached the sample to the machine and we recorder the experiment with a fast camera to visualize the process and on the other hand the machine is connected to a computer to record the results.

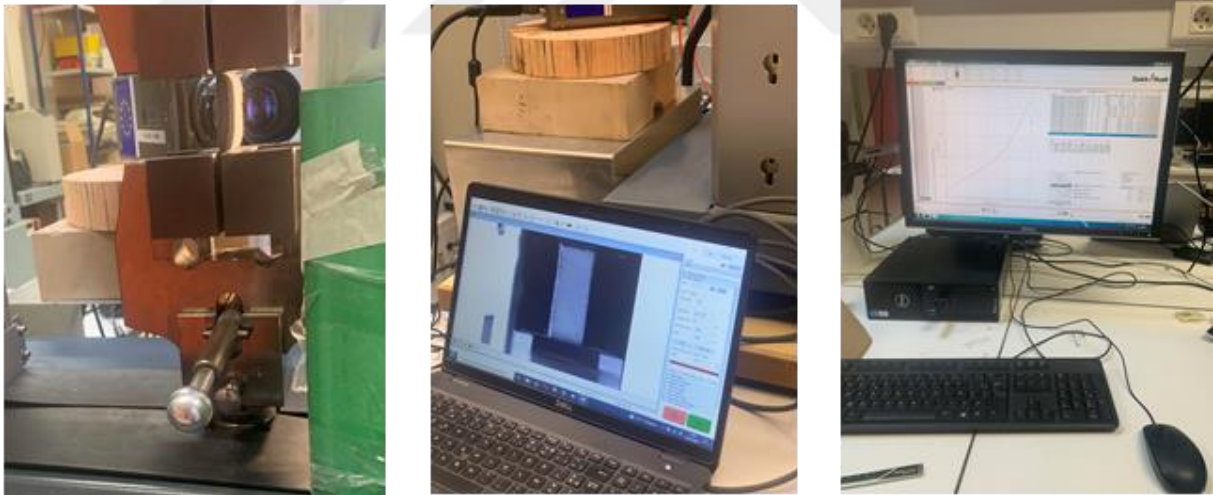


Figure 3.11: Tensile test.

3.5 A NUMERICAL SIMULATION BASED MECHANICAL STUDY ON THE ANISOTROPIC PROPERTIES AND ELASTICITY OF FLAX FIBERS BIOCOMPOSITES

The purpose of this chapter is to study the microstructural properties of the flax fiber biocomposites with a numerical simulation approach based on the finite element method to

predict the young modulus of the biocomposites, determine if they display the proprieties of a RVE (representative volume element) and build a database of structures and their elasticity modulus to be used in the development of a neural network based model to predict this propriety.

3.5.1 Modelling Technique

In this section, X-ray tomographic microscopy images have been processed and used. We had four samples, where each sample is a collection of multiple slices, several crops have been taken from the core of the material in the different slices and then have been used to generate multiple microstructures as explained in Data Processing & Methodology section.

3.5.2 Finite Element Calculation

The simulated microstructures (where the image area ranges from 500x500 micron to the maximum width and height of the microstructure) are implemented in a finite element (FE) model to for the calculation of microstructural effective properties; a two-dimensional plane-stress analysis is assumed noting that 2 machines with an i9 CPU and 100gb of ram have been used for 30 day to get these results. The following table summarizes the simulation's data.

Table 3.2: the simulation's data.

Sample name	notation	Weight [g/m ²]	Voxel size[um]	slices	Observation	Simulated microstructures
Flax Mat 1	FM100C	100	10	701	Clear	46000
Flax Mat 2	FM100N	100	7.5	617	Not clear	160000
Flat Mat 3	FM150C	150	7.5	351	Clear	60000
Flax Mat 4	FM150N	150	7.5	901	Not clear	56000

3.5.3 Geometry

In this part, plane182 element has been selected as a geometry to model 2-D solid structures and used as a plane element. The element is defined by four nodes with two degrees of freedom at each node (translations in the nodal x and y directions) as represented in Figure 3.12 [73]. This technique includes the conversion of each pixel into a plane element. Taking into consideration that the pixel size varies from a sample to another as presented in Data: section. On the other hand Figure 3.13 displays the meshed phase on a 2d image with the use of ANSYS software.

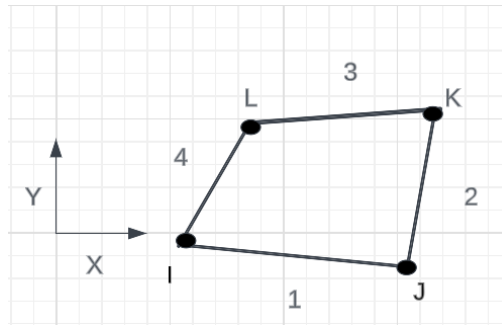


Figure 3.12: Geometry.

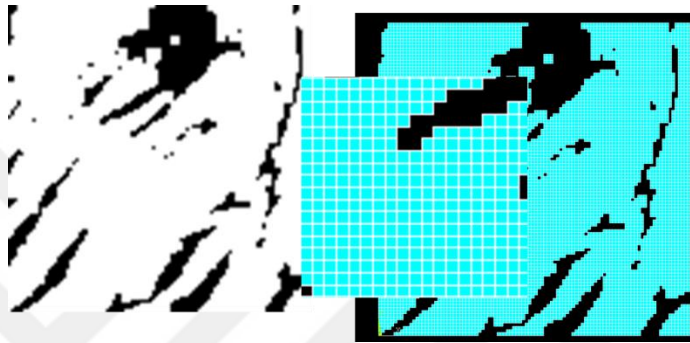


Figure 3.13: Meshed phase.

3.5.4 Material Properties

The model requires some inputs that need to be provided such as E_1 , E_2 which are respectively the flax fibers and the matrix (void in this case) Young's modulus where

$E_1 = 70 \text{ GPa}$ [18], and $E_2 = 0.1 \text{ GPa}$ (a very low value has been attributed to avoid calculation problems). Poisson's ratio is attributed an arbitrary value (0.3).

3.5.5 Loading Conditions

In order to compute the effective properties in the two perpendicular directions attached to the microstructure as represented in Figure 3.14 a static linear analysis is performed.

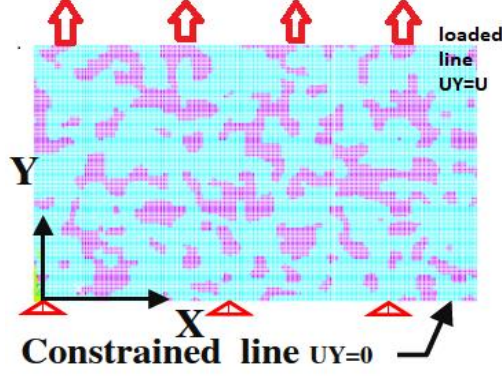


Figure 3.14: Boundary conditions considered in the finite element analysis.

A small displacement of the value of 1px is imposed to all nodes of a given line and all nodes of the opposite line are constrained against the displacement in the same loading direction.

3.5.6 TYPE OF ANALYSE

In this section, we solve a linear elasticity problem to predict the Young's modulus E_X and E_Y in both directions, the anisotropic proprieties of the microstructures, and identify the stress and strain.

The Elasticity modulus in both direction E_X and E_Y is calculated with the following formula:

$$E = \frac{\sigma}{\varepsilon} \quad (3.1)$$

Where σ represents the reaction force per unit surface which is the result of a displacement in a given direction in this case, and ε represents the strain (deformation):

$$\sigma_x = \frac{FX}{DY} \quad (3.2)$$

Where FX is the reaction force on the X axis direction and DY the surface measurement on the Y direction. Similarly, we obtain:

$$\sigma_y = \frac{FY}{DX} \quad (3.3)$$

$$\epsilon_x = \frac{1}{DX} \quad (3.4)$$

From the previous equations (1- 4) we can deduct that:

$$EX = FX * \frac{DX}{DY} \quad (3.5)$$

$$EY = FY * \frac{DY}{DX} \quad (3.6)$$

By the use of equations (3.5) and (3.6), we define the anisotropy with the following formulas:

$$EM = \frac{EX + EY}{2} \quad (3.7)$$

$$anisotropy = \frac{EX}{EY} \quad (3.8)$$

3.6 THE PREDICTION OF YOUNG MODULUS AND ANISOTROPY OF FLAX FIBER BIOCOMPOSITES WITH ARTIFICIAL NEURAL NETWORK

In this section an artificial neural network model is developed to predict the mechanical properties of flax fibers biocomposites based on the dataset that has been built on the finite element simulations.

Objectives:

- The developed ANN model aims to predict the Young's modulus and the anisotropic properties of flax fibers biocomposites.
- Study the possibility and the performance of ANNs to be an alternative of the finite element model.
- Reduce the computational costs of the development of the finite element model.

Methodology

In this study 4 datasets are available to develop the ANN model, each dataset is a set of microstructures of the samples presented in Table 3.2, in each dataset the following columns are used in this work :

- EM : a float value that represents the Young's modulus of the microstructure.
- Anisotropy: a float value that represents the anisotropic property of the microstructure.
- Clear: a Boolean value the shows if the sample is stained or cleared .
- Density: the density of the sample in $\text{g/m}^2\text{D}$.
- Porosity: the porosity ratio of the microstructure.

This work is made in Matlab development environment , the previously mentioned data has been standardized before getting used by the Matlab function `zscores()`, the benefit of this standardization is that it doesn't rely on the original values of the features it can make the data more readable and clarify the impact a feature on an other .

The zscores value is calculated with the following formula:

$$\text{zscore} = (x - \mu) / \sigma \quad (3.9)$$

Where μ is the mean of the dataset and σ is its standard deviation.

For the prediction of the mechanical properties a feedforward neural network is seen to be suitable for our objectives, a set of parameters is pre-selected for the development of the ANN model.

3.6.1 Activation Function Selection:

The default activation function in Matlab for the hidden layer neurons is the tanh which is a function that ranges the value in an interval of [-1,1]:

$$\tanh = \frac{e^x - e^{-x}}{e^x + e^{-x}} \quad (3.10)$$

But in this work Relu is used as an activation function because it has outperformed Tanh after a comparative test :

$$f(x) = \max(0, x) \quad (3.11)$$

Relu has gained a lot of popularity in the deep learning applications due to its performance when compared to other activations functions [74].

For the activation function on the output layer a linear function has been selected instead of the sigmoid function since our objective is to predict continuous values and not a binary classification a linear function seems to be a better choice.

Concerning the architecture of the network many architectures are tested and the most performant is selected later.

To train artificial neural networks, trainlm function is used in matlab and this function includes the use of Levenberg-Marquardt algorithm.

Since the training was done with the neural networks toolbox in Matlab, the default epoch count set to 1000 with a stopping criterion at convergence was used.

Levenberg-Marquardt: It is specially designed for nonlinear least squares curve fitting problems. It aims to find the parameters that minimize the sum of the squared differences between the observed and predicted values in a nonlinear regression problem [77].

The following Figure displays a comparison between the different algorithms used in neural networks:

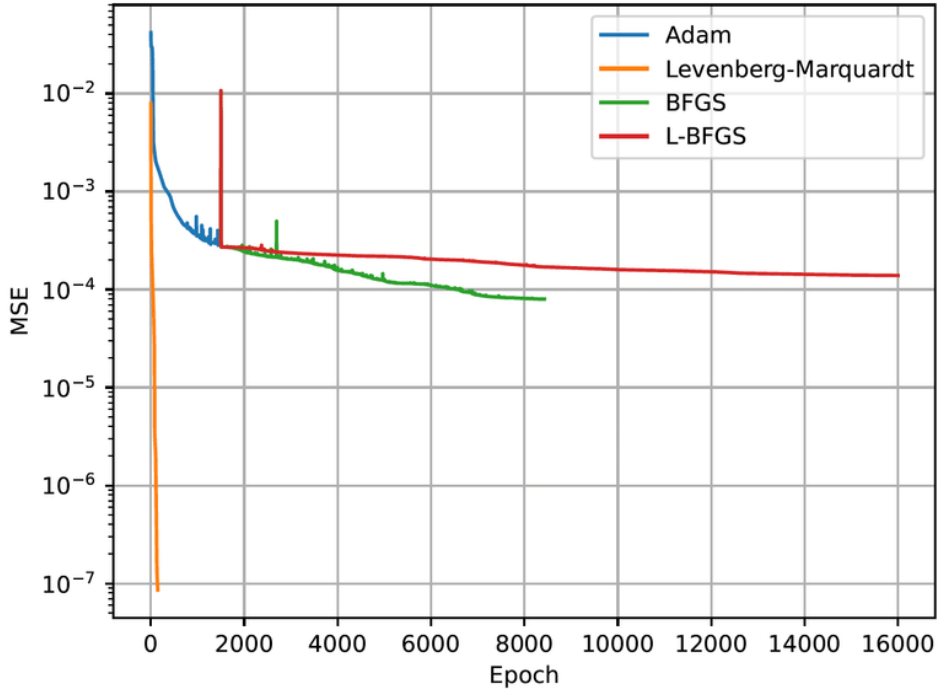


Figure 3.15: A comparison of the performance of the LM algorithm [78].

Figure 3.16 shows clearly an outstanding performance of the Levenberg-Marquardt algorithm where only in 10 epochs it reached low mse values compared to 1000 epoch on the other algorithms.

Since the training is done on Matlab with the neural networks toolbox the default epoch number is used which is set it 1000 with a stopping criteria at the convergence.

As a loss function the mse is selected to evaluate the performance of the network:

$$mse = \frac{1}{n} (actua - forecast)^2 \quad (3.12)$$

for the model architecture several architecture are tested as explained the next section.

Pre-Elementary Tests:

As a pre-elementary test a feed forward neural network with 3 neurons in the input layer, 5 in the hidden layer and 1 neuron in the output layer to confirm the network ability predict the values of a non-linear relation between features the following non-linear function is set :

$$F(x,y,z)= 3x^3+\sin(y^2) + \log(z) \quad (3.13)$$

A dataset of inputs and outputs was generated by using random values as inputs and then they are computed with the function to get an output . The network was trained on this dataset with a ratio of 80% for the training 20% for the validation and test set equally. The results are displayed in the next section.

After this several tests were done on the dataset of FM150N sample, to predict the young modulus property using the porosity and the area as an input and a ratio of 80%,10%,10% was used for the training and validation and test respectively.

In the following Figure 3.16 the best performing neural network architectures are displayed:

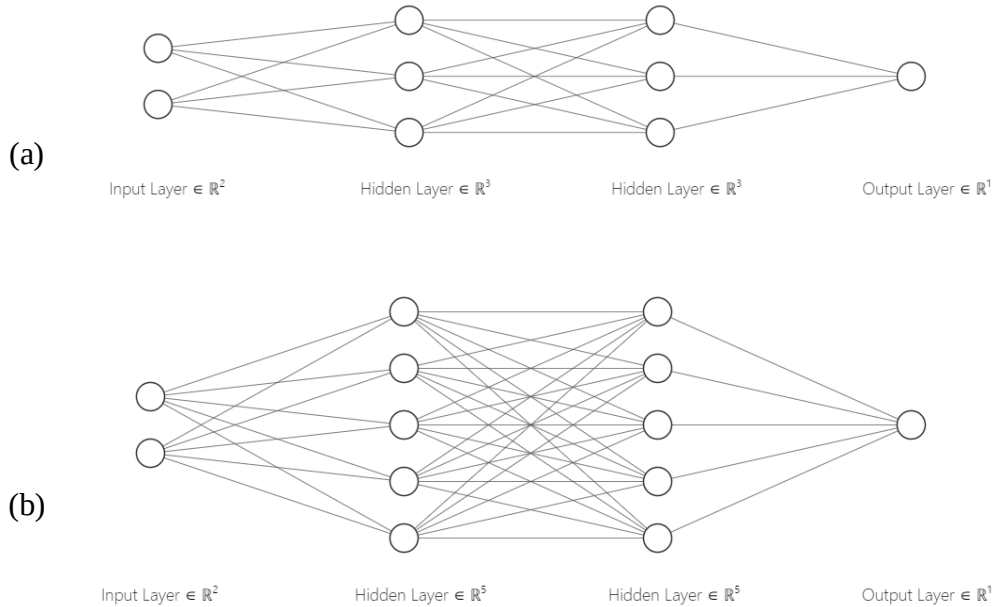


Figure 3.16: A representation of the most performing neural network architectures for the FM150N microstructures.

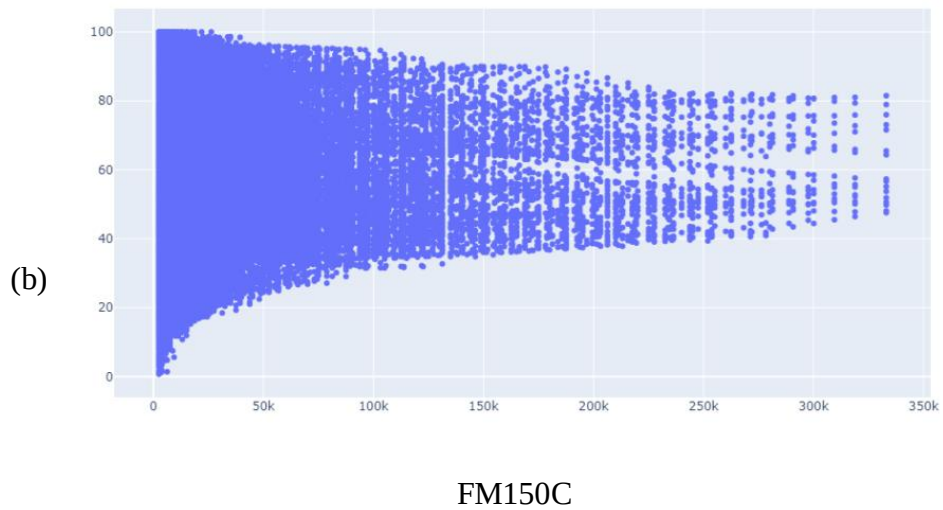
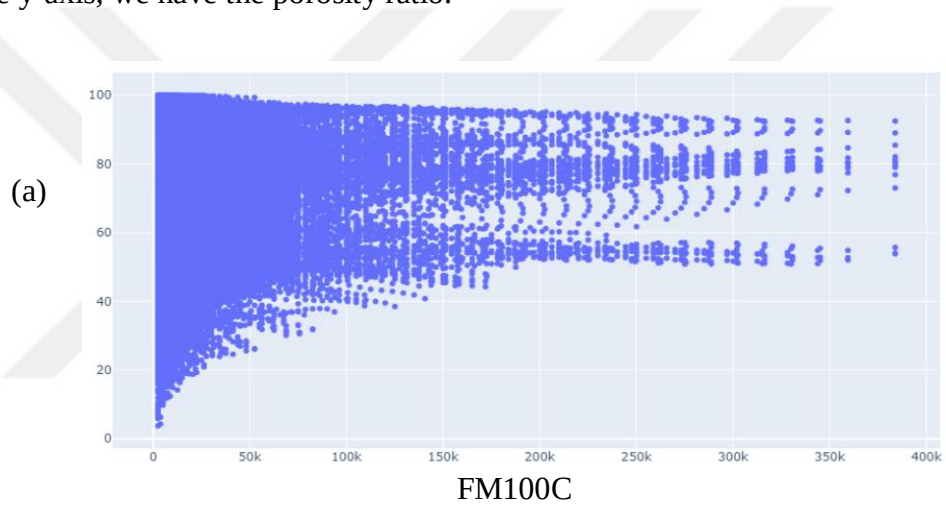
]

4. RESULTS

[In this section the results of the previous experiments are displayed in a form of graphs and tables in order to investigate and extract insights from the data.

4.1 POROSITY ANALYSES RESULTS

The following graphs are made by the use of matplotlib library in python and they represent the porosity analyses results for each sample, on the x-axis, we have the image area in pixels and on the y-axis, we have the porosity ratio.



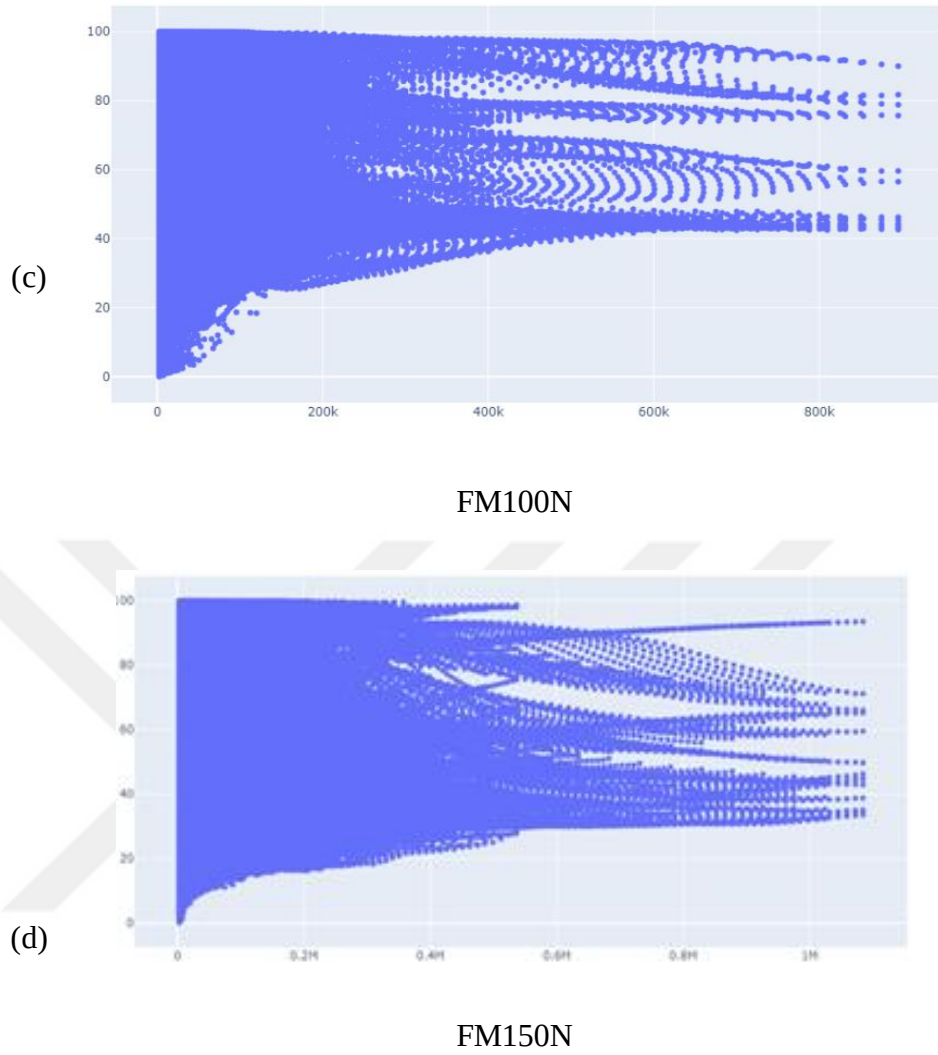


Figure 4.1: porosity analyses results.

4.1.1 Calculating The Porosity Mean And Standard Deviation For The Flax Mat Samples.

In this part we took the original crops which represents the biggest microstructures of the samples as previously mentioned in Data Processing & Methodology section and then calculated the mean and std values of those microstructures. The following Table 4.1 displays the results of this procedure.

Table 4.1: Calculating the porosity mean and std for flax mat samples.

file	sample_name	mean	Std
x351_25_max.csv	FM150N	51,87	16,57
x617_25_max.csv	FM100N	58,99	17,01
x701_25_max_data.csv	FM150C	75,90	12,09
x901_25_max_data.csv	FM100C	61,35	11,28

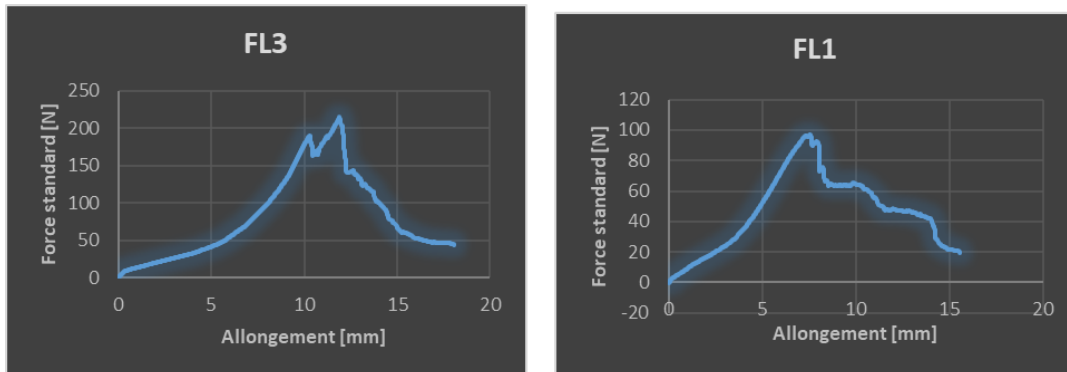
The same procedure is applied to the microstructures after a rotation of 90° in the axis-x direction and the results are displayed in the following Table 4.2 :

Table 4.2: Calculating the porosity mean and std for flax mat samples after the 90° rotation.

file	sample_name	mean	Std
x351_25_max.csv	FM150N	68,437	3,40
x617_25_max.csv	FM100N	72,44	6,44
x701_25_max_data.csv	FM150C	81,00	4,67
x901_25_max_data.csv	FM100C	77,45	5,14

4.2 RESULTS OF MECHANICAL CHARACTERIZATION ON FL1 & FL3 SAMPLES.

After attaching the samples rectangular cuts into the tensile machine the connected computer provided the following graphs as represented in Figure 4.2.

**Figure 4.2:** Tensile test results.

At the end of the experiment both of the samples displayed a permanent deformation as a result of the tensile test as shown in f Figure 4.3 :



Figure 4.3: A permanent deformation on FL1 & FL3 samples after a tensile test.

4.3 RESULTS OF THE NUMERICAL SIMULATION BASED MECHANICAL STUDY ON THE ANISOTROPIC PROPERTIES AND ELASTICITY OF FLAX FIBERS BIOCOMPOSITES

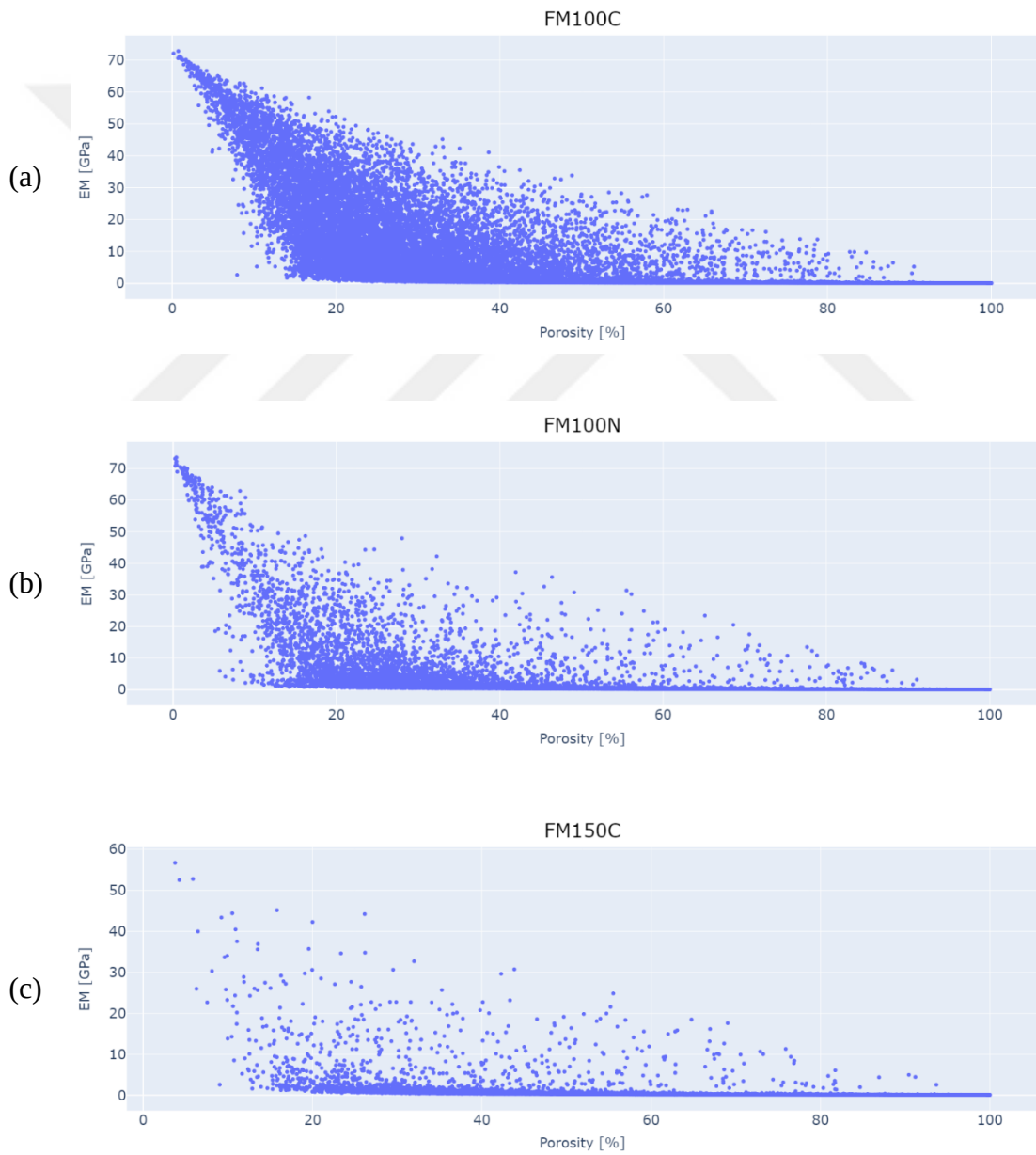
After extensive computations on the microstructures on the different samples presented in Table 3.2 the simulation's data, an example of the results of the FM150N sample is presented in a comprehensive way in Table 4.3, summarizing the key findings of the mechanical properties and anisotropic behavior of the material in question.

Table 4.3: example of FM150N sample's computation results.

FILE	E1	E2	EX	EY	EM	anisotropy
0050_0050_D_cc-10_0_0.dat	70.0	0.1	0.10	0.10	0.10	1.0
0050_0050_D_cc-2_550_50.dat	70.0	0.1	0.31	0.23	0.27	1.14
0050_0050_D_cc-2_600_0.dat	70.0	0.1	14.21	0.27	7.27	52,62
0050_0050_D_cc-2_600_100.dat	70.0	0.1	41.85	36.70	39.27	1.14

The extensive FE computations on different microstructures gave us the possibility to have clear insights on the microstructure's properties and the effect of porosity ratio on these proprieties. The following Figure 4.4 represents the porosity ratio effect on the Young's modulus of for the samples FM100C, FM100N, FM150C and FM150N respectively.

In order to have a better insights on the graphs the data used for each sample has been rebalanced to 46000 microstructure for all the samples some microstructures have been randomly deleted to have a balanced analyses on the graphs.



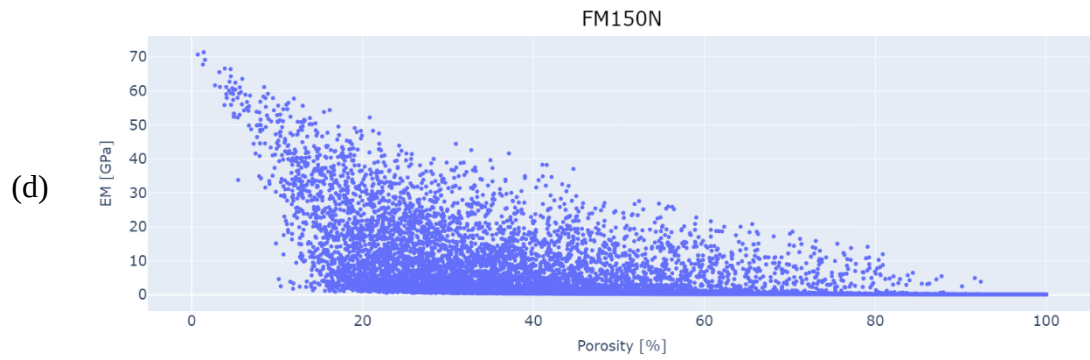
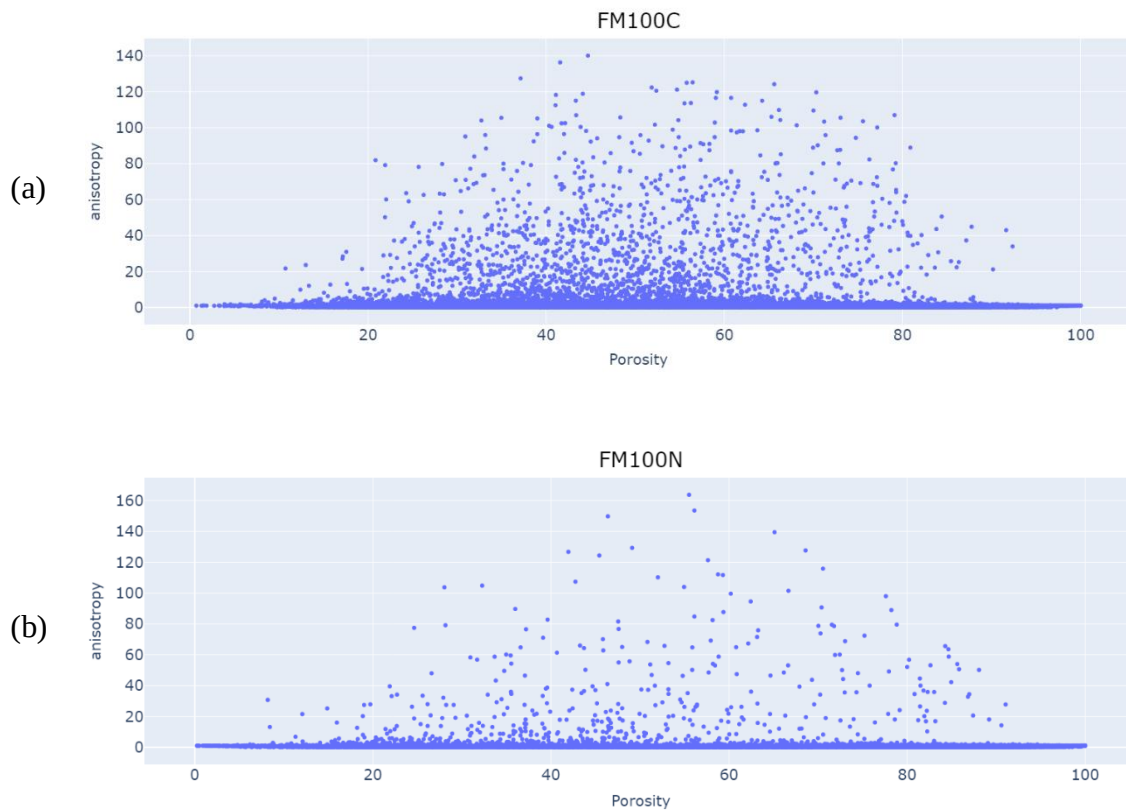


Figure 4.4: the porosity ratio effect on the young's modulus of the samples FM100C, FM100N, FM150C and FM100.

In addition, of analysing the Young's modulus of the samples, visualizing the anisotropic propriety of the samples gives valuable information as represented in the following Figure 4.5.



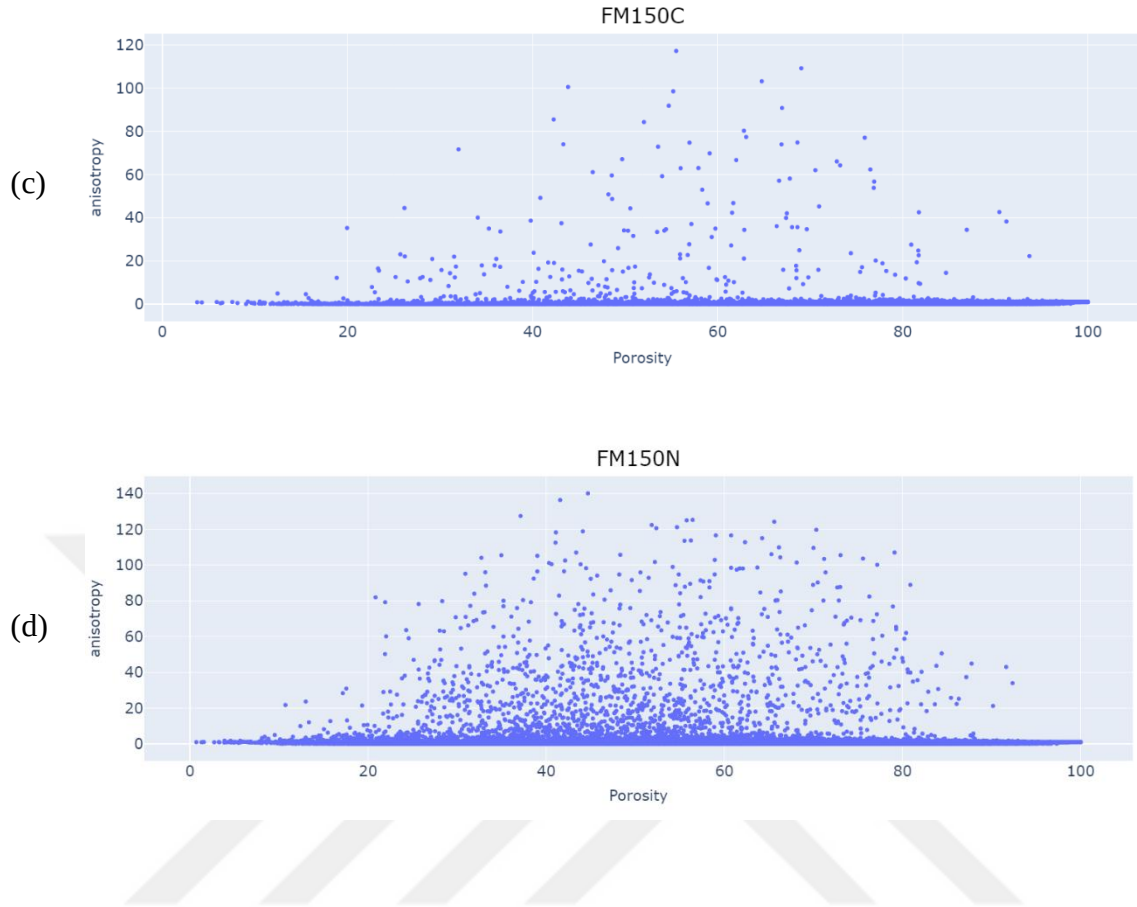


Figure 4.5: a representation of the porosity ratio effect on the anisotropic propriety of the microstructures for the FM100C, FM100N, FM150C and FM100N sample.

For a better understanding of the microstructure proprieties, farther investigations are done as presented in Figure 4.6, which display the anisotropy, and porosity relation with a microstructure area based color scale.

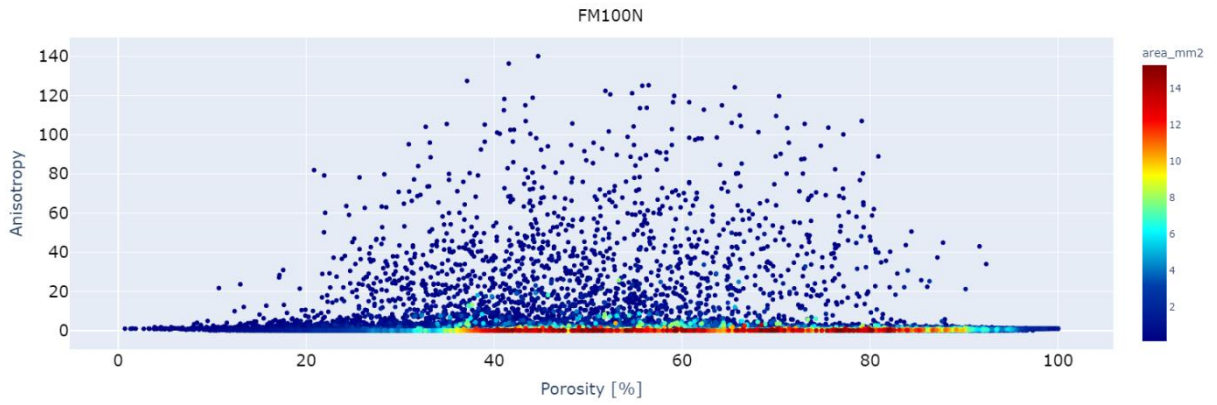


Figure 4.6: a representation of FM150N samples anisotropy and porosity ratio relation with a microstructure area based color scale.

In order to study the isotropic property of the microstructures a zoom into Figure 4.7 as displayed in the following Figure 4.7.

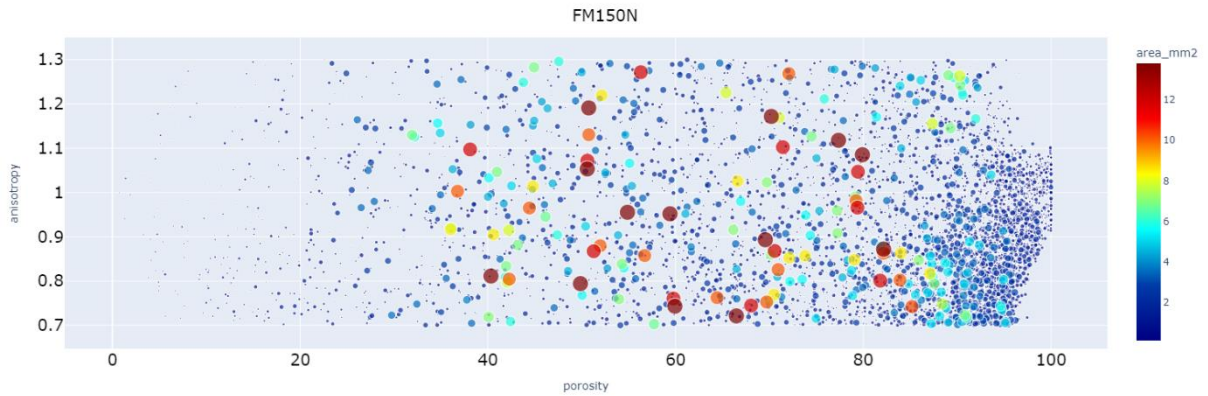


Figure 4.7: an observation of isotropic microstructures on the FM150N sample.

Figure 4.7 is a zoom on the previous figure and it clearly displays that the bigger microstructures can have more isotropic proprieties compared to the small structures.

From the previous analyses , we confirm that the size of microstructures affects its proprieties as a results farther investigations are done on the Young's modulus , the following Figure 4.8 figure represents a zoom in into the graph of porosity ratio and Young's modulus with a structure area based color scaling .

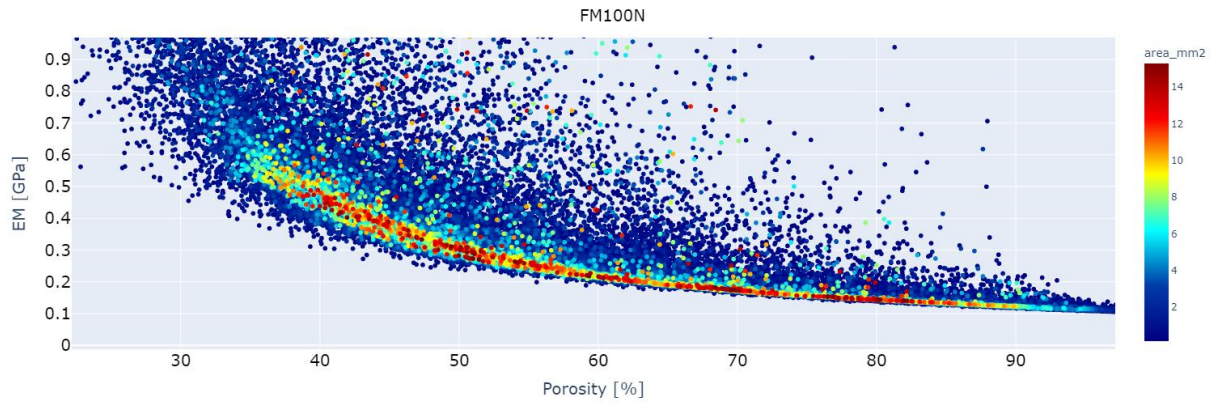


Figure 4.8: a zoom in into the FM150N sample's EM and porosity graph with a structure area based color scale.

Figure 4.8 still shows that we have an exponential down trend and a negative correlation between porosity and EM values but in addition of that it makes the size of the microstructures more clear and we do notice that the bigger structures with an area that is superior to 6 mm² has much lower Young's modulus compared to the smaller once even if they have the same porosity level.

In order to investigate more in the observed down trend, a fit curve is applied to the biggest microstructures and the small ones as displayed in the following Figure 4.9.

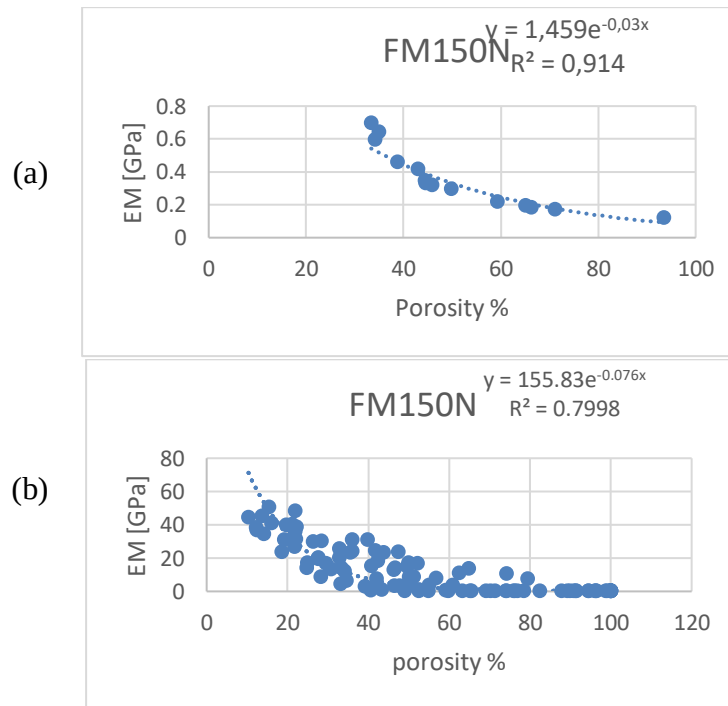


Figure 4.9: a representation of a fit curving for the Young's modulus and porosity graph for the biggest and smallest structures.

In the similar method, we want to observe if there is an exponential trend on the anisotropy and porosity graph as displayed in the following Figure 4.10:

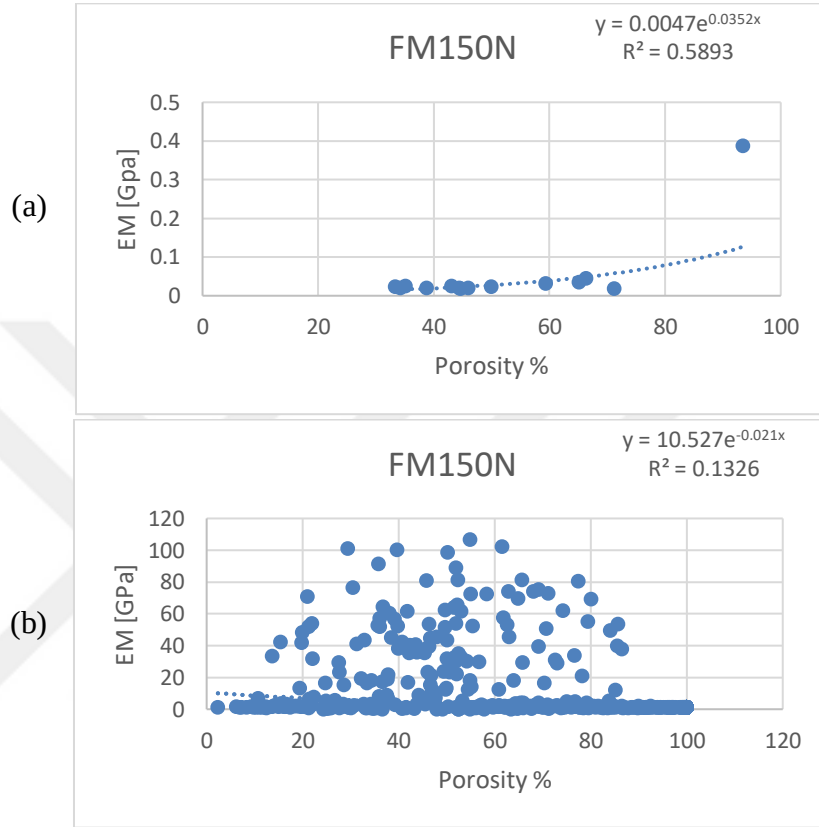


Figure 4.10: a representation of a fit curving for the anisotropy and porosity graph for the biggest and smallest structures.

Figure 4.9 displays clearly an exponential down trend with a fitting value of 0.91 on the biggest microstructures while the smallest ones are less well fitted into the exponential curve.

On the other hand, Figure 4.10 shows that there is a weak exponential fitting for the anisotropy and porosity graph for both of the big and small microstructures.

4.4 RESULTS OF THE PREDICTION OF YOUNG MODULUS OF FLAX FIBER BIOCOMPOSITES WITH ARTIFICIAL NEURAL NETWORK

4.4.1 Pre-Elementary tests results

In a previous section Pre-Elementary Tests: the ability of artificial neural networks on learning and making predictions on non-linear functions the following Figure 4.11 displays this performance.

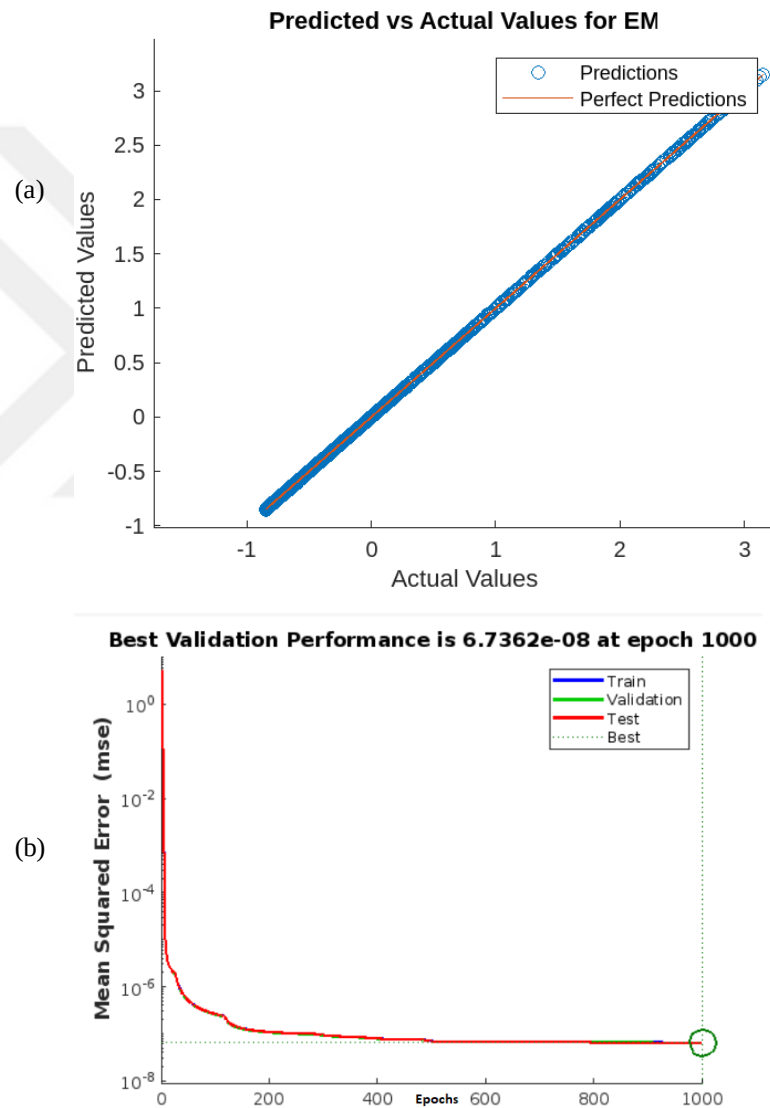


Figure 4.11: Elementary test results on a non-linear function.

As displayed in the Figure 4.11 the neural network clearly managed to predict the output of a nonlinear function with an mse that converges to 0 through all the epochs and as observed on

the first graph all the points are located on the perfect predictions line which confirms that the predicted values and the real values are in agreement.

After proving that the artificial neural networks are capable of making predictions on nonlinear functions. We applied the process that has been mentioned in Pre-Elementary Tests: and the performance of the developed model on FM150N microstructures is displayed on the following Figure 4.12.

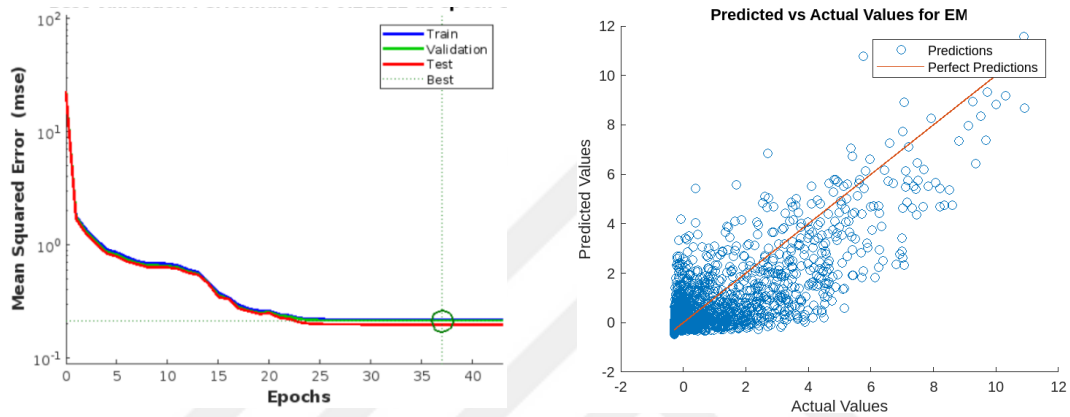


Figure 4.12: The performance of the neural network on predicting the Young's modulus.

With the same architecture we predict the anisotropy propriety and the results are as following:

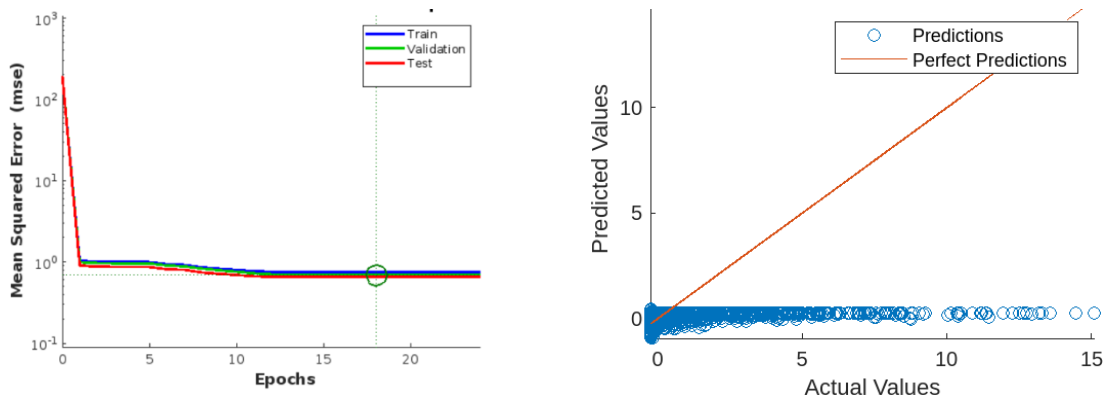


Figure 4.13: The anisotropy prediction performance with neural networks.

Figure 4.12 displays the prediction performance of the Young's modulus with neural networks with an mse value of : 0.2 and it's clear that the predictions are not well fitted on the perfect predictions line so as a results those predictions are not very accurate .

On the other hand Figure 4.13 displays the predictions on the anisotropy feature where an mse value of 0.7 is observed and the predictions are very far from the perfect predictions line which means that the neural network model completely failed to compute this property.

In the previous chapter we deduced that our materials are not an RVE which means that the smaller structures are not representative of the whole material in addition of that the fit-curve of Young's modulus confirmed a weaker fitting for the small structures compared to the biggest ones and Figure 4.13 displayed the complete failure of fitting the anisotropy which means that the dataset structures are heterogeneous where the results of neural networks become very logical , as a result only the biggest structures that are displayed in Figure 4.9 is taken into the dataset.

To find the best neural networks architecture for the new dataset of big structures several architectures of [1,2,3] hidden layers with [3,5,10,15] neurons in each hidden layer and the results of those tests are displayed in the following table:

Table 4.4: The neural networks architectures performance results.

Hidden Layers	Neurons	MSE
1	3	0.023
1	5	0.021
1	10	0.05
1	15	0.026
2	3	0.029
2	5	0.02
2	10	0.08
2	15	0.31
3	3	0.21
3	5	0.05
3	10	0.06
3	15	0.05

Table 4.4 shows the predictions results with different architectures and compares the performance of the neural networks with 2 hidden layers is the most performing one with an mse value of 0.02 at the epoch 8. Figure 4.14 represents the predicted values and the actual ones along with the training graph:

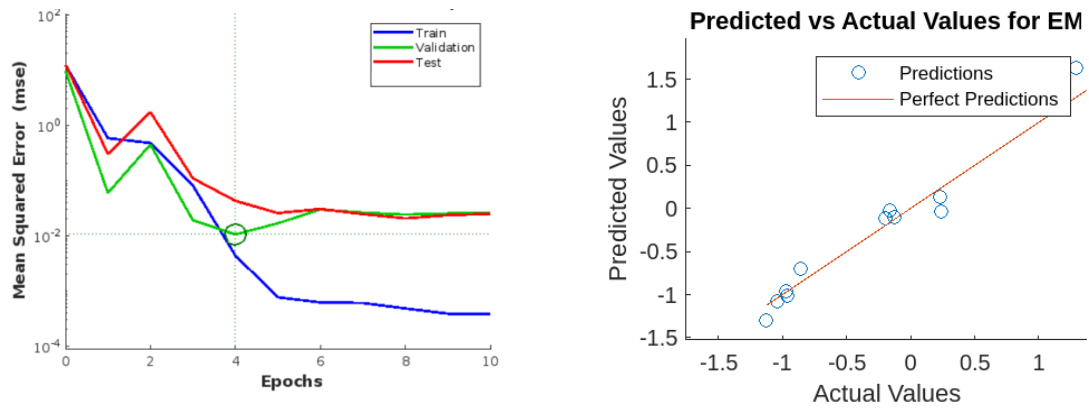


Figure 4.14: Representation of the performance of the best parameters to predict the Young's modulus.

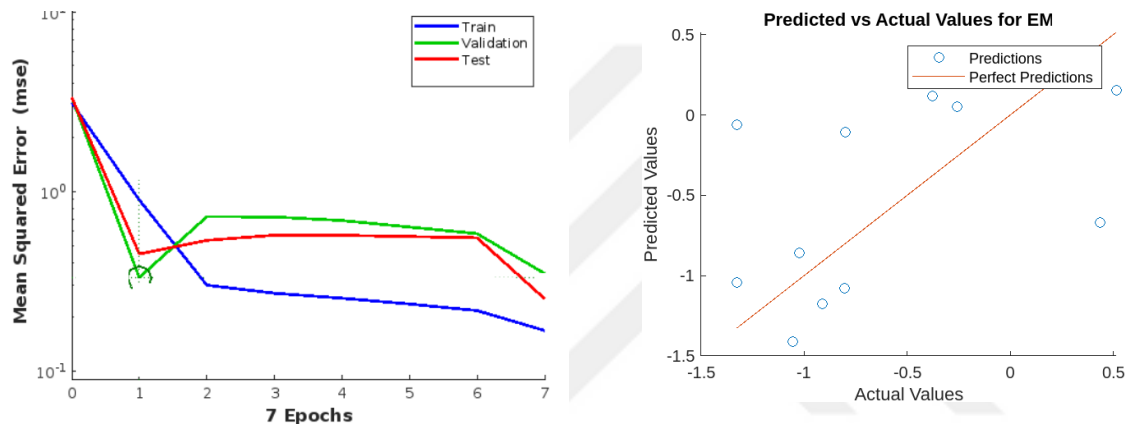


Figure 4.15: The performance of the neural networks with Tanh as an activation function in the hidden layers..

Figure 4.14 shows a good performance of the neural network model to predict the Young's modulus of the biggest structures of the sample FM150N where it displays the predicted values near the perfect predictions line.

But on the other hand, Figure 4.15 displays a weak performance by the use of tanh as an activation function with an mse value of 0.33.]

5. DISCUSSION AND CONCLUSION

5.1 POROSITY ANALYSES

According to the available data, it appears that the porosity measurements for the various flax mat samples vary:

The mean porosity of the Flax Mat 150g No.3 sample is 51.87%, with a standard deviation of 16.57%.

The mean porosity and standard deviation for the Flax Mat 100g No.3 sample are 58.99% and 17.01%, respectively.

With a standard deviation of 11.29% and a mean porosity of 61.35% for the Flax Mat Clear 150g sample.

The mean porosity of the Flax Mat Clear 100g sample is 75.90%, and the standard deviation is 12.10%.

In general, the samples of cleared flax mat seem to be more porous than the samples of stained flax mat. In comparison to the other samples, the Flax Mat Clear 150g sample in particular has a much higher mean porosity.

In order to clear a sample, any impurities or undesired materials are typically removed using a solvent or chemical process. Clearing in the context of a flax mat sample would entail eliminating any non-flax components, such as binders or fillers, that would increase the sample's overall volume without affecting its porosity. The cleared sample would have a higher porosity once these elements were eliminated since more pores would make up more of its volume.

Another possibility is that the clearing procedure itself could enlarge or add to the sample's existing pores. In order to create more pore space and raise the sample's overall porosity, the solvent or chemical used to clear the sample could dissolve or break down some of the materials that were formerly filling in the pore spaces.

The sample's composition, structure, and processing, as well as the testing techniques employed, are some of the possible causes of the variations in porosity values. Porosity readings may also have been impacted by the samples' varying weights, since a thicker or denser sample may have less porosity even when the material composition is the same. The std values for the cleared flax mat samples (11.29% and 12.10%) are generally lower than the std values for the non-cleared samples are (16.57% and 17.01%). This suggests that the porosity measurements for the cleared samples are more consistent and less variable than the measurements for the non-cleared samples.

However, it's worth noting that the Flax Mat Clear 100g sample has a relatively high std value of 12.10%. This indicates that there is still some variability in the porosity measurements, even for the cleared samples.

Overall, the std values are moderately high, indicating that there is a significant amount of variability in the porosity measurements. This variability could be due to various factors, such as sample preparation, testing methods. It's important to carefully control for these factors to minimize variability and obtain more precise and reliable measurements.

5.2 TENSILE TEST

Figure 4.3 is a graphical representation of the results of the performed tensile test on the FL1 and FL3 samples where it shows that the FL3 had more resistance to the applied force (210N) twice as FL1 did and also a longer elongation (18mm) than FL1 and that is explained by the existence of more dense fiber mat (150g/m²) in FL3 and on the other hand FL1 had layers of 100g/m² fiber mat which confirms that denser the fiber layer are the more force resistance we get.

5.3 FINITE ELEMENT ANALYSES

Figure 4.5 is a representation of the porosity ratio effect on the anisotropic propriety of the microstructures for the FM100C, FM100N, FM150C and FM100N sample.

Figure 4.8 displays a clear negative correlation between the porosity ratio and the Young's modulus (EM) as we can observe on all the samples there is an exponential down trend on the EM values while the porosity continues to increase, a maximum Elasticity modulus is

observed at 0% porosity with an approximate value of 70 GPa which is explained by the presence of the material over the whole microstructure which makes its Young's modulus equal to the initial value of flax fibers Young's modulus that we set in the beginning of the simulation.

On the other hand, it is also important to analyze the anisotropic propriety of the samples and its relation with porosity, as we observe on Figure 4.5 all the samples are displaying an anisotropic behavior on the majority of the microstructures, we notice that the interval [20%,80%] of porosity contains the highest anisotropy values comparing to the rest of porosity values.

For a better understanding of the microstructures proprieties, farther investigations are done as presented in Figure 4.6, which display the anisotropy, and porosity relation with a microstructure area based color scale.

Figure 4.6 clearly shows that the smaller microstructures with an area that is inferior to 4mm^2 trends to display more anisotropic proprieties while the bigger structures with an area that is superior to 6mm^2 displays much less anisotropy, it's also important to note that after a zoom on this figure some microstructures displayed an isotropic behavior as shown in Figure 4.7.

Figure 4.7 is a zoom on the previous figure and it clearly displays that the bigger microstructures can have more isotropic proprieties compared to the small structures.

From the previous analyses , we confirm that the size of microstructures affects its proprieties as a results farther investigations are done on the Young's modulus , the following figure represents a zoom in into the graph of porosity ratio and Young's modulus with a structure area based color scaling.

5.3.1 Comparison with Previous Studies

In order to gain further insights into analyses conducted in this study, it is valuable to compare our results with findings from other researchers.

In the work done by Khalvandi et al. (2022) [75] the Young's modulus was predicted based on porosity and the pores shape. The predictions of ANNs and FEA results had good agreement concerning each other and also with the experimental data. The mean squared error

was in the order of 10^{-6} and The absolute difference of ANNs predictions and FEA model were in the [0.004–0.007] range which is better than the mse value that was resulted in this thesis which was in the order of 10^{-2} and this is explain by the difference of nature of the samples and data used in the studies Khalvandi et al. (2022) worked on RVE samples which is not our case which justifies the results accuracy difference but overall the ANNs results were also in agreement with FEM results.

5.3.2 Future work

As a future work using a different type of neural networks like convolutional neural networks (CNNs) can be a great alternative compared to the feedforward neural networks since they can directly take the images as an input and detect the porosity distribution patterns which may lead to a better performance in the prediction of the mechanical behavior of the biocomposites as displayed in the following work [76].

5.4 CONCLUSION

By using structures that were sufficiently large to encompass the microstructural features of the material and small enough to be considered as representative points on the macro scale, we were able to observe a notable disparity in the behavior of the macrostructures. This discrepancy has been clearly demonstrated. It has been shown that an exponential down trend with a fitting value of 0.91 on the biggest microstructures while the smallest ones are less well fitted into the exponential curve. On the other hand, we observed a weak exponential fitting for the anisotropy and porosity for both of the big and small microstructures. These highlighted the substantial differences in the behavior of the material according to its size.

According the previous results, it is possible to confidently conclude that our material does not possess homogeneity. It is evident that a single size or volume of the material does not adequately represent the entire material, including its microstructural features. As a result, we can deduce that our material does not meet the criteria of being a Representative Volume Element (RVE).

The std values for the cleared flax mat samples (11.29% and 12.10%) are generally lower than the std values for the non-cleared samples are (16.57% and 17.01%). This suggests that the

porosity measurements for the cleared samples are more consistent and less variable than the measurements for the non-cleared samples. This variability could be due to various factors, such as sample preparation, testing methods, equipment...etc. It's important to carefully control for these factors to minimize variability and obtain more precise and reliable measurements.

Mechanical properties of our material have been performed through a series of tensile tests on the FL1 and FL3 standard samples, where the obtained graphs showed that the FL3 samples had more resistance to the applied force (210N) twice as FL1 samples did and also a longer elongation (18mm) than FL1 samples. This is explained by the existence of more dense fiber mat (150g/m²) in FL3 samples and on the other hand, FL1 samples had layers of 100g/m² fiber mat which confirms that denser the fiber layer is, the more force resistance we get. It was also found that a deeper analysis of the tensile test results can provide meaningful information about the flax composite behavior if a predictive approach is adopted.

The outputs obtained from the finite element model and the neural network model for the larger structures showed a remarkable consistency. The two models' successful correlation allowed us to drastically cut the computational expenses associated with the study. The use of the artificial neural network (ANN) model, which produced precise predictions for the behavior of our material, proved to be a successful and affordable option.

Utilizing the ANN model, not only produced precise predictions but also offered a sizable computational efficiency benefit. This innovation in computing efficiency creates new opportunities for research of materials with complex microstructural characteristics. In order to better understand material's mechanical behaviors and possibly expand its uses.

Replacement of synthetic composite materials by biocomposite materials is an environmentally friendly alternative and the use of predictive numerical approaches as the ANN model is proved to be a trustworthy tool in this kind of studies.]

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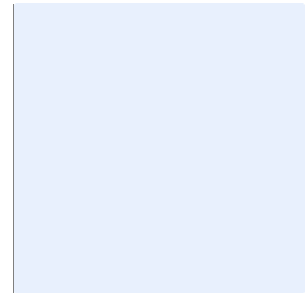
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